FisMat 2013

POLITECNICO DI MILANO

150°

Italian National Conference on

Condensed Matter Physics

(Including Optics, Photonics, Liquids, Soft Matter)

Politecnico di Milano

09-13 september 2013

BOOK OF ABSTRACTS

FisMat 2013 has been a great success, for many reasons. The most relevant is that, for the first time since 2004, the Italian community working in the field of condensed matter physics has had the opportunity to reunite and this chance has not been wasted.

The participation to the event has been impressive: 800 contributions submitted, 900 registered participants, 13 plenary sessions and 70 thematic sessions. All the most important Italian institutions active in this field of research have been adequately represented and all the spectrum of condensed matter physics has been covered with frequent excursions in other branches of science such as chemistry, biology, medicine, cultural heritage.

The scientific level of all the contributions presented at the conference is very high and testify the vitality of our research community. For this reason we decided to public this book of abstract which includes all the oral contributions (more than 500).

We strongly needed this and we will need it even more in the future, this is the reason why the experience of FisMat 2013 will continue with FisMat 2015, which will be held in Palermo.

Ezio Puppin (Conference Chairman)
Antonella Tajani (Scientific Coordinator)

Scientific Committee

Antonella Tajani (CNR)
Lucio Claudio Andreani (Università di Pavia)
Stefano Atzeni (Università di Roma "La Sapienza")
Piero Baglioni (Università di Firenze - CSGI)
Massimo Carpinelli (Università di Sassari - INFN)
Pietro Carretta (Università di Pavia)
Maria Gabriella Castellano (IFN-CNR)
Giovanni Ciccotti (Università di Roma "La Sapienza")
Lamberto Duò (Politecnico di Milano)
Dino Fiorani (ISM-CNR)
Paolo Laporta (Politecnico di Milano)
Paolo Mariani (Università Politecnica delle Marche)
Giorgio Paolucci (ELETTRA)
Nicola Spinelli (Università di Napoli "Federico II")
Francesco Tassone (IIT)

Local Committee

Stefania Mosca (Politecnico di Milano)
Silvia Maria Pietralunga (CNR - IFN, Milano)
Monica Bollani (CNR - IFN, Milano)
Maurizio Contran (Politecnico di Milano)
Claudio Mazzoli (Politecnico di Milano)
Ermanno Pinotti (Politecnico di Milano)
Dario Polli (Politecnico di Milano)
Alberto Tagliaferri (Politecnico di Milano)
Maurizio Zani (Politecnico di Milano)

FisMat 2013 AT A GLANCE

Mon 9	09:00 - 11:00	Registration
	11:00 - 11:30	Opening ceremony
	11:30 - 12:30	Plenary session (Andrea Ferrari)
	12:30 - 13:30	Lunch break
	13:30 - 14:30	Plenary session (Erio Tosatti)
	14:30 - 17:00	Parallel sessions
	17:00 - 18:00	Special event on the Human Brain Project (Egidio D'Angelo)
	18:00 - 19:30	Poster session & happy hour
Tue 10	08:30 - 09:30	Plenary session (Stuart Parkin)
	09:30 - 12:30	Parallel sessions (coffe break 10:30 - 11:00)
	12:30 - 13:30	Lunch break
	13:30 - 16:00	Parallel sessions
	16:00 - 17:00	Plenary session (Fernando Ferroni)
	17:00 - 19:00	Poster session & happy hour
	20:00	Social dinner at the "Museo della Scienza e della Tecnica"
Wed 11	09:00 - 10:00	Plenary session (Roberto Cingolani)
	10:00 - 12:30	Round table
	12:30 - 13:30	Lunch break
	13:30 - 14:30	Plenary session (Francesco Sette)
	14:30 - 17:00	Parallel sessions (beginning of SILS and SISN conferences)
	17:00 - 18:00	Plenary session (Chandrasekar Joshi)
	18:00 - 19:30	Poster session & happy hour
Thu 12	08:30 - 09:30	Plenary session (Dieter Richter)
	09:30 - 12:30	Parallel sessions (coffe break 10:30 - 11:00)
	12:30 - 13:30	Lunch break
	13:30 - 14:30	Plenary session (Massimo Inguscio)
	14:30 - 17:00	Parallel sessions
	17:00 - 18:00	Plenary session (Hardy Gross)
	18:00 - 19:30	Poster session & happy hour
Fri 13	08:30 : 09:30	Plenary session (Janos Haijdu)
	09:30 : 10:30	Plenary session (Daan Frenkel)
	10:30 : 13:30	Parallel sessions (coffe break 10:30 - 11:00)
	13:30	Lunch

Sessions

Monday, September 9

Title	Chairman
Multiferroics	Dino Fiorani
Neural circuit functioning and computation	Alessandro Torricelli
Superconductivity A	Giacomo Ghiringhelli
Metrology and fundamental constants	Paolo La Porta
Environmental physics and energy generation A	Francesco Tampieri
Organic materials and devices A	Marco Sampietro
Plasmonics	Stefano Longhi
Graphene A	Giulio Cerullo
Statistical physics A	Stefano Ruffo
Diamond devices	Ermanno Pinotti

Tuesday, September 10

Title	Chairman
Magnetism and spintronics A	Dino Fiorani
Surface science A	Maria Grazia Betti
Superconductivity B	Angelo Nucciotti
Semiconductors-low dimensional materials A	Stefano Ossicini
Environmental physics and energy generation B	Xuan Wang
Organic materials and devices B	Antonio Cassinese
Strongly Correlated Electron Systems A	Riccardo Bertacco
Graphene B	Roman Sordan
Statistical physics B	Giovanni Jona Lasinio
Biophysics A	Enzo Orlandini
Magnetism and spintronics B	Pietro Carretta
Surface science B	Paola De Padova
Superconducting quantum detectors	Gabriella Castellano

Semiconductors-low dimensional materials B	Stefano Roddaro
Environmental physics and energy generation C	Nicola Spinelli
Electrons and phonons A	Francesco Mauri
Strongly Correlated Electron Systems B	Giacomo Ghiringhelli
Quantum optics A	Paolo Mataloni
Statistical physics C	Amos Maritan
Biophysics B	Laura Cantù

Wednesday, September 11

Title	Chairman
Sensors devices and applications A	Ermanno Pinotti
Surface science C	Marco Finazzi
Superconductivity C	Mikkel Ejrnaes
Plasma physics A	Francesco Pegoraro
SILS A	Antonella Balerna
Electrons and phonons B	Stefano Baroni
Cultural heritage A	Marco Zoppi
Quantum optics B	Lucio Andreani
SISN A	Renato Magli
Spintronics	Riccardo Bertacco

Thursday, September 12

Title	Chairman
Biosensors	Bruno Murari
Quantum optics C	Paolo Mataloni
Silicon Photonics	Francesco Tassone
Plasma physics B	Stefano Atzeni
SILS B	Paolo Ghigna
Photovoltaics A	Giuseppe Gigli
Cultural heritage B	Marcello Picollo
Photonics A	Carlo Sirtori

SISN B	Milva Celli
Microfluidics	Gianluca Galzerano
Sensors devices and applications B	Romeo Bernini
Microscopy A	Giuseppe Nicotra
Soft matter and complexity A	Barbara Ruzicka
Plasma physics C	Paola Mantica
SILS C	Federico Boscherini
Photovoltaics B	Simona Binetti
Ultrafast phenomena A	Christoph Lienau
Photonics B	Francesco Priolo
SISN C	Alessio De Francesco
Biomedical applications A	Paolo Ossi

Friday, September 13

Title	Chairman
Theoretical biology	Giovanni Ciccotti
Microscopy B	Alberto Tagliaferri
Soft matter and complexity B	Paolo Mariani
Plasma physics D	Fulvio Zonca
SILS-AIC Joint session	Alessandro Gualtieri
Photovoltaics C	Aldo Di Carlo
Ultrafast phenomena B	Luca Poletto
Photonic crystals	Silvia Pietralunga
Neurobiosensors	Emilio Carbone
Biomedical applications B	Luca Nardo

Participants

Abbate Sergio	#120	Organic materials and devices B	Tuesday, September 10
Agnello Simonpietro	#102	Semiconductors-low dimensional materials A	Tuesday, September 10
Agostino Angelo	#022	Superconductivity A	Monday, September 9
Al-Mulla Emad A. Jaffar	#038	Organic materials and devices A	Monday, September 9
Albisetti Edoardo	#303	Spintronics	Wednesday, September 11
Alfinito Eleonora	#232	Biophysics B	Tuesday, September 10
Alippi Paola	#130	Strongly Correlated Electron Systems A	Tuesday, September 10
Allevi Alessia	#292	Quantum optics B	Wednesday, September 11
Alpeggiani Filippo	#021	Superconductivity A	Monday, September 9
Altarelli Massimo	#407	SILS C	Thursday, September 12
Amati Matteo	#269	SILS A	Wednesday, September 11
Amodeo Aldo	#111	Environmental physics and energy generation B	Tuesday, September 10
Amodeo Aldo	#115	Environmental physics and energy generation B	Tuesday, September 10
Andreani Carla	#394	Soft matter and complexity A	Thursday, September 12
Angelini Roberta	#460	Soft matter and complexity B	Friday, September 13
Apicella Barbara	#091	Surface science A	Tuesday, September 10
Arciprete Fabrizio	#180	Semiconductors-low dimensional materials B	Tuesday, September 10
Arletti Rossella	#474	SILS-AIC Joint session	Friday, September 13
Armani Francesco	#237	Sensors devices and applications A	Wednesday, September 11
Arosio Paolo	#084	Magnetism and spintronics A	Tuesday, September 10
Atzeni Stefano	#402	Plasma physics C	Thursday, September 12
Avella Adolfo	#209	Strongly Correlated Electron Systems B	Tuesday, September 10
Avella Alessio	#293	Quantum optics B	Wednesday, September 11
Baffigi Federica	#403	Plasma physics C	Thursday, September 12
Bafile Ubaldo	#365	SISN B	Thursday, September 12
Baiesi Marco	#451	Theoretical biology	Friday, September 13
Bajoni Daniele	#321	Silicon Photonics	Thursday, September 12
Baldini Francesco	#309	Biosensors	Thursday, September 12
Baldovin Fulvio	#065	Statistical physics A	Monday, September 9
Balerna Antonella	#409	SILS C	Thursday, September 12
Balucani Marco	#323	Silicon Photonics	Thursday, September 12
Bargigia Ilaria	#441	Biomedical applications A	Thursday, September 12
Barone Paolo	#005	Multiferroics	Monday, September 9
Baroni Stefano	#195	Electrons and phonons A	Tuesday, September 10
Battiato Alfio	#071	Diamond devices	Monday, September 9
Bazzan Marco	#360	Photonics A	Thursday, September 12

Beccara Silvio	#447	Theoretical biology	Friday, September 13
Bejenari Igor	#279	Electrons and phonons B	Wednesday, September 11
Belfi Jacopo	#377	Sensors devices and applications B	Thursday, September 12
Bellini Valerio	#157	Magnetism and spintronics B	Tuesday, September 10
Benenti Giuliano	#145	Statistical physics B	Tuesday, September 10
Bernardi Ettore	#388	Microscopy A	Thursday, September 12
Bernini Romeo	#308	Biosensors	Thursday, September 12
Berrettoni Chiara	#381	Sensors devices and applications B	Thursday, September 12
Bertacco Riccardo	#203	Strongly Correlated Electron Systems B	Tuesday, September 10
Berti Giulia	#088	Surface science A	Tuesday, September 10
Bertotti Giorgio	#077	Magnetism and spintronics A	Tuesday, September 10
Betti Maria Grazia	#240	Surface science C	Wednesday, September 11
Bettotti Paolo	#380	Sensors devices and applications B	Thursday, September 12
Biagioni Paolo	#048	Plasmonics	Monday, September 9
Bietti Sergio	#184	Semiconductors-low dimensional materials B	Tuesday, September 10
Bietti Sergio	#345	Photovoltaics A	Thursday, September 12
Bietti Sergio	#316	Quantum optics C	Thursday, September 12
Bina Matteo	#433	Photonics B	Thursday, September 12
Binetti Simona	#339	Photovoltaics A	Thursday, September 12
Bisogni Valentina	#128	Strongly Correlated Electron Systems A	Tuesday, September 10
Bisti Federico	#062	Graphene A	Monday, September 9
Boarino Luca Boarino	#234	Sensors devices and applications A	Wednesday, September 11
Bollani Monica	#104	Semiconductors-low dimensional materials A	Tuesday, September 10
Bonafos Caroline	#385	Microscopy A	Thursday, September 12
Bondani Maria	#291	Quantum optics B	Wednesday, September 11
Bonfà Pietro	#207	Strongly Correlated Electron Systems B	Tuesday, September 10
Bordignon Sara	#129	Strongly Correlated Electron Systems A	Tuesday, September 10
Bordonali Lorenzo	#159	Magnetism and spintronics B	Tuesday, September 10
Bordone Paolo	#315	Quantum optics C	Thursday, September 12
Borghetti Patrizia	#041	Organic materials and devices A	Monday, September 9
Borgogno Dario	#261	Plasma physics A	Wednesday, September 11
Borisenko Sergey	#094	Superconductivity B	Tuesday, September 10
Boscaino Annalisa	#363	SISN B	Thursday, September 12
Boscherini Federico	#264	SILS A	Wednesday, September 11
Boschini Fabio	#079	Magnetism and spintronics A	Tuesday, September 10
Bosia Federico	#073	Diamond devices	Monday, September 9
Bossoni Lucia	#099	Superconductivity B	Tuesday, September 10
Bottegoni Federico	#301	Spintronics	Wednesday, September 11
Bouzin Margaux	#512	Biomedical applications B	Friday, September 13
Bozzola Angelo	#486	Photovoltaics C	Friday, September 13
Bragheri Francesca	#370	Microfluidics	Thursday, September 12

Brida Daniele	#419	Ultrafast phenomena A	Thursday, September 12
Bridelli Maria Grazia	#282	Cultural heritage A	Wednesday, September 11
Briguglio Sergio	#328	Plasma physics B	Thursday, September 12
Brocca Paola	#149	Biophysics A	Tuesday, September 10
Brunetti Rossella	#197	Electrons and phonons A	Tuesday, September 10
Buatier De Mongeot Francesco	#241	Surface science C	Wednesday, September 11
Buratti Paolo	#257	Plasma physics A	Wednesday, September 11
Bussetti Gianlorenzo	#118	Organic materials and devices B	Tuesday, September 10
Caciuffo Roberto	#095	Superconductivity B	Tuesday, September 10
Caddeo Claudia	#464	Soft matter and complexity B	Friday, September 13
Calegari Francesca	#425	Ultrafast phenomena A	Thursday, September 12
Calidonna Claudia Roberta	#188	Environmental physics and energy generation C	Tuesday, September 10
Callegaro Luca	#025	Metrology and fundamental constants	Monday, September 9
Calloni Alberto	#416	Photovoltaics B	Thursday, September 12
Campi Davide	#278	Electrons and phonons B	Wednesday, September 11
Campione Marcello	#246	Surface science C	Wednesday, September 11
Canazza Giancarlo	#119	Organic materials and devices B	Tuesday, September 10
Cancellieri Claudia	#247	Surface science C	Wednesday, September 11
Canepa Maurizio	#050	Plasmonics	Monday, September 9
Cantù Laura	#146	Biophysics A	Tuesday, September 10
Capati Matteo	#023	Superconductivity A	Monday, September 9
Capitanio Marco	#147	Biophysics A	Tuesday, September 10
Capotondi Flavio	#332	SILS B	Thursday, September 12
Cappello Susanna	#325	Plasma physics B	Thursday, September 12
Caprara Sergio	#204	Strongly Correlated Electron Systems B	Tuesday, September 10
Carabelli Valentina	#502	Neurobiosensors	Friday, September 13
Carlotti Giovanni	#076	Magnetism and spintronics A	Tuesday, September 10
Carretta Pietro	#097	Superconductivity B	Tuesday, September 10
Carretta Stefano	#154	Magnetism and spintronics B	Tuesday, September 10
Carroll Lee	#496	Photonic crystals	Friday, September 13
Cassinese Antonio	#037	Organic materials and devices A	Monday, September 9
Castagna Riccardo	#044	Organic materials and devices A	Monday, September 9
Castiglioni Chiara	#042	Organic materials and devices A	Monday, September 9
Castrovilli Mattea Carmen	#268	SILS A	Wednesday, September 11
Castrucci Paola	#479	Photovoltaics C	Friday, September 13
Cazzaniga Marco	#280	Electrons and phonons B	Wednesday, September 11
Cecchi Stefano	#193	Environmental physics and energy generation C	Tuesday, September 10
Cecconi Fabio	#229	Biophysics B	Tuesday, September 10
Celebrano Michele	#374	Microfluidics	Thursday, September 12
Cesca Tiziana	#052	Plasmonics	Monday, September 9
Chiappini Andrea	#498	Photonic crystals	Friday, September 13

Chiarello Fabio	#256	Superconductivity C	Wednesday, September 11
Chiasera Alessandro	#430	Photonics B	Thursday, September 12
Chiesa Alessandro	#317	Quantum optics C	Thursday, September 12
Chrastina Daniel	#107	Semiconductors-low dimensional materials A	Tuesday, September 10
Ciancio Regina	#205	Strongly Correlated Electron Systems B	Tuesday, September 10
Cicchi Riccardo	#440	Biomedical applications A	Thursday, September 12
Coan Paola	#265	SILS A	Wednesday, September 11
Coduri Mauro	#337	SILS B	Thursday, September 12
Cojoc Dan	#438	Biomedical applications A	Thursday, September 12
Cola Adriano	#181	Semiconductors-low dimensional materials B	Tuesday, September 10
Colle Renato	#276	Electrons and phonons B	Wednesday, September 11
Colombo Annalisa	#043	Organic materials and devices A	Monday, September 9
Colombo Luciano	#196	Electrons and phonons A	Tuesday, September 10
Colonna Stefano	#166	Surface science B	Tuesday, September 10
Comini Elisabetta	#375	Sensors devices and applications B	Thursday, September 12
Continenza Alessandra	#249	Superconductivity C	Wednesday, September 11
Contini Davide	#312	Biosensors	Thursday, September 12
Contini Davide	#442	Biomedical applications A	Thursday, September 12
Convertino Annalisa	#310	Biosensors	Thursday, September 12
Corberi Federico	#144	Statistical physics B	Tuesday, September 10
Cossu Federica	#478	SILS-AIC Joint session	Friday, September 13
Costa Dino	#393	Soft matter and complexity A	Thursday, September 12
Costa Luca	#386	Microscopy A	Thursday, September 12
Cottone Grazia	#067	Statistical physics A	Monday, September 9
Cozzini Stefano	#109	Semiconductors-low dimensional materials A	Tuesday, September 10
Cramer Tobias	#504	Neurobiosensors	Friday, September 13
Crespi Andrea	#497	Photonic crystals	Friday, September 13
Criante Luigino	#499	Photonic crystals	Friday, September 13
Criante Luigino	#373	Microfluidics	Thursday, September 12
Cristelli Matthieu	#225	Statistical physics C	Tuesday, September 10
Cristiani Ilaria	#356	Photonics A	Thursday, September 12
Cristiano Roberto	#172	Superconducting quantum detectors	Tuesday, September 10
Cristofolini Luigi	#461	Soft matter and complexity B	Friday, September 13
Crupi Isodiana	#342	Photovoltaics A	Thursday, September 12
Cuccoli Alessandro	#217	Quantum optics A	Tuesday, September 10
Cuccoli Alessandro	#156	Magnetism and spintronics B	Tuesday, September 10
D'Agostino Stefania	#051	Plasmonics	Monday, September 9
D'Amico Michele	#117	Organic materials and devices B	Tuesday, September 10
D'Angelo Egidio	#009	Neural circuit functioning and computation	Monday, September 9
Dal Conte Stefano	#020	Superconductivity A	Monday, September 9
De Angelis Roberta	#378	Sensors devices and applications B	Thursday, September 12

de Medici Luca	#252	Superconductivity C	Wednesday, September 11
De Padova Paola	#085	Surface science A	Tuesday, September 10
De Renzi Valentina	#415	Photovoltaics B	Thursday, September 12
Debernardi Alberto	#275	Electrons and phonons B	Wednesday, September 11
Della Valle Giuseppe	#490	Ultrafast phenomena B	Friday, September 13
Dellasega David	#330	Plasma physics B	Thursday, September 12
Delmonte Davide	#006	Multiferroics	Monday, September 9
Di Carlo Aldo	#411	Photovoltaics B	Thursday, September 12
Di Cicco Andrea	#335	SILS B	Thursday, September 12
Di Filippo Gianluca	#336	SILS B	Thursday, September 12
Di Fonzo Fabio	#483	Photovoltaics C	Friday, September 13
Di Fraia Michele	#239	Sensors devices and applications A	Wednesday, September 11
Di Garbo Angelo	#452	Theoretical biology	Friday, September 13
Di Giovannantonio Marco	#455	Microscopy B	Friday, September 13
Di Piazza Antonino	#258	Plasma physics A	Wednesday, September 11
Diemoz Paul Claude	#267	SILS A	Wednesday, September 11
Dijkstra Bauke	#471	SILS-AIC Joint session	Friday, September 13
Dinesan Hemanth	#035	Environmental physics and energy generation A	Monday, September 9
Donarelli Maurizio	#165	Surface science B	Tuesday, September 10
Durin Gianfranco	#078	Magnetism and spintronics A	Tuesday, September 10
Ejrnaes Mikkel	#173	Superconducting quantum detectors	Tuesday, September 10
Esposito Emanuela	#053	Plasmonics	Monday, September 9
Esteve Daniel	#250	Superconductivity C	Wednesday, September 11
Faghihi Niloufar	#081	Magnetism and spintronics A	Tuesday, September 10
Falci Giuseppe	#211	Quantum optics A	Tuesday, September 10
Fanfarillo Laura	#096	Superconductivity B	Tuesday, September 10
Fantoni Riccardo	#222	Statistical physics C	Tuesday, September 10
Faraci Giuseppe	#322	Silicon Photonics	Thursday, September 12
Fasci Eugenio	#194	Environmental physics and energy generation C	Tuesday, September 10
Fausti Daniele	#024	Superconductivity A	Monday, September 9
Fazi Laura	#242	Surface science C	Wednesday, September 11
Fazio Rosario	#289	Quantum optics B	Wednesday, September 11
Ferragut Rafael	#484	Photovoltaics C	Friday, September 13
Ferri Fabio	#226	Biophysics B	Tuesday, September 10
Festa Giulia	#349	Cultural heritage B	Thursday, September 12
Filibian Marta	#513	Biomedical applications B	Friday, September 13
Filippone Francesco	#086	Surface science A	Tuesday, September 10
Filipponi Adriano	#398	Soft matter and complexity A	Thursday, September 12
Finazzi Marco	#163	Surface science B	Tuesday, September 10
Fiorentini Vincenzo Fiorentini	#206	Strongly Correlated Electron Systems B	Tuesday, September 10
Fioretto Daniele	#395	Soft matter and complexity A	Thursday, September 12

Flora Francesco	#511	Biomedical applications B	Friday, September 13
Floris Francesco	#238	Sensors devices and applications A	Wednesday, September 11
Fontana Dorotea	#284	Cultural heritage A	Wednesday, September 11
Fontana Raffaella	#351	Cultural heritage B	Thursday, September 12
Fontcuberta Josep	#002	Multiferroics	Monday, September 9
Forneris Jacopo	#074	Diamond devices	Monday, September 9
Fortunelli Alessandro	#090	Surface science A	Tuesday, September 10
Fratesi Guido	#201	Electrons and phonons A	Tuesday, September 10
Frigerio Jacopo	#103	Semiconductors-low dimensional materials A	Tuesday, September 10
Fujii Jun	#306	Spintronics	Wednesday, September 11
Fuzzi Sandro	#031	Environmental physics and energy generation A	Monday, September 9
Gabbanini Carlo	#216	Quantum optics A	Tuesday, September 10
Gaboardi Mattia	#136	Graphene B	Tuesday, September 10
Gabrielli Andrea	#142	Statistical physics B	Tuesday, September 10
Gaggero Alessandro	#175	Superconducting quantum detectors	Tuesday, September 10
Galantucci Luca	#220	Statistical physics C	Tuesday, September 10
Galli Davide Emilio	#224	Statistical physics C	Tuesday, September 10
Gallo Erik Gallo	#334	SILS B	Thursday, September 12
Galzerano Gianluca	#026	Metrology and fundamental constants	Monday, September 9
Gambardella Pietro	#155	Magnetism and spintronics B	Tuesday, September 10
Garlatti Elena	#160	Magnetism and spintronics B	Tuesday, September 10
Garrido Jesus	#017	Neural circuit functioning and computation	Monday, September 9
Gatti Alessandra	#294	Quantum optics B	Wednesday, September 11
Gatto Monticone Daniele	#072	Diamond devices	Monday, September 9
Gerelli Yuri	#436	SISN C	Thursday, September 12
Ghiringhelli Giacomo	#124	Strongly Correlated Electron Systems A	Tuesday, September 10
Giammarchi Marco Giulio	#027	Metrology and fundamental constants	Monday, September 9
Gigli Giuseppe	#410	Photovoltaics B	Thursday, September 12
Giordano Maria Caterina	#500	Photonic crystals	Friday, September 13
Giovenale Emilio	#350	Cultural heritage B	Thursday, September 12
Giulotto Enrico	#183	Semiconductors-low dimensional materials B	Tuesday, September 10
Gizzi Leonida Antonio	#465	Plasma physics D	Friday, September 13
Goletti Claudio	#379	Sensors devices and applications B	Thursday, September 12
Goltsman Gregory	#171	Superconducting quantum detectors	Tuesday, September 10
Gondoni Paolo	#413	Photovoltaics B	Thursday, September 12
Gorini Giuseppe	#437	SISN C	Thursday, September 12
Gosso Sara	#506	Neurobiosensors	Friday, September 13
Grilli Marco	#125	Strongly Correlated Electron Systems A	Tuesday, September 10
Guarcello Claudio	#255	Superconductivity C	Wednesday, September 11
Guardone Alberto	#219	Statistical physics C	Tuesday, September 10
Guarini Eleonora	#392	Soft matter and complexity A	Thursday, September 12

Guarino Anita	#100	Superconductivity B	Tuesday, September 10
Guidi Vincenzo Guidi	#382	Sensors devices and applications B	Thursday, September 12
Gunnella Roberto	#482	Photovoltaics C	Friday, September 13
Gunnella Roberto	#169	Surface science B	Tuesday, September 10
Gurioli Massimo	#495	Photonic crystals	Friday, September 13
Guzzi Rita	#148	Biophysics A	Tuesday, September 10
Hedayat Zadeh Roodsari Hamoon	#492	Ultrafast phenomena B	Friday, September 13
Hilairet Nadege	#472	SILS-AIC Joint session	Friday, September 13
Iadecola Antonella	#251	Superconductivity C	Wednesday, September 11
Isa Lucio	#399	Soft matter and complexity A	Thursday, September 12
Isabella Olindo	#340	Photovoltaics A	Thursday, September 12
Jamet Matthieu	#299	Spintronics	Wednesday, September 11
Jayaswal Gaurav	#212	Quantum optics A	Tuesday, September 10
Jona-Lasinio Giovanni	#218	Statistical physics C	Tuesday, September 10
Jug Giancarlo	#198	Electrons and phonons A	Tuesday, September 10
Koester Petra	#262	Plasma physics A	Wednesday, September 11
Koplak Oksana	#131	Organic materials and devices B	Tuesday, September 10
Kowalczewski Piotr	#343	Photovoltaics A	Thursday, September 12
Krauss Thomas	#494	Photonic crystals	Friday, September 13
Kriegel Ilka	#049	Plasmonics	Monday, September 9
Kuzkova Nataliia	#358	Photonics A	Thursday, September 12
Labate Luca	#443	Biomedical applications A	Thursday, September 12
Lacava Cosimo	#429	Photonics B	Thursday, September 12
Larciprete Rosanna	#135	Graphene B	Tuesday, September 10
Lascialfari Alessandro	#508	Biomedical applications B	Friday, September 13
Lattanzi Gianluca	#122	Organic materials and devices B	Tuesday, September 10
Le Donne Alessia	#341	Photovoltaics A	Thursday, September 12
Leto Giuseppe	#114	Environmental physics and energy generation B	Tuesday, September 10
Lienau Christoph	#488	Ultrafast phenomena B	Friday, September 13
Lillo Fabrizio	#063	Statistical physics A	Monday, September 9
Liscidini Marco	#290	Quantum optics B	Wednesday, September 11
Lisitskiy Mikhail	#254	Superconductivity C	Wednesday, September 11
Liuzzi Giuliano	#036	Environmental physics and energy generation A	Monday, September 9
Lo Russo Sergio	#190	Environmental physics and energy generation C	Tuesday, September 10
Locatelli Emanuele	#069	Statistical physics A	Monday, September 9
Lolli Lapo	#176	Superconducting quantum detectors	Tuesday, September 10
Lorenzana Josè	#001	Multiferroics	Monday, September 9
Lozzi Luca	#414	Photovoltaics B	Thursday, September 12
Luca Perfetti	#418	Ultrafast phenomena A	Thursday, September 12
Lucchetti Liana	#463	Soft matter and complexity B	Friday, September 13
Lupi Stefano	#060	Graphene A	Monday, September 9

Maccarini Marco	#434	SISN C	Thursday, September 12
Macchi Andrea	#400	Plasma physics C	Thursday, September 12
Magazzù Luca	#143	Statistical physics B	Tuesday, September 10
Maggi Silvia	#015	Neural circuit functioning and computation	Monday, September 9
Maiuri Margherita	#480	Photovoltaics C	Friday, September 13
Malizia Andrea	#468	Plasma physics D	Friday, September 13
Mancini Giulia Fulvia	#390	Microscopy A	Thursday, September 12
Manini Nicola	#223	Statistical physics C	Tuesday, September 10
Mantica Paola	#466	Plasma physics D	Friday, September 13
Manzoni Cristian	#422	Ultrafast phenomena A	Thursday, September 12
Mapelli Jonathan	#505	Neurobiosensors	Friday, September 13
Maragliano Luca	#450	Theoretical biology	Friday, September 13
Marenduzzo Davide	#228	Biophysics B	Tuesday, September 10
Mariani Giacomo	#364	SISN B	Thursday, September 12
Mariotti Emilio	#028	Metrology and fundamental constants	Monday, September 9
Maritan Amos	#139	Statistical physics B	Tuesday, September 10
Marongiu Daniela	#412	Photovoltaics B	Thursday, September 12
Marrale Maurizio	#515	Biomedical applications B	Friday, September 13
Marsili Matteo	#064	Statistical physics A	Monday, September 9
Martella Christian	#344	Photovoltaics A	Thursday, September 12
Masiello Guido	#112	Environmental physics and energy generation B	Tuesday, September 10
Masoli Stefano	#013	Neural circuit functioning and computation	Monday, September 9
Massarotti Davide	#253	Superconductivity C	Wednesday, September 11
Mataloni Paolo	#288	Quantum optics B	Wednesday, September 11
Mattevi Cecilia	#055	Graphene A	Monday, September 9
Matthias Bauer	#331	SILS B	Thursday, September 12
Mattoni Alessandro	#087	Surface science A	Tuesday, September 10
Mauri Francesco	#274	Electrons and phonons B	Wednesday, September 11
Maurizio Chiara	#431	Photonics B	Thursday, September 12
Mazza Leonardo	#213	Quantum optics A	Tuesday, September 10
Mazzarella Giovanni	#126	Strongly Correlated Electron Systems A	Tuesday, September 10
Mazzoli Claudio	#003	Multiferroics	Monday, September 9
Mazzolini Piero	#346	Photovoltaics A	Thursday, September 12
Melis Claudio Melis	#510	Biomedical applications B	Friday, September 13
Melloni Andrea	#320	Silicon Photonics	Thursday, September 12
Merlini Marco	#473	SILS-AIC Joint session	Friday, September 13
Mezi Luca	#259	Plasma physics A	Wednesday, September 11
Michailov Michail	#248	Surface science C	Wednesday, September 11
Migliore Michele	#010	Neural circuit functioning and computation	Monday, September 9
Minola Matteo	#270	SILS A	Wednesday, September 11
Mio Antonio Massimiliano	#457	Microscopy B	Friday, September 13

Mistura Giampaolo	#368	Microfluidics	Thursday, September 12
Molinari Elisa	#134	Graphene B	Tuesday, September 10
Mondiali Valeria	#106	Semiconductors-low dimensional materials A	Tuesday, September 10
Monico Letizia	#477	SILS-AIC Joint session	Friday, September 13
Montoncello Federico	#162	Magnetism and spintronics B	Tuesday, September 10
Montorsi Arianna	#208	Strongly Correlated Electron Systems B	Tuesday, September 10
Morandi Vittorio	#384	Microscopy A	Thursday, September 12
Morante J.r.	#376	Sensors devices and applications B	Thursday, September 12
Moras Paolo	#302	Spintronics	Wednesday, September 11
Morpurgo Alberto	#054	Graphene A	Monday, September 9
Mosca Conte Adriano	#354	Cultural heritage B	Thursday, September 12
Motta Mario	#221	Statistical physics C	Tuesday, September 10
Motta Simona	#153	Biophysics A	Tuesday, September 10
Mulser Pietro	#327	Plasma physics B	Thursday, September 12
Murari Bruno	#235	Sensors devices and applications A	Wednesday, September 11
Nappini Silvia	#397	Soft matter and complexity A	Thursday, September 12
Nardo Luca	#439	Biomedical applications A	Thursday, September 12
Narducci Dario	#185	Semiconductors-low dimensional materials B	Tuesday, September 10
Natalello Antonino	#152	Biophysics A	Tuesday, September 10
Natali Dario	#123	Organic materials and devices B	Tuesday, September 10
Nava Giovanni	#432	Photonics B	Thursday, September 12
Nevin Austin	#286	Cultural heritage A	Wednesday, September 11
Nieus Thierry	#016	Neural circuit functioning and computation	Monday, September 9
Nucciotti Angelo	#174	Superconducting quantum detectors	Tuesday, September 10
Olivares Stefano	#214	Quantum optics A	Tuesday, September 10
Olivero Paolo	#361	Photonics A	Thursday, September 12
Onida Giovanni	#199	Electrons and phonons A	Tuesday, September 10
Orlandini Enzo	#227	Biophysics B	Tuesday, September 10
Orlando Tomas	#082	Magnetism and spintronics A	Tuesday, September 10
Orsi Davide	#462	Soft matter and complexity B	Friday, September 13
Ortore Maria Grazia	#230	Biophysics B	Tuesday, September 10
Osellame Roberto	#367	Microfluidics	Thursday, September 12
Ossi Paolo	#509	Biomedical applications B	Friday, September 13
Ossicini Stefano	#178	Semiconductors-low dimensional materials B	Tuesday, September 10
Ottevaere Heidi	#357	Photonics A	Thursday, September 12
Paduano Luigi	#295	SISN A	Wednesday, September 11
Pagliero Alessandro	#338	SILS B	Thursday, September 12
Palma Massimo	#210	Quantum optics A	Tuesday, September 10
Palummo Maurizia	#277	Electrons and phonons B	Wednesday, September 11
Paolucci Giorgio	#405	SILS C	Thursday, September 12
Papagno Marco	#138	Graphene B	Tuesday, September 10

Parlato Loredana	#177	Superconducting quantum detectors	Tuesday, September 10
Paroli Bruno	#404	Plasma physics C	Thursday, September 12
Parravicini Jacopo	#359	Photonics A	Thursday, September 12
Pasquarelli Alberto	#501	Neurobiosensors	Friday, September 13
Pasquini Luca	#191	Environmental physics and energy generation C	Tuesday, September 10
Passoni Luca	#244	Surface science C	Wednesday, September 11
Patimisco Pietro	#428	Photonics B	Thursday, September 12
Patthey Luc	#408	SILS C	Thursday, September 12
Pavesi Lorenzo	#319	Silicon Photonics	Thursday, September 12
Peccianti Marco	#427	Photonics B	Thursday, September 12
Peddis Davide	#083	Magnetism and spintronics A	Tuesday, September 10
Pedio Maddalena	#333	SILS B	Thursday, September 12
Pegoraro Francesco	#324	Plasma physics B	Thursday, September 12
Pernechele Chiara	#004	Multiferroics	Monday, September 9
Perrone Maria Rita	#034	Environmental physics and energy generation A	Monday, September 9
Persano Adorno Dominique	#304	Spintronics	Wednesday, September 11
Petrucci Ferruccio	#348	Cultural heritage B	Thursday, September 12
Petti Daniela	#311	Biosensors	Thursday, September 12
Picollo Federico	#503	Neurobiosensors	Friday, September 13
Picollo Marcello	#281	Cultural heritage A	Wednesday, September 11
Pietralunga Silvia Maria	#391	Microscopy A	Thursday, September 12
Pietropaolo Antonino	#297	SISN A	Wednesday, September 11
Pirri Fabrizio	#307	Biosensors	Thursday, September 12
Pisani Gianluca	#113	Environmental physics and energy generation B	Tuesday, September 10
Placidi Ernesto	#182	Semiconductors-low dimensional materials B	Tuesday, September 10
Plastino Wolfango	#189	Environmental physics and energy generation C	Tuesday, September 10
Poletto Luca	#420	Ultrafast phenomena A	Thursday, September 12
Polignano Maria Luisa	#105	Semiconductors-low dimensional materials A	Tuesday, September 10
Polini Marco	#133	Graphene B	Tuesday, September 10
Politano Antonio	#168	Surface science B	Tuesday, September 10
Polli Dario	#423	Ultrafast phenomena A	Thursday, September 12
Pontiroli Daniele	#192	Environmental physics and energy generation C	Tuesday, September 10
Ponzoni Stefano	#491	Ultrafast phenomena B	Friday, September 13
Porcari Giacomo	#161	Magnetism and spintronics B	Tuesday, September 10
Prestipino Santi	#396	Soft matter and complexity A	Thursday, September 12
Prezioso Stefano	#137	Graphene B	Tuesday, September 10
Priolo Francesco	#318	Silicon Photonics	Thursday, September 12
Quochi Francesco	#039	Organic materials and devices A	Monday, September 9
Radica Francesco	#272	SILS A	Wednesday, September 11
Raimondi Pantaleo	#406	SILS C	Thursday, September 12
Raimondi Valentina	#283	Cultural heritage A	Wednesday, September 11

Rajendran Sai Kiran	#215	Quantum optics A	Tuesday, September 10
Ranguelov Bogdan	#092	Surface science A	Tuesday, September 10
Re Alessandro	#285	Cultural heritage A	Wednesday, September 11
Ricci Fabio	#098	Superconductivity B	Tuesday, September 10
Ricci Francesco	#008	Multiferroics	Monday, September 9
Riccò Mauro	#059	Graphene A	Monday, September 9
Ridolfi Emilia	#179	Semiconductors-low dimensional materials B	Tuesday, September 10
Riedinger Andreas	#444	Biomedical applications A	Thursday, September 12
Riminesi Cristiano	#353	Cultural heritage B	Thursday, September 12
Rinaldi Christian	#305	Spintronics	Wednesday, September 11
Rizi Vincenzo	#033	Environmental physics and energy generation A	Monday, September 9
Roberto Cesario	#329	Plasma physics B	Thursday, September 12
Rocca Mario	#164	Surface science B	Tuesday, September 10
Roddaro Stefano	#101	Semiconductors-low dimensional materials A	Tuesday, September 10
Roethlisberger Ursula	#446	Theoretical biology	Friday, September 13
Rolandi Ranieri	#231	Biophysics B	Tuesday, September 10
Romani Aldo	#352	Cultural heritage B	Thursday, September 12
Romanò Monica	#475	SILS-AIC Joint session	Friday, September 13
Romè Massimiliano	#260	Plasma physics A	Wednesday, September 11
Romeo Francesco	#300	Spintronics	Wednesday, September 11
Rondelli Valeria Maria	#298	SISN A	Wednesday, September 11
Rontani Massimo	#389	Microscopy A	Thursday, September 12
Rossi Barbara	#150	Biophysics A	Tuesday, September 10
Rossi Maurizio	#066	Statistical physics A	Monday, September 9
Ruffinatti Federico Alessandro	#507	Neurobiosensors	Friday, September 13
Ruffo Stefano	#140	Statistical physics B	Tuesday, September 10
Ruggeri Rosa	#456	Microscopy B	Friday, September 13
Ruocco Alessandro	#485	Photovoltaics C	Friday, September 13
Rurali Riccardo	#187	Semiconductors-low dimensional materials B	Tuesday, September 10
Russo Roberto	#236	Sensors devices and applications A	Wednesday, September 11
Rutigliano Maria	#243	Surface science C	Wednesday, September 11
Ruzicka Barbara	#459	Soft matter and complexity B	Friday, September 13
Saba Maria Ilenia	#121	Organic materials and devices B	Tuesday, September 10
Saba Michele	#093	Surface science A	Tuesday, September 10
Sacconi Leonardo	#012	Neural circuit functioning and computation	Monday, September 9
Salluzzo Marco	#202	Strongly Correlated Electron Systems B	Tuesday, September 10
Sampietro Marco	#116	Organic materials and devices B	Tuesday, September 10
Sansone Giuseppe	#493	Ultrafast phenomena B	Friday, September 13
Sassella Adele	#045	Organic materials and devices A	Monday, September 9
Sasso Antonio	#040	Organic materials and devices A	Monday, September 9
Sasso Antonio	#371	Microfluidics	Thursday, September 12

Sbragaglia Mauro	#372	Microfluidics	Thursday, September 12
Scarselli Manuela	#061	Graphene A	Monday, September 9
Schiavi Angelo	#326	Plasma physics B	Thursday, September 12
Scopigno Tullio	#487	Ultrafast phenomena B	Friday, September 13
Sebastiani Federica	#366	SISN B	Thursday, September 12
Secchi Eleonora	#387	Microscopy A	Thursday, September 12
Senesi Roberto	#362	SISN B	Thursday, September 12
Serio Carmine	#032	Environmental physics and energy generation A	Monday, September 9
Sgarlata Anna	#108	Semiconductors-low dimensional materials A	Tuesday, September 10
Siciliano Pietro	#233	Sensors devices and applications A	Wednesday, September 11
Silvestri Ludovico	#014	Neural circuit functioning and computation	Monday, September 9
Sirtori Carlo	#426	Photonics B	Thursday, September 12
Skrbic Tatjana	#448	Theoretical biology	Friday, September 13
Smerieri Marco	#089	Surface science A	Tuesday, September 10
Soavi Giancarlo	#489	Ultrafast phenomena B	Friday, September 13
Solinas Sergio	#011	Neural circuit functioning and computation	Monday, September 9
Solzi Massimo	#158	Magnetism and spintronics B	Tuesday, September 10
Sommariva Marco	#476	SILS-AIC Joint session	Friday, September 13
Sordan Roman	#056	Graphene A	Monday, September 9
Spadaro Maria Chiara	#170	Surface science B	Tuesday, September 10
Spagnolo Bernardo	#141	Statistical physics B	Tuesday, September 10
Spagnolo Vincenzo	#383	Sensors devices and applications B	Thursday, September 12
Spinozzi Francesco	#296	SISN A	Wednesday, September 11
Spirito Davide	#132	Graphene B	Tuesday, September 10
Stagira Salvatore	#424	Ultrafast phenomena A	Thursday, September 12
Stefani Giovanni	#167	Surface science B	Tuesday, September 10
Taioli Simone	#245	Surface science C	Wednesday, September 11
Tampieri Francesco	#110	Environmental physics and energy generation B	Tuesday, September 10
Tantussi Francesco	#046	Plasmonics	Monday, September 9
Taroni Paola	#514	Biomedical applications B	Friday, September 13
Tassi Emanuele	#263	Plasma physics A	Wednesday, September 11
Tavernelli Ivano	#273	Electrons and phonons B	Wednesday, September 11
Tiberto Paola	#007	Multiferroics	Monday, September 9
Tognolini Silvia	#058	Graphene A	Monday, September 9
Toigo Flavio	#314	Quantum optics C	Thursday, September 12
Tommasi Federico	#421	Ultrafast phenomena A	Thursday, September 12
Tommasini Matteo	#057	Graphene A	Monday, September 9
Totani Roberta	#417	Photovoltaics B	Thursday, September 12
Trovato Antonio	#449	Theoretical biology	Friday, September 13
Truccato Marco	#029	Metrology and fundamental constants	Monday, September 9
Trucchi Daniele Maria	#070	Diamond devices	Monday, September 9

Ulisse Giacomo	#075	Diamond devices	Monday, September 9
Valenti Davide	#445	Theoretical biology	Friday, September 13
Valenti Ilaria	#481	Photovoltaics C	Friday, September 13
Valentini Gianluca	#287	Cultural heritage A	Wednesday, September 11
van den Brink Jeroen	#019	Superconductivity A	Monday, September 9
Vanacore Giovanni Maria	#453	Microscopy B	Friday, September 13
Varlamov Andrey	#018	Superconductivity A	Monday, September 9
Vassalli Massimo	#151	Biophysics A	Tuesday, September 10
Vattuone Luca	#047	Plasmonics	Monday, September 9
Vedda Anna	#516	Biomedical applications B	Friday, September 13
Veltri Pierluigi	#467	Plasma physics D	Friday, September 13
Verdini Alberto	#200	Electrons and phonons A	Tuesday, September 10
Viganò Nicola	#271	SILS A	Wednesday, September 11
Violini Nicolò	#435	SISN C	Thursday, September 12
Vitali David	#313	Quantum optics C	Thursday, September 12
Vitiello Miriam Serena	#355	Photonics A	Thursday, September 12
Vobornik Ivana	#127	Strongly Correlated Electron Systems A	Tuesday, September 10
Wang Xuan	#030	Environmental physics and energy generation A	Monday, September 9
Wilson Keith	#470	SILS-AIC Joint session	Friday, September 13
Zaccarelli Emanuela	#458	Soft matter and complexity B	Friday, September 13
Zanella Andrea	#369	Microfluidics	Thursday, September 12
Zani Maurizio	#454	Microscopy B	Friday, September 13
Zavelani-Rossi Margherita	#186	Semiconductors-low dimensional materials B	Tuesday, September 10
Zimbardo Gaetano	#469	Plasma physics D	Friday, September 13
Zivieri Roberto	#080	Magnetism and spintronics A	Tuesday, September 10
Zoli Marco	#068	Statistical physics A	Monday, September 9
Zonca Fulvio	#401	Plasma physics C	Thursday, September 12
Zontone Federico	#266	SILS A	Wednesday, September 11
Zoppi Marco	#347	Cultural heritage B	Thursday, September 12

#001 - Order by disorder mechanism of multiferroic behavior in CuO

Josè Lorenzana (I) – CNR – Istituto dei Sistemi Complessi, Dipartimento di Fisica, Università Sapienza, Roma

G. Giovannetti (CNR-IOM, Trieste), S. Kumar (IFW Dresden), A. Stroppa (CNR-SPIN, L'Aquila), J. van den Brink (IFW Dresden), S. Picozzi (CNR-SPIN, L'Aquila), J. Hellsvik, M. Balestieri (CNR-ISC, Università Sapienza, Roma)

Cupric oxide is multiferroic at unusually high temperatures [1, 2]. Ferroelectricity appears simultaneously with a non-collinear magnetic phase intermediate between the high-T paramagnet and the low-T antiferromagnet. From density functional calculations we find that the low-T magnetic phase is paraelectric and the intermediate magnetic phase ferroelectric, with a size and direction of polarization in good agreement with experiment. By mapping the ab-intio result into an effective spin model we show that the system has a manifold of almost degenerate ground states. In the high-magnetic state non-collinearity and inversion symmetry breaking stabilize each other via the Dzyaloshinskii-Moriya interaction. This leads to an unconventional mechanism of multiferroicity, with the particular property that non-magnetic impurities enhance the effect [3]. We disucss how this kind of multiferrolectricity can be manipulated by imputrities and light pulses and show estimates of the effect in CuO.

[1] T. Kimura et. al., Nature Mat. 7, 291 (2008).
[2] M. Mostovoy, Nature Mat. 7, 269 (2008).
[3] G. Giovannetti, S. Kumar, A. Stroppa, J. van den Brink, S. Picozzi, J. Lorenzana, Phys. Rev. Lett. 106, 026401 (2011);G. Giovannetti, S. Kumar, A. Stroppa, M. Balestieri, J. van den Brink, S. Picozzi, J. Lorenzana, Phys. Rev. Lett. 107, 239702 (2011).

#002 - Magnetoelectric coupling via interface-coupling and phase-separation in multiferroics

Josep Fontcuberta (I) - Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)

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Nanocomposites of polar and magnetic materials are being considered for dual electric and magnetic responsive advanced technologies. Within this approach, most commonly, ferroelectric and magnetic layers are elastically coupled through interfaces in multilayer stacks. However, in epitaxial heterostructures made of these constituting elements, substrate-induced clamping is thought to be a bottleneck that could hamper the necessary piezo or magnetostrictive action, thus substantially cancelling the response. On the other hand, nanocomposites could be self-formed if suitable mesoscopic phase separation of polar and non-polar regions occurs in a magnetic matrix. This is expected to occur in systems where competing magnetic interactions are at play.
We shall overview recent advances in both directions. It will be shown that ferromagnetic/ferroelectric bilayers epitaxially grown with appropriate architecture, can be made to display substantial magnetoelectric response thus reducing the substrate clamping effect. May be more futuristic, it will be shown that mesoscopic phase separation in single-phase materials, such as that occurring in some orthorhombic manganese perovskites, can be exploited to obtain a polar response that can be fully controlled by a magnetic field, keeping memory of its initial state after successive polar loops.
In short, multiferroic materials hold novel phenomena that promise new opportunities in science and technology.

#003 - Resonant X-ray diffraction contribution in understanding multifunctional materials

Claudio Mazzoli - Politecnico di Milano

Multifunctional materials showing coupled electronic orderings, like Multiferroics and Magneto-electrics for example, are extremely appealing for possible futuristic applications in fields as different as information technologies, sensors and energy harvesting, as well as extremely challenging battles for material scientists and solid state physicists. For long time the modelling of such complex systems was essentially out of the scope but in the last ten years the scientific community has produced an enormous effort to investigate and engineer electronic problems down to the microscopic level. In this panorama, Resonant X-ray Scattering experiments have shown its privileged point of view, being able to unravel tiny electronic handles responsible for macroscopic phenomenology of interest. When diffraction is at play, new and exotic orderings can be investigated, sublattice order parameters spotted and finally coupling mechanisms of electronic origin revealed. I will surf on the last contributions of RXD on this class of materials, showing how the complementarity with neutrons and the specificity of X-ray directly provides the scientific community with fundamental information, otherwise essentially inaccessible.

#004 - Magneto-electric characterization of $BiMn_7O_{12}$ polymorphs

Chiara Pernechele - Dipartimento di Fisica e Scienze della Terra, Università di Parma

Francesco Mezzadri (CNR- IMEM, Parma), Michele Buzzi (PSI, Villigen Switzerland), Davide Delmonte, Massimo Solzi (Dipartimento di Fisica e Scienze della Terra, Università di Parma), Gianluca Calestani (Dipartimento di Chimica e GIAF, Università di Parma), Riccardo Cabassi, Fulvio Bolzoni, Edmondo Gilioli (CNR- IMEM, Parma)

Magnetoelectric multiferroics are actracting wide interest concerning the realization of multifunction devices due to the coexistence of electrical and magnetic ordering. Possible applications can be envisaged in the field of magnetic recording, for improving the reading and writing speed and also in spintronics for the development of new devices based on the additional degrees of freedom

given by ferroelectricity [1].

An interesting material belonging to the class of lone-pair driven multiferroics is $BiMn_7O_{12}$ with structure of quadruple perovskite [2], in which ferroelectricity is induced by the stereochemical effect produced by the Bi^{3+} ion.

$BiMn_7O_{12}$ samples obtained by solid state reaction synthesis under high pressure and high temperature conditions show the existence of three different phases: monoclinic (1.5% Mn^{4+}), rhombohedral (3.0% Mn^{4+}) and cubic (4.5% Mn^{4+}) as a function of Mn^{4+} content [3].

In the present work we will discuss the magnetoelectric characyetisationof the three polymorphs. $\chi(T)$ measurements confirm that the low temperature ordered state for each phase is antiferromagnetic and the presence of a small net momentum value can be ascribed to spin canting induced by Dzyaloshinskii-Moriya interaction. The hysteresis loop shape seems also to be characteristic of the different crystal structure. From the dielectric characterization appears that while monoclinic sample presents two clear peaks at the two magnetic ordering temperature confirming magnetoelectric coupling, the rhomobhedral one shows no clear signs of dielectric constant anomalies at the magnetic transition temperatures. The magnetic measurements in applied electric field show an important effect on the zero field cooling curve measured after electric field poling, thus bringing $BiMn_7O_{12}$ among the most interesting multiferroics materials.

[1] R. Ramesh et al., Nat. Mater. 6 21-29 (2007).
[2] A. Prodi et al., Nat. Mater. 3 48 - 52 (2003).
[3] F. Mezzadri et al., Chem. Mater, 23(16) 3628 (2011).

#005 - Homochiral magnetic cycloids driven by ferroelectric polarization in multiferroic $BiFeO_3$

Paolo Barone – CNR – Istituto Superconduttori, Materiali Innovativi e Dispositivi, UOS L'Aquila

Roger D. Johnson (Clarendon Lab., Univ. of Oxford and ISIS facility, Rutherford Appleton Lab.-STFC, UK), A. Bombardi (Diamond Light Source, UK), R. J. Bean (C.M.M.P., Univ. College London, UK), S. Picozzi (CNR-SPIN UOS L'Aquila) P. G. Radaelli (Clarendon Lab., Univ. of Oxford, UK), Y. S. Oh (Rutgers Center for Emergent Materials and Univ. of New Jersey, USA), S-W. Cheong (Rutgers Center for Emergent Materials and Univ. of New Jersey, USA), L. C. Chapon (Institut Laue-Langevin, Grenoble)

Multiferroic materials are of great interest to the condensed matter physics community as they may form, e.g., key components in future low energy data storage devices. Of all multiferroics studied thus far, $BiFeO_3$ attracts the greatest attention, as it displays multiferroicity at room temperature, where most require cooling below liquid nitrogen temperatures. In $BiFeO_3$ ferroelectricity is the consequence of an improper structural transition at T_c ~1100K to the polar space group *R3c*, whereas the magnetic ordering transition occurs at T_N ~ 640K. The structure can be described locally as G-type antiferromagnetic, but with a long period modulation (a ~ 62 nm) in the hexagonal basal plane, that has been experimentally identified as a cycloidal modulation. While the structural and magnetic transitions are not coincidental, on the basis of general symmetry considerations an inhomogeneous magnetoelectric coupling is expected, where ferroelectric polarization appears to be coupled not only with the magnetization density but also with its gradient. Starting from the experimental observation of homochiral magnetic domains in a ferroelectric monodomain BiFeO3, we theoretically analyzed the coupling between magnetism and ferroelectricity via a combined approach based on a spin-model complemented by relativistic density-functional simulations, unveiling the crucial role of ferroelectric polarization in determining the vector chirality of the magnetic cycloidal phase.

#006 - Study of complex thermally induced field dependent magnetization reversal in BiFe0.5Mn0.5O3, a potentially RT type-I multiferroic

Davide Delmonte - Università di Parma

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We have recently synthesized BiFe0.5Mn0.5O3, a novel multiferroic belonging to the class of bismuth-based double perovskites, in high pressure/high temperature conditions. In this system the electric properties are ascribed to the stereochemical effect induced by the 6s2 lone pair of the Bi ion, while magnetism depends on the complex pattern of interactions involving iron and manganese. Single-crystal X-ray diffraction allowed us to determine the crystallographic structure of the system as a B-site disordered perovskite and suggests the presence of antiferroelectricity. The magnetic characterization indicates an unconventional magnetic behavior producing a weak ferromagnetic transition around 420 K followed below 288 K, by a field-dependent reversal of the magnetization process. We registered the higher negative value of the magnetization -0.75 emu/g, for an applied field of 70 Oe. Larger fields gradually inhibit the magnetization reversal process, which is completely suppressed at 1.5 KOe. Despite the actual interpretation of the magnetization reversal process [1], our studies give a different explanation of this phenomenon.

By performing temperature dependent neutron diffraction experiments, we determined the spin ordering scheme of the system as a G-type structure, involving the sole presence of AFM interactions. However the low-temperature magnetism of BiFe0.5Mn0.5O3 shows intricate mechanisms. Such mechanisms evidently confirmed a different origin, that is weaker in energy than the AFM leading contribution. Thanks to Fe-57 Mossbauer spectroscopy we have been able to discriminate the presence of iron ions with a dramatically different behaviour: a little part of them being ordered at RT, due to the presence of iron-rich clusters, and a large population of paramagnetic ones that gradually gets ordered with a continuous mechanism taking place at 288 K, when the long range antiferromagnetism occurs driven by the manganese ions ordering. The current results suggest that the weak ferromagnetic effects observed can be due to uncompensated Dzyaloshinkii-Moriya interactions characterized by different D vectors and thermal

dependencies as could be for the Fe-O-Fe, Mn-O-Mn and Fe-O-Mn interactions. This mechanism is responsible for the magnetization reversal and allows to justify its strong dependence on the applied magnetic field, according also to the low magnitude of the magnetic response. As a consequence, in absence of a sufficiently large field, the magnetization goes down to negative values below 250 K but can be easily reversed up simply increasing the external field [2].

Furthermore we measured a magnetodielectric effect that can partially controlled by an external magnetic field and other interesting evidence of magnetoelectricity in this intriguing compound.

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[2] D. Delmonte et al., submitted (2013).

#007 - Magnetic and magnetotransport properties of multiferroics materials

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Multiferroic materials simultaneously exhibiting ferroelectric and magnetic ordering are a particularly attractive class of materials in view of their applications resulting from the coupling between order parameters. They can be used in spintronics and as multi-state memory devices which can be addressed either electrically or magnetically.

Bismuth-iron ferrite $BiFeO_3$ (BFO) is the most studied multiferroic system because both polar and magnetic order coexist at room temperature. BFO is a G-type antiferromagnet, where each Fe^{+3} spin is surrounded by six nearly antiparallel spins on the nearest Fe neighbors. A weak canting moment originates from the local magnetoelectric coupling to the polarization. Several experimental measurements, including the presence of a magnetic hysteresis loop in single crystals, suggested that at very low temperatures a weakly ferromagnetic state exists. In the last decade, an enhanced spontaneous magnetization has been observed in $BiFeO_3$ thin films produced by pulsed laser deposition (PLD), presumably owing to their more disordered/polycrystalline structure.

In this work, BFO layers were deposited by PLD (T = 650°C, P = 200 mTorr (O_2)) on both Si and $SrTiO_3$ substartes with a 60 nm $SrRuO_3$ interlayer used as bottom electrode for ferroelectric hysteresis characterization. The epitaxial nature of the films on the (100), (110) and (111) crystallographic directions was confirmed by XRD. The typical BFO film thickness is between 100-200 nm. Phase and composition of the films were confirmed by X-ray diffraction and Energy Dispersive X-ray spectroscopy.

The magnetization behavior in the temperature range 5 – 300 K has been studied in all deposited films. Magnetoresistance response (MR) has been measured as a function of temperature in the same temperature interval and in the field range 0 – 70 K using a standard four-point technique. The MR ratio for a given value of magnetic field H is defined as MR = [R(H)) - R(H=0)] / R(H=0) X 100.

For T < 100 K, the films exhibiting the highest magnetic signals display a high-field, non-saturating, negative MR associated with a low-field positive MR; the position of the local maximum decreases with measuring temperature. Above 100 K, a nearly parabolic MR with positive curvature is measured, indicating the onset of an ordinary magnetoresistance effect. Correspondingly, magnetic hysteresis loops change from a highly ferromagnetic state to a much weaker ferromagnetic contribution superimposed to a diamagnetic phase.

#008 - Magneto- and electroresistance in ferromagnet-ferroelectric junctions

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Vincenzo Fiorentini (Università di Cagliari)

Multiferroic junctions combining metallic ferromagnets and insulating ferroelectrics are a promising -and fashionable- avenue to obtain electroresistance and magnetoresistance modulation of tunneling exploiting polarization switching in the ferroelectric interlayer. We report on investigations of the electronic structure and diffusive transport properties of the $Sr/RuO_3/PbTiO_3/SrRuO_3$ multiferroic junction in the two polarization states of the junction, and depending on the interface structure (symmetric Sr-Ru, symmetric Ti-Sr, and mixed asymmetric). We use gradient density functional theory for the electronic structure and Bloch-Boltzmann transport theory. We find that the switching of polarization causes a large asymmetry of the tunneling potential, which in turn gives rise to a large electroresistance both in-plane and across the junction. The different magnetization induced by polarization at the two interfaces (tunable by the polarization states) also causes magnetoresistance, simply by changing the conductivity in the two spin channels. We are now extending the calculation to ballistic transport and to systems with differently magnetized bottom and top metals.

#009 - Beyond structure-function relationship: dynamic properties of the cerebellar network in a realistic model

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Realistic modeling is an approach based on the careful reconstruction of neurons and synapses starting from biological details at the molecular and cellular level. This technique, combined with the connection topologies derived from histological measurements, allows a faithful reconstruction of neuronal networks. Finally, the advent of specific software platforms (PITHON-NEURON) and of super-computers allows large-scale network simulation to be performed in reasonable time. This approach inverts the logics of original theoretical models, which anticipated an intuition on how the network should work. In realistic modeling, network properties "emerge" from the numerous biological properties embedded into the model. Since theoretical models have usually been unsatisfactory in predicting core central nervous system functions, and since these latter are in fact critically determined by biological details, realistic modeling provides the opportunity of bridging computational investigations to biology. A first issue is that realistic networks are spiking allowing an unprecedented analysis of the neural code. A second advantage of realistic networks is that of including any requested non-linear time-dependent processes down to molecular dynamics, extending network properties to the time domain. Similarly, by being able to incorporate arbitrary connection topologies, realistic networks extends their properties into the 3D space domain. Thus network analysis is projected into a multidimensional hyperspace allowing for the investigation of spatio-temporal dynamics.

This approach has recently allowed the realistic modeling to the cerebellar cortical network. The neurons (over 105) are reproduced at a high level of detail generating millisecond precision spike timing and uncovering complex phase-relationships extended over the entire neuronal population. The spike organization in bursts adds complexity to the neural code engaging special time- and frequency-dependent mechanisms in neurons and synapses. The recurrent nature of connections, combined with special non-linear neuronal membrane properties, causes population oscillations, resonance and phase-reset coordinating neuronal activity in the time, space and phase domains. This complex set of mechanisms, associated with others changing synaptic efficacy like long-term plasticity, determine a distributed spatiotemporal processing of incoming input patterns leading to macroscopic properties like gain control, filtering, and learning. The model is currently being used in the context of the HUMAN BRAIN PROJECT to investigate the cerebellar network and brain functions.

#010 - Neural circuits computation and functions in the olfactory bulb

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The circuits that carry out sensory processing in the olfactory bulb have been investigated experimentally in terms of odor selectivity and dynamics of cell responses, usually in single cells or in small randomly selected sets of cells. This has limited a clear understanding of the spatio-temporal dynamics of the mitral-granule cell network in representing an odor input, which requires simultaneous recording from a relevant subset of the cells activated by an odor. The functional effects of network-wide processes, in relation to the patterns of glomeruli activated by different odors, thus remain relatively unknown and difficult to explore experimentally.

To aid in solving this problem we constructed a large scale 1D model of the olfactory bulb [1] to analyze how the spatio-temporal dynamics of lateral inhibition produce glomerular-related cell clusters. We are extending that approach with a new 3D model for processing natural odorants. For this purpose, we model the glomerular activity in a $\approx$ 2 mm^2 area of the olfactory bulb (about 1/20th of the entire system). Several 3D reconstructions of mitral cells with full dendritic trees [2] were analyzed to extract morphological parameters to generate a population of some 700 synthetic 3D mitral cells, 5 for each glomerulus. Approximately 20000 granule cells were randomly inserted into the model and connected using a collision detection algorithm. The activity elicited in 127 glomeruli in the dorsal olfactory bulb during presentation of 19 natural odorants [3] was then used to drive self-organization of the network under different conditions of odor input. Movies visualizing the network activity and network self-organization during an odor presentation will be shown and discussed. This is the first implementation of an olfactory bulb microcircuit using realistic 3D cell properties and network connectivity. It provides a new framework for investigating the functions of a brain microcircuit.

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[2] Igarashi et al., J. Neurosci. 32:7970 (2012).
[3] Vincis et al., Nat. Neurosci. 15:537 (2012).

#011 - Ensemble neuronal responses in a large-scale realistic model of the cerebellar cortex

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Realistic simulation of central networks remains a challenge due to the complexity of internal connectivity and cellular mechanisms involved. We have recently built a realistic model of the cerebellar granular layer [1], which has now been extended to include the molecular layer and Purkinje cells (PC). The model is built in NEURON-PYTHON and is fully scalable, thus allowing to simulate large-scale networks of arbitrary size. The model is made of conductance-based multicompartmental neurons and incorporates dynamic synaptic mechanisms. The model accounts for the principal neuronal types (granule and Golgi cells in the granular layer;

Purkinje cells and stellate cells in the molecular layer) and for their density and connectivity (including gap-junctions between Golgi cell dendrites). As in the real network, mossy fiber (mf) branching gives origin to clusters of glomeruli aligned along the parasaggittal plane. The functionality of this cortical cerebellar network model was validated using input patterns, whose impact has been demonstrated previously. (1) Low frequency random mf inputs, simulating background resting activity, induced low frequency oscillations in the granular layer. (2) High frequency bursts delivered to specific mf bundles activated multiple activity spots within the granular layer, with a center-surround configuration. (3) Collision of inputs from multiple active mf bundles generated either coincident excitation or inhibition [2]. (4) Low-frequency MF bursts were reliably transmitted through the granular layer toward PCs aligned along the vertical axis as well as to PCs laying along the parallel fiber axis. Conversely, high-frequency bursts were strongly amplified and transmitted toward PC aligned along the vertical axis but not along the parallel fiber axis [3].These results, by closely matching experimental recordings, suggest that the model network can be further used to investigate the mechanisms of cerebellar functioning.

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#012 - Advanced optical techniques to explore brain structure and function

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Understanding brain structure and function, and the complex relationships between them, is one of the grand challenges of contemporary sciences. Thanks to their fexibility, optical techniques could be the key to explore this complex network. Here, we briefly review recent advancements in optical methods applied to three main issues: anatomy, plasticity and functionality. We describe novel implementations of light-sheet microscopy to resolve neuronal anatomy in whole fixed brains with cellular resolution. Moving to living samples, we show how real-time dynamics of brain rewiring can be visualized through two-photon microscopy with the spatial resolution of single synaptic contacts. The plasticity of the injured brain can also be dissected through cutting-edge optical methods that specifically ablate single neuronal processes. Finally, we report how nonlinear microscopy in combination with novel voltage sensitive dyes allow optical registrations of action potential across a population of neurons opening promising prospective in understanding brain functionality. The knowledge acquired from these complementary optical methods may provide a deeper comprehension of the brain and of its unique features.

#013 - The intrinsic and synaptic responsiveness of a new realistic Purkinje cell model

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The latest discoveries on Purkinje cell (PC) physiology suggest that the mechanisms of PCs intrinsic excitability have to be revisited Starting from available models, we have constructed a new PC model in Python-NEURON, which explicitly accounts for the Axon Initial Segment (AIS) and a part of the axon including the first node of Ranvier (RVN). The fast Na+ channels are located in AIS, soma with initial dendrite and RVN. The K+ delayed rectifier channels are located only in the soma. The Ca^{2+} and Ca^{2+}-dependent K+ channels, including SK2, as well as intracellular Ca^{2+} dynamics have been updated. The new model configuration now generates simple spike (SS) firing reproducing the experimental input-output curve. SSs initiate in AIS and then back-propagate into the soma decaying sharply inside the dendritic tree. Activation of parallel fiber (pf) generates a short burst followed by a pause caused by Stellate cells. Following a complex spike (CS), SS activity is interrupted independently of the inhibitory synaptic input. Interestingly, the model can shift its state from silent to autorhythmic (configuring a bistable behavior) upon transient current injection or activation of CFs. The pf and granule cell ascending axon (aa) synapses have been modeled using a stochastic release mechanism activating AMPA synaptic receptors. The facilitation and depression profiles of pf and aa synapses faithfully reproduce the experimental data. This model provides a valuable tool to further investigate the Purkinje cell function in cerebellar network models.

#014 - Exploring whole-brain anatomy on the micron-scale with confocal light sheet microscopy

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Understanding the mechanisms underlying brain function is one of the biggest challenges of contemporary science. Our knowledge of the functioning of neural cells, as well as of the mechanisms underlying neuronal synapses, has advanced in recent years. However, our cognition of the complex architecture of the network between neurons lags a long way behind. In fact, mapping neuronal soma and projections throughout the whole brain challenges current imaging technologies, since macroscopic volumes need to be reconstructed with microscopic resolution.

Several techniques, combining mechanical slicing with optical microscopy, have been proposed in the last years to map brain anatomy (KESM, MOST, fMOST, STP). However, the time needed to prepare and image a single mouse brain at micron resolution ranges from several weeks to months.

A different approach to map the anatomy of the whole brain is based on light sheet microscopy. In this technique, the sample is enlightened with a thin sheet of light and the fluorescence emission is collected along an axis perpendicular to the illumination plane. Coupled with specimen clearing methods based on refractive index matching, light sheet microscopy allows imaging of large samples, as entire mouse brains. We recently set up a novel implementation of this method (confocal light sheet microscopy, CLSM) capable of obtaining micron-scale reconstruction of entire mouse brains labeled with fluorescent proteins. CLSM, combining light sheet illumination and confocal detection, allows deep imaging inside macroscopic cleared specimens with high contrast and speed.We will present several results about whole-brain mapping with CLSM in various types of mouse models in which different neuronal populations have been labeled with fluorescent markers. The high-resolution whole-brain optical tomographies affordable with our technique allows mapping the distribution of selected types of neurons throughout the entire brain.

Such whole-brain high resolution cellular atlases will provide a robust foundation also for the emerging field of brain simulation, which aims to take advantage of the exceptional computational power now available to simulate the complex machinery of the brain. In this framework, we will describe our role in the Human Brain Project, one of the two FET Flagships recently approved by the European Commision, which will attempt to simulate human brain through all its levels of organization.

#015 - Electrophysiological characterization of the striatal FSI microcircuitry: a combined experimental and modeling study

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Giovanni, Thierry Nieus, Stefano Taverna (IIT, Genova)

Parvalbumin-expressing, fast-spiking interneurons of the striatum (FSIs) are thought to play a central role in cognitive and motor tasks, yet functional interactions between synaptically connected FSIs are relatively unknown. Here, we investigated the interplay of firing activity between pairs of genetically identified FSIs in vitro. FSI pairs were mostly interconnected through both electrical and GABAergic synapses. Gap junctions (GJ) promoted membrane potential coupling, which mediated a loose coordination of firing activity; however, the hyperpolarizing phase of GJ-mediated spikelets caused a fast, repetitive inhibition of action potential firing during prolonged, supra-threshold DC current injection. These effects were dependent on the dendritic location of GJ in a new multi-compartment model of FSI pairs which reproduced the main electrical responses characterized in experimental recordings. Simulations showed that maximal inhibition of spike firing occurred when GJ were located at a distance of 100-150 µm from the soma. Finally, spike silencing occurred even in the absence of GABAergic synapses, or persisted after complete block of GABAA receptors. The dual pattern of functional coordination mediated by electrical synapses endows FSIs with peculiar dynamic properties which may play a major role in organizing striatum-dependent behavior.

#016 - Investigating the interplay between intrinsic and evoked activities in cultured neuronal networks by dimensional reduction techniques

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High density microelectrode arrays (MEAs) provide extracellular recordings from thousand of electrodes (www.3brain.com) and offer novel capabilities to investigate electrophysiological signaling in cultured neuronal networks and in ex vivo brain tissues. In this study we report on our recent technological and data analysis advancements to investigate the propagation and the interplay of spontaneous and electrically evoked activities in cultured networks. To do so, a novel high density MEA with on-chip stimulating electrodes was realized. It provides whole-array recordings from 4096 electrodes (pitch of 81 um, active area of 8 mm by 8 mm) and electrical stimulation from 16 electrodes located every 8 recording sites. Here, this device was used to interface hippocampal neuronal networks. From the second week in vitro these cultures display a peculiar intrinsic firing regime characterized by periodic synchronized network-wide bursts. These network bursts originate from specific ignition sites of the cultured network (i.e. characterized by more excitable cells) and can propagate through the entire network. These propagations are informative of the underlying network connectivity and their classification based on their spatiotemporal patterns might elucidate the network's organization and its ongoing dynamic. Previous studies have described the trajectories of these propagations by tracking their center of activity trajectory (CAT). Although CATs provide a good overall description of spatiotemporal patterns, they are not suited for fine studies on these propagations. Here we have adopted a more rigorous approach by applying dimensional reduction techniques that take advantage of the redundancy and of the sparseness of multi-unit recordings. Our results show that by Principal Component Analysis (PCA) we can properly reconstruct the time course of spatiotemporal propagations with a minimal set of three components (i.e. explaining ~ 90% of the variance of the trajectories). The PCA classification based approach allowed us to characterize both intrinsic and electrically evoked network-wide propagations. Interestingly, our results show that electrical stimulation can evoke (i) distinctive propagations that depend on the specific spatial-temporal properties of the stimulus as well as (ii) propagations that are already expressed in the intrinsic 'repertoire' of network bursts. Here we will discuss these results and our observations on the interplay between intrinsic and electrically evoked network-wide propagations.

#017 - Millisecond-scale regulation of spike timing by distributed synaptic plasticity at the cerebellum input stage

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Biological neuronal networks have evolved precise processes regulating the number and positioning of spikes [1] by operating in a continuously changing environment. Spike timing has been revealed in afferent sensory pathways and in cortical networks [2], in which millisecond-scale correlations among neurons are thought to improve information storage capacity and computational capabilities [3]. Spike timing can be controlled by long-term synaptic plasticity [4], which regulates the strength and dynamic properties of synapses. Nevertheless, it remains unclear how distribution of synaptic weights could fine-tune spike timing in central networks expressing multiple distributed forms of synaptic plasticity.

This issue is especially relevant for the cerebellum, which is endowed with several forms of long-term synaptic plasticity and has been predicted to operate as a timing and a learning machine. Here a computational model has been used to simulate the impact of multiple synaptic weight variations in the cerebellar granular layer network. In response to mossy fiber bursts, synaptic weights at multiple connections regulated either spike number and positioning in granule cells. The weight at mossy fiber to granule cell synapses finely tuned the delay of the first spike and the weight at mossy fiber and parallel fiber to Golgi cell synapses regulated the duration of the time-window during which the first-spike could be emitted. Moreover, the weights of synapses controlling Golgi cell activation regulated the strength of granule cell inhibition and therefore the number of spikes that could be emitted (from 0 to 3 spikes). Interestingly, different combinations of synaptic weights optimized either first-spike timing precision or spike number, efficiently controlling transmission and filtering properties. These results predict that distributed synaptic plasticity regulates the emission of quasi-digital spike patterns on the millisecond time scale and allows the cerebellar granular layer to flexibly control burst transmission along the mossy fiber pathway.

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#018 - Quantum fluctuations and dynamic clustering of fluctuating Cooper pairs

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We develop the general approach for description of fluctuation phenomena in the whole phase diagram of a dirty superconductor above the upper critical field line $H_{c2}(T)$. First of all we derive the exact expression for the fluctuation conductivity in two dimensional superconductors as a function of temperature and magnetic field in the whole domain of the normal phase. Focusing on the vicinity of the quantum phase transition near zero temperature we arrive to the conclusion that as the magnetic field approaches the critical field $H_{c2}(0)$ from above, a peculiar dynamic state consisting of the clusters of coherently rotating fluctuation Cooper-pairs forms, which we identify as the precursor of Abrikosov lattice. We estimate the characteristic size and lifetime of such clusters and indicate in the corresponding domain of the phase diagram, where such phenomenon can be observed. The derived values allow us to reproduce qualitatively the available results for the quantum fluctuation contributions to the in-plane conductivity, magnetization, and the Nernst coefficient. The developed approach gives possibility to study in details also other important manifestations of the fluctuation phenomena, attracted attention of superconductive community in last decade: the giant Nernst signal and opening of pseudo-gap above the transition temperature. Careful study of the role of fluctuations in the latter phenomenon allows us to predict the new type of zero-bias anomaly in tunneling conductivity of superconducting films. All theoretical results are provided by the computer programs allowing to fit experimental data and extract the necessary information concerning microscopic parameters of the studied superconducting systems.

#019 - Spin-orbital separation in the quasi 1D Mott-insulator Sr_2CuO_3

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As an elementary particle the electron carries spin h/2 and charge e. When binding to the atomic nucleus it also acquires an angular momentum quantum number corresponding to the quantized atomic orbital it occupies (e.g., s, p or d). Even if electrons in solids form bands and delocalize from the nuclei, in Mott insulators they retain their three fundamental quantum numbers: spin, charge and orbital. The hallmark of one-dimensional (1D) physics is a breaking up of the elementary electron into its separate degrees of freedom. The separation of the electron into independent quasi-particles that carry either spin (spinons) or charge (holons) was first observed fifteen years ago. Using Resonant Inelastic X-ray Scattering on the 1D Mott-insulator Sr_2CuO_3 we now observe also the orbital degree of freedom separating. We resolve an orbiton liberating itself from spinons and propagating through the lattice as a distinct quasi-particle with a substantial dispersion of ~ 0.2 eV.

#020 - Tracking the dynamics of the pairing glue in a cuprate superconductor with ultrashort laser pulses

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The mechanism explaining the formation of Cooper pairs in high-T_c superconductors has not reached any final consensus. A pairing mechanism involving the coupling with phonons or excitations of electronic origin, or a cooperative contribution of both these bosonic degrees of freedom has been proposed to trigger the superconductivity in these compounds. Experiments performed at equilibrium conditions are able to reconstruct the spectrum of the pairing glue but they don't allow to infer any precise information about the relative weight of the electronic and phononic contributions to the glue.
We tackle this problem by measuring the optical response of a $Bi_2Sr_2Ca_{0.92}Y_{0.08}Cu_2O_{8+\delta}$ crystal using broadband ultrafast spectroscopy. Exploiting the simultaneous spectral and temporal resolution of this technique, we are able to study the temporal evolution of the dielectric function on a broad energy range and to disentangle unambiguously the electronic and phononic contribution of the glue on the basis of their different temporal dynamics. On the time scale faster than the effective temporal resolution of the experiment and the typical electron-phonon thermalization time, the quasiparticles are already thermalized with the excitations of electronic origin, such as spin fluctuations or loop currents, participating to the glue. The strength of this interaction ($\lambda=1.1$) and its spectral distribution fully accounts for the high critical temperature of the system [1].
The non-equilibrium optical response of the same system, recently measured with unprecedentedly high temporal resolution (<10 fs), fully confirms the previous physical scenario and exhibits, on a broad energy range, an additional temporal dynamics occurring on a time scale of few femtoseconds (10 fs). These recent results constitute the direct observation of the relaxation process between electronic carriers and the bosonic excitation of electronic origin. Furthermore they takes on crucial importance for the formulation of a microscopic model aiming to describe the non-equilibrium physics of photoinduced carriers in strongly correlated systems.

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#021 - Josephson and two-dimensional plasma waves in nanoparticles of layered superconductors

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High-Tc cuprate superconductors are strongly anisotropic systems that support two kinds of plasma waves [1-3]: the Josephson plasma wave (JPW), arising from tunnel coupling of the superfluid density along the c-axis, and quasi-2D plasmons, resulting from

plasma oscillations of the condensate along the conductive planes, while normal electrons are responsible for dissipation. The characteristic frequency of JPWs, the Josephson plasma frequency, provides a good estimate of the strength of interplane Josephson coupling, especially in multilayered materials, where inter- and intra-bilayer couplings give rise to both longitudinal and transverse-optical JPWs. Josephson tunneling may be relevant to high-Tc superconductivity, as it is suggested by the fact that the Josephson frequency correlates with the critical temperature [1,4].

In this work we first discuss the electrodynamic description of Josephson and quasi-2D plasmons in the long-wavelength limit, and show that they can be macroscopically modelled with a strongly anisotropic dielectric tensor. We then generalize the concept of confined surface plasmon excitations – which is widely exploited in the context of usual metallic nanoparticles [5] – to the field of layered superconductors, calculating the characteristic frequencies of surface plasmons in the quasi-static limit. For the case of spherical geometry, an analytic solution of the electrostatic equations is available, leading to a general formula that shows the occurrence of coupling between low-energy JPWs and quasi-2D plasmons in confined multilayered superconductors. The results can be applied to the interpretation of far-infrared experiments with the sphere-resonance method [4,6] or electron-energy-loss spectroscopy, the latter involving the whole spectrum of multipolar surface modes.

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#022 - Structural modulation by chemical substitution in single crystal HT$_c$ superconductors

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Stacks of Intrinsic Josephson Junctions (IJJs) with atomic size are naturally present in layered high-Tc superconductors (HTS) such as $Bi_2Sr_2CaCu_2O_8+$ (Bi-2212), $La_2-xSrxCuO_4$ (LSCO) and Rare Earth-123.[1-3]. Among the possible IJJs applications, high frequency devices can take advantage from the large Josephson plasma frequency found in some HTS IJJs. In particular, Y-123 has the highest Josephson plasma frequency and its properties can be modulated by cationic substitutions, as already noticed for Pb doped Bi-2212 [4]. In a future context of IJJs exploitation, HTS whiskers, like the ones belonging to the Y-123 system, are suitable to realize studies and devices based on IJJs, which require high homogeneity of the IJJs properties on the micrometric scale. Their highly crystalline nature, low defect concentration and excellent superconducting features provide this aspect.

In this work, a study is presented on the structural and superconducting variations induced by doping with elements able to favor the increase of the superconducting critical temperature and the yield of the synthesis process. Elements (Al, Sb, Te, Ga) addition was systematically modulated in the nominal cationic stoichiometry of (Y,Ca)BCO-123. The effects of the elemental incorporation in the structure were investigated using single crystal X-ray diffraction technique and SEM/EDS measurements to obtain information on cationic distribution. In particular, single crystal X-ray diffraction successfully correlate the cationic insertion with the substitution sites, highlighting sometimes a modification of coordination frameworks of copper [5]. The electrical characterization indicates corresponding changes in the conducting properties of the materials.

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#023 - Hidden ferronematic order in underdoped cuprates

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We study a model for low doped cuprates where doped holes form magnetic vortices and, due to short-range interaction, aggregate into stripe segments which are composed of vortex-antivortex pairs. Since a vortex in a XY spin system in two dimensions can be mapped to a 2D topological charge, whose sign depends on the winding number of the vortex, we can treat each pair as an electric dipole. We argue that a state with macroscopic polarization is stabilized, which we call a ferronematic. This state can be characterized as a charge nematic which, due to the net polarization, breaks inversion symmetry and also exhibits an incommensurate spin modulation. We find that incommensurability and macroscopic polarization are directly related and thus they can represent a reasonable order parameter to describe this broken symmetry state. We show that our calculation can reproduce the doping dependent spin structure factor of lanthanum cuprates in excellent agreement with experiments. As a further step a Monte Carlo analysis provides information on the temperature and doping evolution of these complex phases as well as on the thermodynamic phase transitions.

#024 - Resonant coherent phonon generation in superconducting YBCO thin films

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The role played by phonons and high energy excitation of electronic origin in Cuprates superconductivity is still controversial. The interconnections between low energy vibrations and the high energy electronic response are intimately connected to the formation of the superconducting phases in the cuprates and still heavily debated. We show here the possibility of exploiting the presence of a coherent vibrational response in time domain spectroscopy to establish a direct link between c-axis vibrational modes and the electronic charge excitations in optimally doped YBCO.

#025 - Thermal noise correlations in quantum Hall effect devices: experimental check of a theorem by Battiker

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Johnson-Nyquist expression for the mean-square voltage spectral density function of thermal noise in a two-terminal element has been extensively verified in over wide ranges of temperature, frequency and resistance of the two-terminal element. Most accurate investigations are given by Johnson noise thermometry experiments, where a base accuracy of a few parts per million was recently achieved. A generalization of the Johnson-Nyquist expression was derived in 1990 by Markus Büttiker [1]. Buttiker's expression is a statement about equilibrium noise *correlations* in multiterminal devices, and predicts the cross-spectral density functions between noise voltages measured at different terminal couples. The proof of Buttiker's expression deals also with the case of nonreciprocal electrical networks, for which the expression has its most interesting form.

Quantum Hall effect (QHE) gives an ideal physical model to verify Büttiker's expression. QHE devices are multiterminal and exhibit a high degree of nonreciprocity. With the same devices, different networks can be obtained by short-circuiting together two or more terminals; the resulting network transresistances are simple fractions of the quantized Hall resistance.

Measurements of voltage noise correlations have been carried out with a digital correlator and ultra-low-noise amplifier on a 6-terminal quantum Hall effect device. The device was in a screened probe provided with coaxial leads, kept at 1.3 K and under a magnetic field of 9 T. For all the configurations tested, the predictions of Büttiker's expression were verified within the experimental uncertainty of a few percent.

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#026 - Frequency metrology and high-precision molecular spectroscopy in the near-infrared spectrum

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Molecular laser spectroscopy combined with the technology of optical frequency combs is nowadays a research subject that is very much alive for several reasons. Absolute frequency measurements of vibration–rotation transitions provide precise information on the potential energy surface and relevant perturbation effects, precision measurements on molecular beams or cold molecular samples allow one to check the stability of fundamental constants, furthermore, narrow molecular resonances serve as high-quality frequency standards in the infrared (IR) region and knowledge of their absolute frequencies is extremely useful for the application of them in telecommunications.

We report on an extensive spectroscopic investigation of the absorption spectrum of the H_2O molecule in the wavelength range from 1.38 to 1.41 µm. Both linear and sub-Doppler regime of interactions were exploited. In the linear case, based upon the combination of precision measurements of water vapor absorption profile at wavelength around 1.39 µm and sophisticated and extremely refined spectral analysis procedures, we report on new method (Doppler broadening thermometry) for the spectroscopic determination of the Boltzmann constant with a combined uncertainty of $24 \times 10{-6}$ [1]. The measurement of the sub-Doppler line-center frequencies, performed with absolute frequency calibration by using a GPS-disciplined fiber based optical frequency comb, has been performed with an overall uncertainty of 30 kHz [2]. The investigated water line pairs have been chosen with a lambda scheme, so as to share the excited energy level and allow an accurate determination of the rotational energy separations of the fundamental vibrational state. The retrieved energy separations agree, by less than 80 kHz, with recent findings provided by the so-called MARVEL procedure for spectral data inversion, thus yielding a very stringent test of its accuracy.

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#027 - Study of fundamental laws with positronium and antihydrogen

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The Aegis Collaboration at CERN, Geneva

Gravity and Quantum Theory of Fields form the basis of the description of the physical world. Among their fundational basis, the Weak Equivalence Principle and the CPT Theorem, respectively.

Tests of fundamental symmetries such as gravity for antimatter (antihydrogen systems) and positronium can now be conducted and are planned at the Antiproton Decelerator of CERN, Geneva. The Aegis (Antimatter Experiment Gravity Interferometry Spectroscopy) experiment, under commissioning at CERN, aims at testing the validity of the Weak Equivalence Principle with Antimatter and performing detailed studies of antihydrogen and positronium spectroscopy that have impact on the CPT Theorem validity.

#028 - High precision spectroscopy of Francium isotopes for APV measurements

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The facility for production and trapping of radioactive Francium in Legnaro National Laboratories has recently given new results. The main problem with this alkali is the very weak flux that makes it necessary optimization of each relevant parameter, first of all the trapping efficiency. After the measurement with unprecedented precision of the D_2 trapping and of the D1 repumping lines, we dedicated ourselves to the search for new methods of detection of the unknown transitions and to strategies to increase the number of trapped atoms. Light Induced Atom Desorption effect has been successfully applied. We will discuss the main features of the experimental setup, the offline preparation of the measurements on a Rubidium trap and the results on the 210 u.m.a. Francium isotope obtained in the 10 beam time days of this last year. The final goal is the preparation of Atomic Parity Violation experiment that, due to the good theoretical calculation predictions, could allow low energy tests of the Standard Model. LNL experiment is the only running one on Francium atom at the moment, but 2 complementary facilities are in construction at Triumf (Canada) and at the Tohoku University (Japan). Collaboration with the japanese group has been started at the end of last year.

#029 - Fabrication of stacks of intrinsic Josephson junctions for metrological applications

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Nowadays, programmable arrays with thousands of in-series Josephson junctions (JJs) are the most common devices used at metrological institutes to represent the voltage standard. Whatever basic element they use (SIS, SINIS or SNIS junctions, with S: Superconductor, I: Insulator, and N: Normal metal), all of them are based on the Nb and Al technology, which implies the need for liquid helium temperatures for their operation, with corresponding complications in the experimental setup and consequent remarkable costs. On the other hand, high temperature superconductors show a layered crystal structure, which can be viewed as a series of atomically flat intrinsic JJs. Therefore, a new technology providing thousands of highly packed, in-series JJs working at liquid nitrogen temperatures is theoretically possible.

In the present work we explored such a possibility by fabricating stacks of intrinsic JJs out of high-quality BSCCO and YBCO single crystals with high aspect ratios (whiskers). In the case of BSCCO, stacks have been produced by means of a photolithographic process exploiting both a single cleaving and a double cleaving technique. Although these two methods differ in the typical cross section area of the stacks, both require the use of a Focused Ion Beam (FIB) to etch trenches forcing the current to flow normal to the superconducting planes. Stacks with about 100 junctions have been produced and characterized. However, their properties show a shift in the doping regime compared to pristine crystals. This seems to be related to the presence of laterally implanted Ga ions in the stack sidewalls, as nano-XRF characterization by means of synchrotron radiation (space resolution about 150×110 nm^2) has pointed out. In the case of YBCO, stacks were fabricated by means a of a process involving no photolithography and no cleaving, but the use of FIB could not be avoided. Also in this case a decrease in the critical temperature has been observed, but this seems to depend on the cross-section area in the sense of a larger decrease for smaller stacks, which sets a lower limit for stack fabrication able to work at liquid nitrogen temperature. Attempts of observing junction switching and Shapiro steps for this material are currently under way.

#030 - Implementation of high dynamic Raman lidar system for 3D map of particulate optical properties and their time evolution

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Fast scanning lidar system can provide aerosol volume distribution and time evolution in atmosphere. Usually fast scanning lidar has a relative simple configuration. Multi-wavelength depolarization and Raman measurements gave us more information about the particulate shape, type and dimension. The most Raman lidars use high power laser source in order to get enough Raman scattering signal. One of a challenge for Raman lidar system is to have enough dynamic range to satisfy the measurements both for pure molecule Rayleigh scattering and high dene aerosol, such as dust storm, volcano emitted aerosol and high polluted urban aerosol. The estimation of microphysical properties requires independent measurements of both backscatter and extinction coefficient at several wavelengths (multi-wavelength Raman lidar). Additional information can be retrieved from simultaneous measurements of the depolarization signal and water vapor mixing ratio, since those measurements are particularly useful to correlate aerosol optical properties with their shape and hygroscopicity.

A new, versatile prototype of polarization, Raman scanning lidar system (named AMPLE - Aerosol Multi-wavelength Polarization LIDAR Experiment) has been designed and implemented at Napoli Research Unit of CNISM. AMPLE is a project of the scientific co-operation between CNISM and the Beijing Research Institute of Telemetry (BRIT) and represents the first action of the recently founded Italy-China Laser Remote Sensing Joint Research Center.

The AMPLE system has been designed to perform volume scanning of the atmosphere and to retrieve high quality 3D map of particlulate optical properties and their time evolution. The AMPLE system is equipped with a doubled and tripled Nd:YAG diode-pumped laser that is specifically designed for this device, with a repetition rate of 1KHz and average optical power of 0.6 W at 355 nm, 1.5W at 532 nm and 1W at 1064 nm. The relative high repetition rate laser source can increase the detectable signal dynamic range. Each detected signal is acquired by multi-channel scalers with a raw spatial resolution varying from 30 cm to 30 m. Moreover, polarization purity of laser line allows to perform polarization measurements at both 355 and 532 nm. This device is installed in the Beijing city area, which is strongly affected from anthropogenic pollution and sand dust from Gobi desert.

A second unit of AMPLE has been realized for the National Institute for Geophysics and Volcanology (section of Catania) to be installed on the slope of Mt. Etna. This second system is configured as polarized scanning lidar. It will allow to monitor the ash emission during Mt. Etna explosive activity so that the plume mapping and the estimated particulate mass concentrations will be retrieved.

#031 - High resolution-time of flight-aerosol mass spectrometer: an innovative tool to characterize fine particulate matter

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Stefania Gilardoni (CNR - ISAC, Bologna)

Fine atmospheric particulate matter is composed by solid and liquid particles suspended in the atmosphere, characterized by an aerodynamic diameter smaller than 2.5 μm ($PM_{2.5}$) and often below 1 μm (PM_1). Fine particles are ubiquitous pollutant at urban, rural, and remote locations. In urban environment and during the coldest seasons $PM_{2.5}$ daily average concentration is often above the limit set by the European Air Quality Directive of 25 μg m^{-3}.

Fine particles are responsible for impairment of air quality and altering earth radiation budget by direct and indirect effects. Understanding their composition and microphysical properties will help to limit their emission sources, to understand the mechanisms responsible for their effect on climate, and to unveil the properties relevant for negative health effects.

The High Resolution-Time of Flight-Aerosol Mass Spectrometer (HR-TOF-AMS) is an innovative measurement technique that analyses simultaneously chemical composition, size distribution, and mixing state of fine particles at high time resolution. Atmospheric particles are sampled through a critical orifice that focuses submicron particles into a narrow beam. Particles are accelerated by ultrasonic expansions (10^{-5} Torr) into a time of flight chamber were their size is determined. At the end of the chamber, particles are vaporized by impaction on a 600°C oven, and ionized by electron ionization at 70 eV. Molecular fragment ions are then identified based on their mass to charge ratio in a second time of flight chamber. The high resolution of mass spectrometer allows the quantification of organic and inorganic molecular fragments and the elemental analysis of organic aerosol. In the framework of national and international research projects (ARPA-ER Supersite project and EU-PEGASOS project), two HR-TOF-AMSs have been deployed at a rural and an urban site within several field experiments over the last three years. Observations supported the identification of fine particle emissions sources, and allowed the understanding of the link between particle microphysics and atmospheric processes.

#032 - Fourier transform spectrometers from space applied to atmospheric physics and earth observations

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In recent years Fourier Transform Spectrometers have been widely used to develop space missions dedicated to Numerical Weather Prediction, Climatology, and, in general, Earth Observations (EO). This technology will remain in the forefront of satellite space applications at least for the next 20 years. In fact, after the success of the Infrared Atmospheric Sounding Interferometer (IASI), the French Space Agency will continue with the IASI Next Generation (IASI-NG), while ESA and EUMETSAT have plan to put an

imaging FTS in the geostationary orbit. Although the instruments for EO space applications have a moderate spectral resolution (in the range 0.1 to 1 cm^{-1}) they still pose a formidable challenge in terms of data transmission and dissemination to the user community. Based mostly on the experience of the authors with the IASI mission, this paper review science and applications of modern satellite FTIR technology. This will be done considering the case of IASI. The Infrared Sounding Interferometer (IASI) has been developed in France by the Centre National d'Etudes Spatiales (CNES) and is flying on board the Metop-A (Meteorological Operational Satellite) platform, the first of three satellites of the European Organization for the Exploitation of Meteorological Satellite (EUMETSAT) European Polar System (EPS). IASI has been primarily put in orbit to work for a meteorological mission, hence its main objective is to provide suitable information on temperature and water vapour profiles. The instrument has a spectral coverage extending from 645 to 2760 cm^{-1}, which with a sampling interval $\Delta\sigma = 0.25$ cm^{-1} gives 8461 data points or channels for each single spectrum. Data samples are taken at intervals of 25 km along and across track, each sample having a minimum diameter of about 12 km. With a swath width on Earth's surface of about 2000 kilometers, global coverage is achieved in 12 hours, during which the instrument records about 650000 spectra. IASI science involves spectroscopy of atmospheric gases, with H_2O and CO_2 playing the most important role, and radiative transfer. Applications have mostly to do with the retrieval of surface parameters (temperature and emissivity) and the atmospheric state vector (temperature, humidity, ozone) along with trace gases which are important for air quality (e.g., CO) and global warming (CO_2, N_2O, CH_4). The paper will first review the science and spectroscopy in the form and quality needed for modern satellite spectrometers, the radiative transfer, and finally will show retrieval of surface and atmospheric parameters. The case of trace gases will be shown as well. The basic concept of correlation interferometry developed by the authors will be presented and discussed in the context of trace gas retrieval.

#033 - Atmospheric monitoring with Raman LIDAR at the Pierre Auger observatory

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One of the techniques adopted by the Pierre Auger observatory to detect ultra high energy cosmic rays is based on air fluorescence detection. The knowledge of atmospheric properties during data acquisition is of primary importance. Together with other instruments, a Raman LIDAR, that has taken data for about one year, provide measurements of the aerosol optical transmission. This presentation describes the hardware designs, the operational procedures, and the analyses performed on the collected data: aerosol optical properties and their vertical distributions.

#034 - Sensitivity of solar and terrestrial HR profiles to the vertical distribution of aerosol properties

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Aerosol composition and sources in the Mediterranean basin are quite complex, including not only anthropogenic aerosols from human activities of the industrialized surrounding regions, but also natural aerosol from desert areas (e.g. northern Africa) and the Mediterranean Sea. As a consequence, several studies indicated that the aerosol radiative forcing is among the highest in the world during Mediterranean summers. The effects of the aerosol optical property profiles on aerosol direct radiative effects (DREs) and heating rates (HRs) profiles are investigated in this study to contribute to the characterization of the aerosol radiative impact in the Mediterranean basin. More specifically, clear-sky, instantaneous, and daily average aerosol DREs and HR profiles in the short-wave (SW, 0.3–4 µm) and long-wave (LW, 4-80 µm) spectral range are calculated by a radiative transfer model. Compared to the SW aerosol DRE, the LW aerosol DRE has received much less consideration, even if aerosols with large particles, such as dust or sea salt, can exert significant LW-DREs at the surface. SW and LW DREs are generally opposite at the ToA and surface, respectively. Thus, it is very important to understand how these aerosol DREs, occurring at different atmospheric levels (surface, ToA and within the aerosol column) act together and alter the atmospheric energy budget.

The used radiative transfer model is based on aerosol optical and microphysical properties from ground-based sun-sky photometer measurements and aerosol vertical profiles from lidar measurements. Radiosonde measurements (see also http://esrl.noaa.gov/raobs/) at the meteorological station of Brindisi that is 40 km north-west of Lecce are used to define vertical profiles of density, pressure, temperature, and water vapor from 1 up to 20 km altitude.

Lidar measurements are regularly performed at the Mathematical and Physics Department with a Raman lidar identified as UNILE (UNIversity of LEcce) lidar, which is operative within the European Aerosol Research LIdar NETwork (EARLINET) since May 2000. The UNILE lidar nowadays employs an f/4 Newton telescope with a 30-cm-diameter mirror and a frequency-tripled Nd-YAG laser (355 nm) that delivers pulses of about 350 mJ of energy at a repetition rate of 30 Hz. A sun/sky photometer operating within AERONET is also operative at the UNILE lidar site since 2003. The photometer measures direct sun radiance in eight spectral channels between 340 and 1020 nm (340, 380, 440, 500, 675, 870, 940, and 1020 nm). Sky measurements are performed at 440, 675, 870, and 1020 nm through a wide range of scattering angles from the Sun.

The techniques used to retrieve vertical resolved aerosol optical properties from combined multi wavelengths lidar and sun/sky photometer measurements will be analyzed.

#035 - Absolute frequency spectroscopy for the determination of the 17O/16O amount-ratio in water

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In the last decade, laser absorption spectroscopy has been widely used for highly-accurate measurements of stable isotope ratios, relative to international standard materials [1]. In contrast, almost no effort has been reported on the development of new technologies for amount-of-substance ratio determinations, which would be extremely important to address the issue of long-term comparability of isotope-ratio data. We propose a new method for the measurement of the $^{17}O/^{16}O$ isotope amount-ratio in water, based on the use of a pair of offset-frequency locked extended-cavity diode lasers at 1.4 µm. This method enables one to acquire absorption spectra with an extremely high fidelity, exploiting the highly accurate, absolute, and repeatable frequency axis [2]. One of the two lasers, namely the slave laser, is continuously scanned across a pair of $H_2^{16}O$ and $H_2^{17}O$ lines at 7183.5 cm^{-1}, while interacting with a water vapor sample inside a multiple reflections cell at a total pressure of 15 Torr and a temperature of 298.15 K, thus producing absorption spectra with a SNR exceeding 4000. The determination of the amount-ratio is performed through a careful analysis of the acquired spectra, by using semi-classical line profiles. In this respect, the influence of the choice of the line shape model on the $^{17}O/^{16}O$ determinations has been investigated. The performance of the spectrometer, in terms of reproducibility, has been carefully assessed by an Allan variance analysis. Finally, the effective use of the Kalman filtering technique has been demonstrated and compared to the usual approach of spectral averaging, yielding a precision of 0.6 ‰ from repeated spectral acquisitions over a time span of 6000 s [3]. The future developments involve implementing an active temperature stabilization of the cell, which can improve the current figures, quantifying the accuracy of our method and extending the determinations to the other isotopologues of water.

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#036 - Search for Martian methane with TES data: development of a dedicated radiative transfer code. First results.

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Since methane was first reported in the Martian atmosphere, in 2004, an extraordinary effort has been undertaken to understand its origin, evolution and removal from the atmosphere, on time scales much less than the UV photodestruction rate of ~ 350 years. Much of the work, using orbital data, so far has focused on the analysis of the data coming from two instruments: the Planetary Fourier Spectrometer (PFS) on the Mars Express, and the Thermal Emission Spectrometer (TES) on the Mars Global Surveyor. Here we focus on the TES data, because of their abundance (several millions of spectra per Martian year), the more extensive spatial coverage, and better spatial resolution. Unfortunately, the spectral resolution of TES (5 and 10 cm^{-1}) is challenging to the detection of methane using the ν_4 band centered at 1306 cm^{-1}. For this reason, an accurate atmospheric model, and a reliable radiative transfer code are required, in order to assess the reliability of the methane column abundance retrieval with TES data, and whether methane exhibits a regular seasonal cycle or not. From this perspective, we have developed a dedicated pseudo-monochromatic radiative transfer model, based on a model developed for the analysis of the Earth atmosphere, whose main advantage is the analytical parameterization of the optical depths layer-by-layer, with the ability to calculate the analytical Jacobians with respect to the gas concentrations and to the state vector. In the present work, the main theoretical elements of this model and the first results are shown.

#037 - Charge transfer at the interface betweenT6/PDI-8CN2 heterostructures

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We report on the observation of an interfacial charge transfer effect in high quality Sexithiophene (T6)/ N,N'-bis (n octyl)-dicyanoperylenediimide (PDI-8CN2) heterostructures, composing the active channels of field-effect transistors (HeOFETs). Bilayered heterostructures with different T6 and PDI-8CN2 thicknesses have been fabricated and characterized by means of electrical measurements, Atomic Force Microscopy and ex-situ Ultraviolet Photoemission spectroscopy (UPS, with He I and He II photons). Bulk films of T6 showed HOMO and (calculated) LUMO energy positions basically aligned to literature results, while PDI-8CN2 energy levels differ from the expected configuration, with the HOMO being 2.8eV below the Fermi edge, in principle making possible the matching between the T6-HOMO and PDI-8CN2-LUMO levels. Indications of charge transfer at organic/organic interface have been obtained by means of both electrical measurements and UPS analysis. In comparison with single layer (unipolar) devices, the electrical response (output and transfer-curves) of HeOFETs shows the presence of ambipolar transport, a considerable enhancement of the active channel conductivity, the shift of the threshold voltages and a negative trans-conductance behaviour. The energy level scheme constructed from UPS data will be presented for various bilayered heterostructures, suggesting the possible occurrence of different phenomena at the hetero-interfaces, such as interface dipoles or band bending.

#038 - Poly(lactic acid) as a biopolymer-based modified clay nanocomposite

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In this study, Thiohydroxamic Acids (THA) synthesized from vegetable oil; and sodium montmorillonite clay, (Na-MMT) were used to prepare organoclay (OMMT). The clay modification was carried out by stirring the clay particles in an aqueous solution of THA at which the clay layer thickness increased from 1.23 to 2.67 nm. This OMMT was then used for nanocomposite production to improve the property balance of poly(lactic acid) (PLA) by solution casting process. The nanocomposite was characterized using various apparatuses. The X-ray diffraction (XRD) and transmission electron microscopy (TEM) results confirmed the production of nanocomposite. PLA modified clay nanocomposite shows higher thermal stability and significant improvement of mechanical properties in comparison with pure PLA. The use of THA as a modifier will reduce the dependence on petroleum-based surfactant. In addition to its applications such as films, textile fibers and medical puposes, this nanocomposite represents a good candidate to produce disposable packaging because they have good mechanical, thermal properties, fabricability and processability.

#039 - Photophysical properties of NIR emitting lanthanide complexes with organic ligands

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Lanthanide (Ln) coordination complexes with organic ligands have been investigated for their potential in optoelectronics as electroluminescent materials [1] and optical gain media [2]. In particular, Er(III) complexes have been envisaged as novel near-infrared (NIR) materials for plastic optical amplifiers. Ln complexes benefit from the high absorption cross-section of the organic ligands, possibly resulting in very efficient Ln emission sensitization [3,4], and from their solubility in polymers, which allows to reach highly concentrated materials without the drawback of metal clustering and consequent emission quenching. Most reports on Ln complexes have addressed NIR emission quenching by ligand vibrational groups [1], and much is still to be learned on the ligand-centered excited-state dynamics and the high-excitation regime.

We report on the whole photocycle dynamics, as well as on the NIR emission quantum yield and saturation properties of a model class of monometallic and polymetallic Er(III) and Yb(III) coordination complexes with 8-quinolinolato (Q) as the organic ligand [4,5]. Photoexcited singlet excitons in the Q ligands decay to triplet states on the 10 ps time scale, much faster than expected on the basis of the heavy-ion effect. In turn, triplet excited states undergo a fast decay on the 100 ps time scale as a consequence of ligand-to-metal energy transfer. Near-infrared emission lifetime and quantum yield measurements confirm that Er(II) and Yb(III) sensitization is very efficient in Q complexes, attaining values close to 100%. High-excitation experiments with subnanosecond laser pulses show that in monometallic complexes Er(III) excited-state population reaches up to inversion threshold at a pump level corresponding to one excitation per complex. Yb(III) Q complexes have been successfully incorporated into silica sol-gel glasses. The doped sol-gel glasses behave as solid-state solutions and photophysical studies show that the emission properties of the incorporated complexes are preserved in the silica matrices [6].

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#040 - Surface-enhanced Raman based on highly uniform active substrates obtained using block copolymers

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In this communication, we discuss the application of ordered, ultrahigh-density templates of nano-textured Ag-particles obtained by self-assembling of inorganic-containing polystyrene-block-poly(4-vinylpyridine) copolymer (PS-b-P4VP) micelles, for the spectroscopic surface-enhanced Raman of higly diluted molecules and for imaging in-vitro of red blood cells (RBCs).
Hexagonal arrays of PS-b-P4VP micelles, with selective inclusion of Ag nanoparticles (NPs) in the polar core, prepared by in situ reduction of a suitable precursor, are obtained by polymer self-assembly upon fast solvent evaporation during spin coating on the supporting substrate. UV irradiation and/or plasma oxygen treatment remove the polymer matrix leaving immobilized nano-islands of Ag-NPs. Such a kind of SERS-active substrate consists of a reproducible and uniform two-dimensional hexagonal array of silver clusters with a diameter ranging from 25 to 30 nm (single particles having typically diameters of 5 nm) and nano-island gap distances of the order of 5-8 nm on silicon and 15 nm on glass, while giving rise to high enhancement factors and addressing the issue of SERS reproducibility. The basic substrate supporting the plasmonic coating used in this work is either of silicon or glass. This last allows working in back scattering configuration permitting real time monitoring, via microscopy, of the RBCs on which Raman measurements are being carried out. The template is thus applied for surface-enhanced Raman analysis of the red blood cell (RBC) membrane in confocal micro-Raman configuration demonstrating to have SERS imaging potential thanks to the uniformity of the nano-textured substrate. The first experimental evidence of SERS imaging of a red blood cell membrane in-vitro is demonstrated.

#041 - Donor-to-acceptor core-level shift in molecular blend/metal interfaces

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Interface phenomena at the nanoscale level are of crucial importance in the emerging fields of nanoscience. Two-dimensional donor-acceptor blends contacting a metal surface make up an effective interface in charge injection devices. In such systems, the important question that arises is how the molecule/metal interaction plus the intermolecular interactions affect the molecular electronic level alignment, i.e., how do the Highest Occupied Molecular Orbital, HOMO, and the Lowest Unoccupied Molecular Orbital, LUMO, align with respect to the metal Fermi energy. This is a key issue for injection devices based on donor-acceptor blends, since it defines the energy barriers for hole and electron injection. However, the HOMO and LUMO alignment is not easy to elucidate in complex multi-component, molecular/metal systems. Here we demonstrate that core-level photoemission from donor-acceptor/metal interfaces can straightforwardly and transparently determine molecular level alignment. We focus on 2D crystalline networks, and carry out a systematic investigation over a number of donor-acceptor/metal systems. In particular, we use Au(111), Cu(111) and Ag(111) as substrates, perfluorinated copper-phthalocyanine ($F_{16}CuPc$) and perfluoropentacene (PFP) as aromatic acceptors, and copper-phthalocyanine (CuPc) and pentacene (PEN) as electron donors. For each combination, XPS spectra show a characteristic binding energy shift in core-levels as a function of molecular donor/acceptor ratio, irrespectively of the molecule or the metal. Such shift reveals how the level alignment at the molecule/metal interface varies as a function of the donor-acceptor stoichiometry in the contact blend. We also show that the energy level alignment is barely affected by donor-to-acceptor charge transfer, and majorly determined by the electron potential created by donor (high attractive potential) or acceptor (low attractive potential) molecules in their vicinity, i.e., by the average change in work function.

#042 - Structure and vibrational dynamics of long CN chains investigated with IR and Raman spectroscopy

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Polyynes (linear sp-carbon chains, C_N) have been observed as intermediates in the production of fullerenes and nanotubes [1]. They are also relevant in astrophysics [2] and many natural products do contain short polyyne moieties. Similarly to other nanostructured carbons, polyynes are of great interest in molecular electronics. Among π-conjugated systems, polyynes have the simplest one-dimensional structure (alternated sequence of single and triple CC bonds) and have been subject of several theoretical studies [3-7]. Due to instability at ambient temperature, the synthesis of long sp-carbon chains has been a challenging endeavor [8]: the strategy followed was the introduction of large endcapping groups providing steric hindrance, which prevents reactions at the polyyne framework. Furthermore, by choice of the end groups it is possible to change the chain structure, reaching an almost vanishing bond length alternation (cumulenes). We present a study based on vibrational spectroscopy and DFT calculations on polyynes and cumulenes, which provide general guidelines for the analysis of the vibrational and structural features of sp-carbon based materials. Based on longitudinal optical phonons of the infinite sp-carbon chain, we have carried out the complete assignment of the observed IR and Raman CC stretching features (2300 – 1900 cm^{-1} range) for chains with n = 4 – 20 triple bonds. We show polarization effects induced by unsymmetrical capping and deviations from chain linearity in long polyynes. Moreover, Raman markers of cumulenes have been identified and compared with the spectroscopic signature of alternated polyynes.

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#043 - Transparency in PMMA glasses:correlation between optical properties and positron annihilation lifetime spectroscopy measurements

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Cell-cast process is the industrial method of choice used for obtaining high-quality, optically transparent PMMA sheets. This route is characterized by two steps: first, a pre-polymerization of the monomer, in which only modest monomer conversion (15-20 %) is achieved. Second, an additional amount of monomer and a small amount of initiator are added to the pre-polymer, and the resulting syrup is introduced into the casting mold. The polymerization of the syrup contained between two glass plates clamped together is carried out by heating the mold to a preset temperature. Polymerization has been tuned in order to reduce the monomer residual to less than 1% in weight, in line with standard international requirements. Finally, the PMMA sheet needs to be annealed at a higher temperature in order to relax internal strain.

We have verified that different annealing temperatures provide for different transparency (optical absorption) of the PMMA sheets, even though Nuclear Magnetic Resonance (NMR), and Thermo-Gravimetry Analysis (TGA) measurements give equivalent results, indicating that no variation of the chemical formula and local structure occurs. In particular, we verified that the optical absorption drops to below 84 dB/km at 470 nm only when the annealing temperature is somewhat larger than the PMMA glass transition temperature. We found that the amount of residual monomer and the polymer molecular weight are also correlated to the optical measurements results. These in turn influence the polymer transition glass temperature, measured by Differential Scanning Calorimetry (DSC).

By carrying out accurate optical measurements on large sheets, we could verify that optical absorption in this range of visible wavelengths is mainly related to Rayleigh scattering. This has microscopic origin in the structural inhomogeneities of the polymer material. These inhomogeneities have been studied and identified as free volume cavities by the Positron Annihilation Lifetime Spectroscopy (PALS) technique. Data on the positronium lifetime and the mass density of the studied polymers were correlated. A linear relationship was found between the mass density and the free volume cavity size of the PMMA samples. The results indicate that a degradation of the optical properties is associated with a volume free increase inside the polymers. Besides, density gradient widths at the polymer-vacuum surfaces were observed by use of a positron beam with variable implantation energy.

#044 - Visualizing light-polarization through photo-polymerization processes

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We report an investigation on single-beam polarization-driven light-channelization, scattered light-distribution and photo-polymerization anisotropy in organic mixtures irradiated with CW or nano-pulsed laser at different wavelengths and intensities (lambda = 405, 488, 532 nm; 50 mW/cm^2 to 2 W/cm^2). The organic mixture is composed of multi-acrylate monomer (TPGDA, DPHPHA, PHPHA) and di-ketones. The induced photo-polymerization permits the visualization, at a glance, of the polarization state of the incident laser light. By irradiating the mixture in absence of oxygen, polymer structures are clearly evident in the area that has been directly irradiated. The addition of 1-halolalkanes (1-Chloro-alkanes and 1-Bromo-Butane) in the system increases the angle of the light scattering (higher than 73 °). This effect is influenced by the halogen added in the system. The described phenomena could be explained on the basis of interference between excited electrons and the incoming electromagnetic field and/or on the basis oriented polymerization (correlated with oriented polymer shrinkage).

#045 - Organic droplet epitaxy for the growth of rubrene-based heterostructures

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Recently, organic droplet epitaxy [1] has been proposed as a powerful tool for driving the growth of organic heterostructures with a high degree of crystallinity and with a nanopatterned surface. These characteristics, particularly relevant when thinking of applications in solar cells, are demonstrated to be achievable when proper materials are selected. In particular, the interface and surface energy of the materials to be combined into the heterostructures are the key parameters.

Here, we discuss the growth and properties of organic crystalline heterostructures grown by organic molecular beam epitaxy [2] coupling rubrene with different materials and different ways [1,3]. Following this approach, the balance of interface and surface energy can be tuned and different properties found, while crystallinity is always preserved. Studying the surface morphology, crystal structure and macroscopic optical properties of the different heterostructures, pronounced differences are observed and discussed considering the general conditions for organic droplet epitaxy.

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#046 - Near-field interaction with plasmonic waveguides and individual nanoemitters

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One of the major perspectives in plasmonics foresees its application to integrated photonic platforms based on a translucent network, where optical and electronic processing can be accomplished in an integrated fashion. Within this frame, the ability of plasmonics to transfer optical information from individual nanoemitters to the conventional (far-field) optics world, and vice-versa, represents a key element.

Due to the inherently non propagating nature of the electromagnetic field associated with surface plasmons (SP) and to the small size of the involved nanostructures, unconventional optical diagnostic methods must be used to analyze plasmonic systems. We have employed near-field microscopy joined with polarization control to investigate plasmonic waveguides and the interaction with nanoemitters consisting of individual carbon nanotubes (CNT).

A specific setup of Scanning Near-field Optical Microscopy (SNOM) has been designed and realized, which enables both emission and collection mode operations, the latter upon space and polarization controlled far-field illumination. The setup is used to assess the propagation properties of Gold waveguides comprised of thin metal layers deposited on glass and lithographically patterned at Université de Bourgougne, Dijon, in order to obtain tapered ends. Thanks to a regular grating of grooves inscribed at the beginning of the waveguide and enabling SP launch through far-field illumination, the propagation of the supported plasmon modes along the waveguide down to the taper end is analyzed by mapping the collected near-field intensity. The ability in concentrating electromagnetic intensity close to the tapered end is assessed as a function of the nanostructure geometry, revealing the crucial role of edge modes in ruling the cutoff size [1].

The interaction in the near-field with individual single wall CNTs, either deposited on glass substrates or part of two-electrode light emitting devices produced at Ludwig Maximilians Universität, München, is also studied. The inter-band emission is first analyzed and correlated with the CNT morphology, reconstructed through the shear-force methods. Modifications of the emission and plasmon-mediated excitation (e.g., remote excitation [2]) are investigated with sub-diffraction spatial resolution.

Work supported by NanoSci ERA+ Project "E2-PLAS".

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#047 - Acoustic surface plasmon: from Be (0001) to Au(111)

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The existence of collective electronic excitations with acoustic dispersion is relevant for plasmonic devices as well as for catalysis since a wavevector independent group velocity allows for a distortion free propagation of a plasmonic signal while the vanishing energy for vanishing wavevector results in non-negligible thermal excitation probability.

The existence of the ASP is connected with the presence of a 2-dimensional electron gas oscillating in counterphase with the electrons of the underlying 3-dimensional substrate.

The ASP has been firstly predicted theoretically [1] and then observed experimentally firstly on Be(0001) [2] and later on Cu(111) [3] and on Au(111) [4]. It is a relatively robust excitation since it survives to some extent to surface nanostructuring [5] while it is killed as soon as the Shockley surface state at Γ is destroyed e.g. by oxygen adsorption. According to theory the slope of the dispersion is determined by the Fermi velocity of the surface state: while for Be(0001) and Cu(111) the experimentally measured dispersion is in very good agreement with theoretical prediction, for Au(111) there is an unexpected and large difference [4] whereby the experimental slope of the dispersion is nearly twice as large as expected.

In order to clarify this issue we have reinvestigated the ASP dispersion on Au(111) using ELS-LEED and HREELS [6]. Our measurements show that there are in fact two losses with a nearly linear dispersion with parallel momentum: the higher energy one reproduces the data of ref. [4] while the lower energy one has a significantly lower slope. First principles Theoretical calculations show that the high energy loss feature is due to an interband transition while it is the low energy one which corresponds to the ASP of Au(111). The latter mode exists in spite of running within the continuum of interband transitions.

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#048 - Dynamics of multi-photon luminescence in gold nanoantennas

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Multi-photon photoluminescence (MPPL) microscopy has become a widespread tool in high spatial resolution imaging, especially of biological tissues. In plasmonics, MPPL processes are very attractive in noble-metal nanoparticles and nanoantennas in view of the spectroscopic and sensing applications made possible by the resonant behavior of the electron plasma oscillations. It is now well-established that two-photon photoluminescence (2PPL) in gold results from two sequential single-photon absorption events and that its dynamics is ruled by the relaxation time of the excited hole distribution in the *sp* band after the first photon absorption [1]. Noticeably, higher order processes have been reported in the literature for gold dipole antennas, where four-photon photoluminescence (4PPL) has been observed [2]. However, the occurrence of 2PPL or 4PPL appears so far to be elusively random, and no firm basis has been set for the 4PPL process.

In this work we perform two-pulse nonlinear correlation measurements of gold MPPL, by splitting sub-100-fs pulses in a Michelson interferometer and coupling them into a confocal optical microscope. While rough gold films generate solely 2PPL, resonant single-crystal gap antennas [3] produce strong 4PPL. For both 2PPL and 4PPL, two-pulse correlation shows a single-exponential incoherent tail that directly probes the 1 ps relaxation time of the nonequilibrium *sp* distribution, which therefore represents the intermediate excited configuration for both cases. Based on this observation and on the gold band structure, we are able for the first time to shed light onto the 4PPL process and suggest that in the case of 4PPL the intermediate nonequilibrium *sp* distribution is created by a coherent three-photon *sp→sp* transition, as implied by energy and parity conservation, followed by a single-photon *d→sp* transition [4].

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#049 - Near infrared plasmonics with vacancy doped copper chalcogenide nanocrystals

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In recent years, the investigation of copper based chalcogenide (Cu2-xE, E = S, Se, Te) nanocrystals (NCs) has attracted an increasing attention. An appealing characteristic typical for the entire family of copper chalcogenides is the ability to hold localized surface plasmon resonances in the NIR. The high carrier density of ~1021/cm3 is a result of copper vacancies in the structure. The active control of the vacancy density in the structure via oxidation and reduction allows for the control of the plasmon resonance. This provides an additional means of tunability of the plasmon resonance with respect to noble metal nanoparticles [1-4].

In this contribution, the investigation of the optical properties of copper chalcogenide NCs will be presented. Our results are based on steady state and ultrafast spectroscopy. We report on the tunability of the localized surface plasmon resonance of this type of semiconductor NCs and on its influence on their excitonic properties. We suggest that this material system may offer a unique platform to study at the nanoscale the interaction between excitons and plasmons.

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#050 - Au-Ag alloy nanoparticles 2D-arrays: fabrication and surface-enhanced Raman spectroscopy application

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Alloy nanoparticles (NPs) have attracted much interest because of their unique catalytic, electronic and optical properties. In particular, the NPs localized surface plasmon resonance (L-SPR) can be tuned by controlling the alloy composition. Achieving this goal often requires complex fabrication techniques . Here we propose an extremely easy method, based on a self-organization approach, to fabricate well-ordered 2D arrays of Au-Ag alloy NPs with changing composition across the substrate. This feature makes our arrays very promising for designing surface-enhanced Raman spectroscopy (SERS) substrates, provided a precise control

of the nanofabrication process.

The NPs are fabricated by the consecutive deposition of the two metals onto self-organized nanopatterned LiF(110) substrates. The preparation procedure allowed to obtain a linearly varying composition of the NPs on a single LiF substrate. The NPs plasmonic resonance blue-shifts linearly across the substrate with the increase of Ag content, as predicted for homogeneous alloys. The arrays morphology has been studied by scanning electron microscopy and atomic force microscopy. The arrays consist of NPs coherently aligned with a few nanometers interparticle spacing and narrow size distribution in the few tens-of-nm range. The arrays morphology is uniform over a several millimeters area and despite the varying composition.

These NPs arrays have been employed as SERS substrates after the adsorption of Rhodamine-6g and 4-mercapto benzoic acid. The intensity trend of the Raman spectra is directly correlated to the NPs composition, i.e. to the plasmonic resonance wavelength. A strong field enhancement was found, as confirmed also by theoretical simulations, allowing to detect a nanomolar concentration of the test-molecules.

#051 - Dipole decay dynamics engineering within the discrete dipole approximation

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Over the last years there was a considerable effort to control the modification of spontaneous emission, and the radiative decay rate engineering (RDE) has become a central issue in nanophotonics. Metallic nanoparticles or nanostructures seem to be good candidates to achieve this goal: thanks to localized surface plasmons, these objects are able to strongly perturb the electromagnetic fields in their surroundings and to modify both the excitation and the emission rates of proximate emitters, i.e. fluorophores, chromophores, and QDs.

A theoretical control of the electromagnetic coupling between localized surface plasmons and point-like sources of radiation becomes thus a challenging topic in nano-photonics and plasmonics.

Here a classical electrodynamics description of a metal-emitter system is adopted to analyze the perturbations induced by nanoparticles to the spontaneous decay rate of a single emitter assumed point-like, in a regime of weak coupling in which a macroscopic description of metal is assumed to be valid [1]. A Discrete Dipole Approximation (DDA) approach [2-3] is presented as an useful and accurate tool to investigate coupling problems involving geometries not analytically solvable. Initially preliminary checks place the method on a firm ground: the method is applied to Ag nanospheres and nanoshells, which represent two analytically solvable cases, and it is shown to lead to an excellent agreement with exact results.

The approach is then used to consider the response of elongated nanoparticles, like Ag prolate spheroids and nanocones. The analysis sheds light on the important contributions that elongated nanoparticles could provide in enhancing the decay rates of a dipole source. Results demonstrate how the optical response of conically-shaped nanoparticles can be affected by the distance and the orientation of the emitter of radiation, as well as by other geometrical parameters. The particular symmetry of these plasmonic objects results in peculiar features: the absorption efficiencies of the modes depend on the distance of the source of radiation in a counterintuitive way, and this is explained in terms of the excited charge density distributions.

The possibility to simulate arbitrary shaped nanostructures and several dipole-metal configurations presented with this work, could thus open new avenues for an aware use of surface plasmons in fluorescence spectroscopy applications or for fundamental studies on light-matter interaction [4].

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#052 - Luminescent ultra-small gold nanoparticles obtained by ion implantation in silica

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Noble metal nanoparticles (NPs) are widely investigated for their plasmonic properties as efficient scatterers and/or absorbers of light in the visible and near-infrared range. Nevertheless, noble metal NPs made by 100 down to 5 atoms can be of special interest when dealing with luminescence as they encompass the transition between bulk and mo-lecular regimes, where discrete electronic levels emerge, whose energy separation is larger than thermal energy even at room temperature. Therefore, efficient radiative re-laxation can be in principle achieved under direct HOMO-LUMO excitation or under interband photo-stimulation [1].

Recently, our group started a systematic investigation of the optical properties of ultra-small (i.e., made by few atoms) molecule-like Au NPs obtained by ion implantation in silica. Indeed, ion implantation provides a well-controlled way to produce local super-saturation in silica allowing to efficiently control the early stages of nucleation and growth of implanted species by working very close to the critical size of nucleation (i.e., 2-3 Au atoms in silica). This can be achieved (i) by tailoring the implantation conditions (multi-energy implantation scheme, maximum concentration close to the Au solubility limit) and (ii) by a careful control over the annealing of the damage introduced in the implanted silica which can act as a non-radiative recombination channel for luminescent NPs [2]. By correlating EXAFS and photoluminescence (PL) characterizations, our results clearly show that molecule-like Au NPs

made by 5-50 atoms in silica exhibit intense room temperature PL emission in three different spectral regions around 750 nm, 980 nm and 1200 nm, under 488 nm Ar laser excitation. Such PL bands progressively fade as the average Au NP size is in-creased above 50 atoms upon thermal annealing above 600-700 °C.

We further investigated the correlation of such Au PL with the energy transfer process to Er^{3+} ions in Au-Er co-implanted silica [3]. The results clearly show that the 980 nm PL band of Au NPs is partially quenched by the Er^{3+} absorption level at 980 nm that acts as an effective de-excitation channel for Au PL through which the photon energy is transferred from Au NP to Er, eventually producing the emission at 1.5 microns.

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#053 - Fiber optic plasmonic nanoprobes: towards multifunctional photonic devices and components

Emanuela Esposito - CNR - Istituto di Cibernetica, Pozzuoli

Alessio Crescitelli, Armando Ricciardi, Marco Consales, Giuseppe Quero, Antonello Cutolo, Andrea Cusano (Università del Sannio, Dipartimento di Ingegneria Elettronica - Corso Garibaldi 107, 82100, Benevento)

The integration of nanostructures within optical fibers is giving rise to a new generation of highly functionalized all in-fiber nanoprobes which, being easily and remotely connectable to complex illumination systems and demodulation units, may partially overcome the issue related to the extreme integration of all the components required at lab-on-chip level.

We have recently proposed and demonstrated a valuable fabrication route for the integration and patterning of functional materials at micro and nano-scale onto optical fibers, posing the basis for a new and emerging technological vision named "Lab on Fiber". The validation of the proposed process has been carried out through the realization, directly onto the fiber tip, of 2D metallo-dielectric nano-crystals supporting local surface plasmon resonances (LSPR). We demonstrated the effectiveness of the proposed methodology to realize versatile technological platforms at nano-scale to be used for label-free chemical and biological sensing as well as basic component for novel polarization sensitive photonic devices. To demonstrate the strength of our method, we fabricated and characterized a first lab-on-fiber platform based on a 2D hybrid metallo-dielectric nanostructure supporting localized surface plasmon resonances (LSPRs).

Specifically, we first demonstrate how, by taking advantages from the large set of degrees of freedom (metal and dielectric thickness, periodic or aperiodic patterns) exhibited by the platform, it is possible to tailor the field distribution of the plasmonic mode enabling the control on the refractive index sensitivity of the final device. With a view towards surface sensitivity (which indeed is the key parameter in chemical and biological applications), we experimentally observed that the proposed device is able to detect the formation of nano-sized overlays over very limited active areas. Moreover, we demonstrate how is it possible, by properly choosing the geometrical parameters, to control the number and the field distribution of the excited LSPR posing new basis for optimal resonance engineering.

Finally, we show how to obtain polarization sensitive devices starting from the same technological platform, by breaking the circular crystal symmetry at both unit cell or entire lattice levels (with elliptical holes and different periods in the two perpendicular directions, respectively).

#054 - Interaction effects in suspended graphene devices

Alberto Morpurgo (I) - University of Geneva

I will discuss a number of recent experiments on suspended graphene devices, where different effects due to Coulomb interactions are visible. As a first example, I will discuss transport through suspended graphene nano-ribbons that form spontaneously during current annealing of graphene. In these ribbons, the half-integer quantum Hall effect due to non-interacting Dirac fermions emerges – upon the application of a perpendicular magnetic field- from the transport regime characteristic of nano-ribbons, dominated by the formation disorder –induced random quantum dots. I will then move on to discuss multi-terminal devices based on suspended graphene (and its multilayers), for which we have developed a rather reproducible fabrication technique. The focus of this part of the talk will be on graphene bilayers, both a zero and at high magnetic field.

#055 - Interfacial engineering for graphene synthesis and applications

Cecilia Mattevi (I) - Imperial College London

Low cost high quality graphene production and its scalable and reliable deposition onto large areas remain challenging. Solubilization of graphene could potentially be a valuable option that allows large-scale production and processing. In this regard, we focused our attention on oxygen-functionalized graphene that is a water-soluble material. Here, I will present our work on enabling novel pathways for large area electronics and energy storage devices using solution processable chemical derivatives of graphene. Correlation between electrical, structural and chemical properties of chemically derived graphene thin films along with novel tunable opto-electronic properties, such as photoluminescence and giant IR absorption, will be discussed. Further, understanding of the atomic structure evolution of chemical derived graphene upon thermal treatment will be reviewed as an invaluable tool to design novel functionalized graphene and novel graphene interfaces. I will then demonstrate how new processing methods can be applied in designing novel highly porous graphene three-dimensional structures for energy storage devices.

#056 - Gigahertz multi-transistor graphene integrated circuits

Roman Sordan (I) - Politecnico di Milano

Erica Guerriero, Laura Polloni, Laura Giorgia Rizzi, Massimiliano Bianchi (Politecnico di Milano, Via Anzani 42, 22100 Como), Ashkan Behnam, Enrique Carrion, Eric Pop (University of Illinois at Urbana−Champaign, Urbana, Illinois 61801, United States)

Information technology is driven by the continuous progress of digital electronics, which has been following Moore's law for almost 50 years, becoming a multi-trillion dollar industry in the process. As silicon technology is approaching some fundamental limits, alternative materials are being widely investigated. While many studies have focused on individual devices based on low-dimensional materials (e.g., 1-D nanotubes, 2-D graphene, MoS_2), their operation in digital circuits at high, technologically-relevant frequencies has so far not been demonstrated.
In this talk, the first experimental realization of integrated graphene digital circuits operating at gigahertz frequencies will be presented. In contrast to previous reports on high-frequency graphene electronic circuits, which typically consisted of a single graphene transistor integrated with a few passive components, the present circuits were made by integrating several transistors on a single channel of CVD-grown monolayer graphene. The transistors were incorporated into direct-coupled active stages, each exhibiting over-unity voltage gain and in/out signal matching. Each stage also exhibits a very low on-state resistance so charging/discharging of the gate capacitance of the next stage is very fast, enabling operation at gigahertz frequencies. The fabricated circuits are versatile and can also be used in a wide range of applications in analog electronics, some of which will be discussed in this talk.
The first gigahertz multi-transistor graphene integrated circuits demonstrated here pave the way for the application of graphene in high-speed digital and analog circuits in which high operating speed could be traded off against power consumption and circuit complexity.

#057 - Infrared and Raman spectroscopy of molecular graphenes

Matteo Tommasini - Politecnico di Milano

L. Brambilla, G. Zerbi (Dipartimento di Chimica, Materiali e Ingegneria Chimica 'Giulio Natta', Politecnico di Milano), K. Müllen (Max-Planck-Institut für Polymerforschung, Mainz, Germany)

In this contribution we will analyze the vibrational spectra of polycyclic aromatic hydrocarbons with selected shapes (see Figure), which can be regarded as the molecular finite size parents of graphene. Even though Raman spectroscopy is widely used for characterization of graphene samples [1], we will show that IR spectroscopy is also worth to be considered and can add interesting information which is directly related to molecular topology and edge termination. By converse, Raman spectroscopy of molecular graphenes is more sensitive to the extended π-conjugated core of these sp^2 carbon systems and carries information on confinement effects [1a].
We will report on the analysis of the IR spectra through DFT calculations. This clearly shows that the strong IR signals found in the lower wavenumber region (say below 1000 cm^{-1}) are generally associated to out-of-plane CH bending vibrations whose position and relative intensities are dependent upon the edge topology of the molecule considered. More specifically, a statistical analysis carried out on the simulated IR spectra of a set of about 50 polycyclic aromatic hydrocarbons allows to classify the molecules in groups of similar topology, based on the similarities among their IR spectra.
Furthermore, we will address here also the resonant Raman behavior of these selected molecular graphenes, both from the

experimental and theoretical point of view. We will report on the calculations of the resonant Raman response of C42, C48 and C96 by TDDFT and we will show that the ID/IG ratio does depend on the excitation wavelength, similarly to what is known for graphite [2, 1b].

We finally notice that, through DFT calculations, it is possible to show that the equilibrium structure of C96 in vacuo turns out to be slightly curved and chiral (non planar, propeller-like). This is interesting since it reveals that the chiral variant of Raman spectroscopy (namely ROA) could be very profitably used to investigate deviations from planarity in graphitic materials, similarly to the exemplary case of another non-planar chiral polycyclic aromatic hydrocarbon, hexahelicene [3].
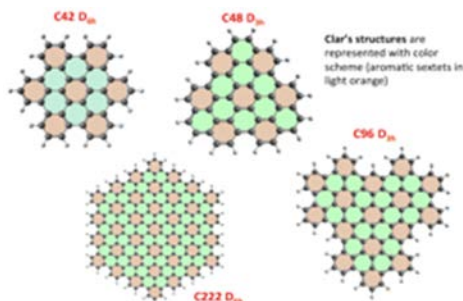
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#058 - Graphene image potential states at the graphene/Cu interface

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Due to its outstanding electronic, mechanical, and thermal properties, graphene has created much interest in the scientific as well as the technologic community. More and more publications have emerged since 2004 and testify to its implementation in sensors, field emitters, nanoelectronics, nanocomposite materials, and many more. In these devices a crucial role is played by the interaction of graphene with metal substrates. A very sensitive probe for understanding the graphene-substrate coupling is represented by Image Potential States (IPSs) [1,2,3]; these unoccupied states are characterized by a large spatial expansion into the vacuum of the associated wavefunctions and hence depend sensitively on the graphene-metal interaction [4, 5].

In this work, we studied the properties of IPSs at the weakly coupled interface graphene/copper by means of angle-resolved non-linear photoemission, employing femtosecond laser pulses as photon source. This technique is a powerful tool for investigating the unoccupied electronics states at surfaces; infact, while the occupied electronic states of graphene on metal substrates have been carefully investigated in the vicinity of the Fermi level, the unoccupied electronic states at interfaces have not been characterized or discussed in detail yet. By comparing the spectra collected on graphene/Cu(111) and on graphene grown on Cu polycrystalline foil, we were able to identify the Shockley surface state, the n=1 image state of the Cu(111) surface and, for the first time, the symmetric n=1 IPS of a single layer of graphene. The binding energy and the effective mass of these states are measured and compared with those of graphite in order to understand the role of the interaction with the metallic substrate.

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#059 - Magnetism and hydrogen interaction in graphene probed by muons

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When positive muons are implanted in materials with low free electrons density, like most of the carbon nanostructures, they capture an electron and form muonium (Mu), a light isotope of hydrogen. The μSR technique allows to follow the evolution of the muon spin after its implantation, thus probing the interaction of a single hydrogen atom with the material.

In this work the interaction of Mu with graphene is investigated. Due to the relatively large muon penetration depth, gram-scale

samples are required, so the first ?SR experiment in graphene was performed on chemically-produced material [1]. Unlike other types of nanostructured carbon, here an evident muon spin precession was observed. Although it is usually the fingerprint of magnetic order, here it was demonstrated to originate from muon-hydrogen nuclear dipolar interactions. The μ-H distance, fitted from the observed spin evolution, is dm-H » 1.75 Å which matches the inter-proton distance in a CH2 group. This proves the formation of CHMu (analogous to CH2). This CHMu proved to be stable up to 1250 K where the signal still persists. Three possible trapping sites are present in graphene: in-plane vacancies, zig-zag and armchair edges. The different dipolar fields acting on the muon in these defects allow to distinguish among these different sites. These results also rule out the formation of defect induced ferromagnetic or antiferromagnetic order in chemically synthesized graphene [2].

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#060 - Plasmonic excitations in topological insulators

Stefano Lupi – Dipartimento di Fisica, Università Sapienza, Roma

Plasmons are the quantized collective oscillations of electrons in metals and doped semiconductors. The plasmons of ordinary, massive electrons are since a long time basic ingredients of research in plasmonics and in optical metamaterials.
Plasmons of massless Dirac electrons were instead recently observed in a purely two-dimensional system like graphene and their properties are promising for new tunable plasmonic metamaterials in the terahertz and the mid-infrared frequency range.
Dirac quasi-particles are known to exist also in the two-dimensional electron gas which forms at the surface of topological insulators due to a strong spin-orbit interaction. Therefore, one may look for their collective excitations by using infrared spectroscopy. Here we first report evidence of plasmonic excitations in a topological insulator (Bi_2Se_3), that was engineered in thin micro-ribbon arrays of different width W and period 2W to select suitable values of the plasmon wavevector k. Their lineshape was found to be extremely robust vs. temperature between 6 and 300 K, as one may expect for the excitations of topological carriers. Moreover, by changing W and measuring in the terahertz range the plasmonic frequency vP vs. k we could show, without using any fitting parameter, that the dispersion curve is in quantitative agreement with that predicted for Dirac plasmons.

#061 - 3D multifunctional carbon nanotube networks

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The bulk synthesis of mm-thick carbon nanotube (CNT) macrostructures is developed through sulphur-addition strategy during ambient-pressure chemical vapour deposition with ferrocene used as catalyst precursor. The macrostructures are made of long and entangled CNTs, forming a random skeleton with open pores.
The macrostructures are characterized by electron microscopies and Raman spectroscopy. Transmission electron microscopy analysis shows the presence of Fe nanoparticles throughout the nanotubes. Due to the presence of these particles, the whole network exhibits a marked magnetic responsiveness even at room temperature.
Owing to its lightweight and super-hydrophobicity (contact angle higher than 150°) arising from the highly porous structure, the sponge easily floats on water this makes it easy moving it with a magnet to absorb oil from water polluted regions. A CNT sponge is able to absorb oil up to 200 times of its initial weight. Once the sponge becomes saturated, it can be ignited so that the absorbed oil is eliminated. In this process, the fire blows over without destroying the sponge, which is hence ready to be reused. Besides, the sponge is also able to absorb selectively organic solvents (e.g. dichlorobenzene) from water.
The in-situ scanning electron microscopy analysis evidenced that the network electrical conductivity linearly increases with the applied compression, due to increase of percolating pathways under loads. The network sustains compressions up to 75% and elastically recovers its morphology and conductivity during the release period, thus being interesting also for pressure-sensing applications.

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#062 - Lithium electronic states after intercalation on SiC buffer layer

Federico Bisti – Università de L'Aquila

Gianni Profeta (Università de L'Aquila, CNR-SPIN, L'Aquila), Hendrik Vita (Fritz-Haber Institut der Max-Planck Gesellschaft, Germany), Francesco Perrozzi, Maurizio Donarelli (Università de L'Aquila), Paolo Moras (CNR-ISM, Trieste), T. Seyller (Technische Universität Chemnitz, Germany), K. Horn (Fritz-Haber Institut der Max-Planck Gesellschaft, Germany), L. Ottaviano (Università de L'Aquila, CNR-SPIN, L'Aquila)

Lithium deposition on graphene was recently proposed as a possible viable way to make graphene superconducting [1]. If graphene interlayer state is shifted at the Fermi level a strong enhancement of the electron-phonon coupling was predicted. The theoretical prediction is based on the simple model of isolated graphene layer with Li on top forming a $\sqrt{3}$ x$\sqrt{3}$ reconstruction (the LiC_6 system) [1]. A real system that can approximate this condition is the graphene layer obtained from the buffer layer of the 6H-SiC(0001) 6 $\sqrt{3}$ x6$\sqrt{3}$ −R30° reconstructed surface by Li intercalation. Previous experimental studies have demonstrated buffer layer decoupling using Li intercalation [2,3]. Furthermore, two theoretical models have been proposed for the interpretations of this effect that differs in the Li adsorption [4,5].

In this work we have investigated the electronic structure of this system. The LEED patterns and the core level photoemission spectra obtained are in agreement with the previous studies [2]. The ARPES data revealed the presence of new low energy states near the Fermi level, never investigated before. Theoretical calculations, using the two proposed structural models [4,5], allow to assign these new features to Li states. These states originate from the reconstruction of the SiC surface states after Li absorption.

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#063 - Systemic risk at high frequency: price cojumps and Hawkes factor models

Fabrizio Lillo (I) - Scuola Normale Superiore di Pisa

Instabilities in the price dynamics of a large number of financial assets are a clear sign of systemic events. By investigating a set of 20 high cap stocks traded at the Italian Stock Exchange, we find that there is a large number of multiple cojumps, i.e. minutes in which a sizable number of stocks displays a discontinuity of the price process. We show that the dynamics of these jumps is not described neither by a multivariate Poisson nor by a multivariate Hawkes model, which are unable to capture simultaneously the time clustering of jumps and the high synchronization of jumps across assets. We introduce a one factor model approach where both the factor and the idiosyncratic jump components are described by a Hawkes process. We introduce a robust calibration scheme which is able to distinguish systemic and idiosyncratic jumps and we show that the model reproduces very well the empirical behaviour of the jumps of the Italian stocks.

#064 - Why do complex systems look critical?

Matteo Marsili (I) - Abdus Salam International Centre for Theoretical Physics, Trieste

The study of complex systems is limited by the fact that only few variables are accessible for modeling and sampling, which are not necessarily the most relevant ones to explain the systems behavior. In addition, empirical data typically under sample the space of possible states.
We study a generic framework where a complex system is seen as a system of many interacting degrees of freedom, which are known only in part, that optimize a given function. We show that the underlying distribution with respect to the known variables has the Boltzmann form, with a temperature that depends on the number of unknown variables. In particular, when the influence of the unknown degrees of freedom on the known variables is not too irregular, the temperature decreases as the number of variables increases.
This suggests that models can be predictable only when the number of relevant variables is less than a critical threshold.
Concerning sampling, we argue that the information that a sample contains on the behavior of the system
is quantified by the entropy of the frequency with which different states occur. This allows us to characterize the properties of maximally informative samples:
Within a simple approximation, the most informative frequency size distributions have power law behavior and Zipf's law emerges at the crossover between the under sampled regime and the regime where the sample contains enough statistics to make inference on the behavior of the system. These ideas are illustrated in some applications, showing that they can be used to identify relevant variables or to select most informative representations of data, e.g. in data clustering.

#065 - Scaling symmetry, renormalization, and time series modeling - The case of finance

Fulvio Baldovin (I) – Dipartimento di Fisica, Università di Padova

We present and discuss a stochastic model of financial assets dynamics based on the idea of an inverse renormalization group strategy. With this strategy we construct the multivariate distributions of elementary returns based on the scaling with time of the probability density of their aggregates. In its simplest version the model is the product of an endogenous auto-regressive component and a random rescaling factor embodying exogenous influences. Mathematical properties like increments' stationarity and ergodicity can be proven. Thanks to the relatively low number of parameters, model calibration can be conveniently based on a method of moments, as exemplified in the case of historical data of the S&P500 index. The calibrated model accounts very well for many stylized facts, like volatility clustering, power law decay of the volatility autocorrelation function, and multiscaling with time of the aggregated return distribution.
In agreement with empirical evidence in finance, the dynamics is not invariant under time reversal and, with suitable generalizations, skewness of the return distribution and leverage effects can be included. The analytical tractability of the model opens interesting perspectives for applications, for instance in terms of obtaining closed formulas for derivative pricing. Further important features are: The possibility of making contact, in certain limits, with auto-regressive models widely used in finance; The possibility of partially resolving the endogenous and exogenous components of the volatility, with consistent results when applied to historical series.

#066 - Quantum Monte Carlo study of quantized vortices in 4He

Maurizio Rossi - Dipartimento di Fisica e Astronomia, Università degli Studi di Padova

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Diagonal and off-diagonal properties of 2D [1] and 3D 4He systems doped with a quantized vortex have been investigated via the Shadow Path Integral Ground State (SPIGS) method using the fixed-phase approach [2]. Under such approximation the vortex acts as a static external potential; thus, the resulting Hamiltonian can be treated exactly with Quantum Monte Carlo methods providing the exact solution for the modulus of the wave function.
As functional form for the phase we choose first the standard Onsager-Feynman (OF) ansaz [3], and then we improve it by including also back-flow (BF) corrections [2]. Under the OF phase ansaz we find an hallow vortex core in agreement with previous results obtained with Density Functional[4], variational[5] and Diffusion Monte Carlo [6]. The introduction of BF provides only a small correction to the energy, but has a dramatic effect on the structure of the vortex that turns out to have a partially filled core. These results resembles the ones obtained in 2D with Green Function Monte Carlo [2] and in 3D with variational Shadow Wave Functions

[5,7].
We have studied also a vortex in solid 4He because of the possible connections with a super-solid phase. We find that the vortex do no affect in a sensible way both the structural properties of the solid and the off-diagonal ones. We deduce that a quantized vortex cannot auto-sustain itself and conclude that the considered wave functions can be an appropriate representation of a vortex in solid Helium only if a condensate is already present.

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#067 - Multiphoton absorption of myoglobin-nitric oxide complex: relaxation by D-NEMD of a stationary state

Grazia Cottone - Dipartimento di Fisica e Chimica, Università di Palermo

Gianluca Lattanzi (Dipartimento di Scienze Mediche di base, Università di Bari "Aldo Moro" TIRES e INFN, Bari), Giovanni Ciccotti (Dipartimento di Fisica, Università Sapienza, Roma), Ron Elber (Institute of Computational Engineering and Sciences (ICES) and Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, United States)

The photodissociation and geminate recombination of nitric oxide in myoglobin, under continuous illumination, is modeled computationally. The relaxation of the photon energy into the protein matrix is also considered in a single simulation scheme that mimics a complete experimental setup. The dynamic approach to non-equilibrium molecular dynamics is used, starting from a steady state, to compute its relaxation to equilibrium. Simulations are conducted for the native form of sperm whale myoglobin and for two other mutants, V68W and L29F, illustrating a fair diversity of spatial and temporal geminate recombination processes.
Energy flow to the heme and immediate protein environment provide hints to allostery. In particular, a pathway of energy flow between the heme and the FG loop is illustrated. Although the simulations were conducted for myoglobin only, the thermal fluctuations of the FG corner are in agreement with the large structural shifts of FG during the allosteric transition of tetrameric hemoglobin.

#068 - Thermal fluctuations and denaturation bubbles in circular DNA

Marco Zoli – Università di Camerino

The separation of the complementary strands in DNA is a template for fundamental biological functions as replication and transcription in which the double helix has to unzip, or open temporarily, to expose the bases hidden in its core and allow for a reading of the genetic code.
The breathing of DNA and bubble formation are dynamical processes shaped by the strong thermal fluctuations of the base pairs and also by the ambient conditions. While fully atomistic descriptions are computationally intractable due to the myriad of degrees of freedom even in short sequences, theoretical investigations start from mesoscopic models representing the interactions at the level of the nucleotide units. Close to the reality models have to include the twisting of the individual strands around the helical axis and the bending of the axis itself.
I have recently developed a computational method, based on the path integral formalism [1-4], suitable for application to Hamiltonian models which incorporate the sequence specificity of the double helix. As the base pairs thermal displacements with respect to the ground state are computed in the path configuration space, the formation of fluctuational openings can be monitored as a function of temperature. Helix untwisting, openings loci and bubble sizes for specific sequences can be predicted in a broad temperature range. Structure characterization and nanobubbles formation are particularly relevant for the use of DNA in nanosensing applications.

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#069 - Survival probability of interacting particles in one dimension

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The diffusion of particles confined within a channel of radius comparable with their size is a paradigmatic example of anomalous diffusion with important applications in biology and nanotechnology. We present a study of hard particles in a confined geometry (single file diffusion [1], [2]), in contact with a thermal bath. Being impenetrable, particles cannot exchange their order; under this extreme constraint, the motions of the individual particles are correlated and for sufficiently long times $\langle x^2 \rangle \approx t^{1/2}$. By means of analytical techniques (reflection principle [3]), numerical simulations and experiments performed in microfluidic devices, we study the survival probability of the Single File system in the presence of two absorbing boundaries. More precisely, we can calculate the probability that all the particles, started within a certain region of length L, are still in this region after a time t. Moreover, it is

possible to analytically reconstruct the emptying process of the channel by calculating the probability that exactly n particles out of N have left the survival region. Despite the presence of the strong subdiffusive regime, surprisingly all these survival probabilities decay exponentially with t, and can be obtained by using non-interacting Green functions and basic results of probability theory.

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#070 - CVD Diamond: from detection of high-energy and nuclear radiation to concentrated solar conversion

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Since the early 90's CVD diamond has been acquired an increasing interest from the scientific and industrial community about its capability to detect intense ionizing radiation beams with an outstanding damage radiation resistance. During the last decade, CVD diamond demonstrated the potential to overcome limitations connected to the use of natural diamond stones, by ensuring minor production costs and reproducible physical properties. Many research groups reported results on polycrystalline diamond films as a sensitive material to ionizing radiation, but problems of signal stability and material homogeneity hampered the transition from a research to a production level. The relatively recent technological advances in CVD diamond homoepitaxy allowed single-crystal films becoming a standard material, with physical properties even superior than natural diamond. The scientific and technological challenge is now focused, at an industrial level, on the control of the films defect density and, at a R&D level, on developing device structures able to maximize the performance of the specific device designed for each specific application. We report on the development of x-ray dosimeters and fast neutron spectrometers characterized by performance superior than the commercial ones. On the other hand, polycrystalline diamond still acquired additional interest for large area applications. Owing to its electron emission capability connected to conditions of negative electron affinity, polycrystalline CVD diamond was employed as an efficient thermionic emitter in a novel-concept conversion module for concentrated solar systems. We report on the tailoring of the physical properties of polycrystalline CVD diamond films as well as on the advanced development activity of the related conversion module.

#071 - Characterization of ion-implanted single-crystal diamond with spectroscopic ellipsometry

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We use variable-angle spectroscopic ellipsometry and transmittance measurements to evaluate the variation of the complex refractive index of ion implanted single-crystal diamond. Both electronic and nuclear damage regimes are investigated by considering different ions and energies for the implantations. An increase is found in both real and imaginary parts of the refractive index for all considered fluences [1].
The index depth variation is determined in the whole wavelength range between 250 and 1690 nm. The dependence from the vacancy density is evaluated, highlighting a deviation from linearity in the high-damage-density regime. A considerable increase (up to 5%) in the real part of the index is observed, attributed to an increase in polarizability, thus offering new microfabrication possibilities for waveguides and other photonic structures in diamond.

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#072 - Bright single colour centres in CVD diamond emitting in the 750 - 800 nm region

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Single luminescent centres in diamond attracted increasing attention due to their applications in quantum cryptography and computation, as well as experiments on the foundations of quantum mechanics. The most widely investigated centre is the NV-defect (Nitrogen Vacancy pair), which possesses very promising properties that make it suitable for quantum information processing, but has several drawbacks with respect to an employment as single photon source. Such drawbacks consists mainly in a broad spectral emission, the low count rate due to an high excited state lifetime and the presence of a shelving state. In this work we present a study on single photon emitters in Chemical Vapor Deposition (CVD) diamond in the near-IR region that can surpass the performance of NV centres within the above mentioned criterions.
Several CVD single crystal samples with a nitrogen concentration around 1 ppm and polycrystalline of electronic grade purity were damaged with MeV carbon atoms and/or exposed to high temperature annealing (1000 – 1500 °C) in order to activate impurities already present in the crystal and observed with confocal microscopy. We notice that this procedure leads to the formation of three kind of centres, with emission wavelength around 755, 765 and 772 nm respectively in all the sample used, uniformly distributed with a mean distance in the order of 10 μm. The Photo Luminescence (PL) emission is almost confined into the Zero Phonon Line (ZPL), which is <5 nm width in all cases and count rate that can reach 200 kHz. Radiative lifetimes measured from the second-order auto-correlation function are in the order of 1-2 ns and almost in half of the investigated emitters the shelving state effect is not present. Part of this centres shows photoblinking, probably due to disturbing neighbouring impurities, but annealing at highest temperatures reduces this effect. PL emitted light and also absorbance cross-section are polarization-sensitive with a dipole-like structure.
In addition, Solid Immersion Lenses (SIL) using a focussed ion beam milling were realized in order to increase the light collection efficiency from the colour centres that suffers from the high refractive index mismatch between diamond and air.
The attribution of these centres is still unclear, but on the basis of sample processing the centres have to be attributed native impurities and eventual induction of vacancies in the CVD crystals.

#073 - Experimental/numerical analysis of strains in irradiated single-crystal diamond

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We present a phenomenological model and Finite Element simulations to describe the depth variation of mass density and strain of ion-implanted single-crystal diamond. Several experiments are employed to validate the approach: firstly, samples implanted with 180 keV B ions at relatively low fluences are characterized using high-resolution X-ray diffraction (HR-XRD); secondly, the mass density variation of a sample implanted with 500 keV He ions well above its amorphization threshold is characterized with Electron Energy Loss Spectroscopy (EELS). At high damage densities, the experimental depth profiles of strain and density display a saturation effect with increasing damage and a shift of the damage density peak towards greater depth values with respect to those predicted by TRIM simulations, which are well accounted for in the model presented here. The model is then further validated by comparing TEM-measured and simulated thickness values of a buried amorphous carbon layer formed at different depths by implantation of 500 keV He ions through a variable-thickness mask to simulate the simultaneous implantation of ions at different energies.

Our results suggest the intriguing possibility of 'strain engineering' the properties of sub ensembles of colour centres in diamond, where the strain fields are engineered by controlled ion implantation into the sample. This would allow some tuning of the centre properties (including frequency, polarisation and allowed transitions) whilst also potentially separating differently aligned colour centres, with applications to ensemble protocols for quantum information processing and quantum sensing.

#074 - Fabrication and characterization by means of focused ion beams of a diamond detector with integrated graphitic micro-electrodes

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The utilization of focused MeV ion micro-beams has been recently proven to be suitable for the direct lithography of highly conductive graphitic channels buried in an insulating single-crystal diamond matrix [1]. The micrometric resolution of a focused ion beam is an ideal tool for the fabrication of radiation hard, low capacitance, fast operation, multi-electrode geometries, enabling for the development of high resolution position sensitive solid state detectors [2].

In this work, the microfabrication of a multi-electrode diamond detector is presented, and its performance for ionizing radiation detection is investigated by means of the Ion Beam Induced Charge (IBIC) technique.

The detector was fabricated using a 2 MeV He ion micro-beam scanning on a homoepitaxial, 50 μm thick, detector grade CVD diamond sample.

The charge collection efficiency of the device was studied by means of IBIC experiments using a 4 MeV He micro-beam, which allowed to probe the charge transport properties of the detector within the first 10 μm in depth from the sample surface. IBIC experiments were carried out under different bias voltage conditions and under different arrangements of the sensitive electrodes.The IBIC experiments allowed to map the charge collection efficiency of the device as a function of the position of the ion beam raster scan, enabling an exhaustive characterization of the electrostatics and of the electronic properties of the detector. Electric field distribution and carrier lifetimes were interpreted in the framework of the Shockley-Ramo-Gunn theory, allowing to identify the role of carrier species in the induced charge pulse formation mechanism.

The same IBIC characterization procedure was adopted on a twin diamond detector with surface metallic electrodes; the comparison between the experiments allowed us to qualify the features and the limits of the ion beam micro-fabrication technique for the development of effective diamond particle detectors.

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#075 - Use of carbon nanotubes cathodes in electron sources

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Cold cathodes are electron sources whose operation is based on the field emission effect decribed by Fowler and Nordheim in 1928. Advances in cold cathodes open the way to a large range of applications like for example flat-panel displays, portable X-ray tubes and high power microwave amplifiers. In this last devices, when the operation frequency is in the range of THz, electron beam with high current density are required.

In this context, field emission based cathodes represent a valuable alternative to the commonly used thermionic cathodes. Their possibility to work at room temperature leads in fact to many advantages such as small dimensions, simplification in the electron gun design, longer life time.

Carbon nanotubes (CNTs) are among the most studied and famous field emitters employable in cold cathodes. In the last twenty years, since their discovery, the CNTs have been widely investigated demonstrating their good quality as field emitters, in terms of

high aspect ratio, low threshold electric field and good stability. However only in 2010 it has been demonstrated the possibility to employ a CNTs cathode in an electron gun for a TWT. Nevertheless the opportunity to integrate CNTs cold cathode in electron gun has still to be investigated more in detail.

In this work we present a carbon nanotubes electron source assembled with a low cost technique. We used a carbon nanotube cathode that reached the remarkable current density of 0,6 A/cm^2. The cathode has been assembled with an external grid in a compact electron source that achieved a maximum output current density of 45 mA/cm^2. This study is mainly focused on the possibility to integrate carbon nanotubes cathodes in linear vacuum device such as Klystron or traveling wave tubes (TWT).

The CNTs have been synthesized with a thermal CVD technique using 5 nm patterned evaporated nickel as catalyst. The realized cathode has been characterized in terms of electron field emission in diode configuration. The cathode anode distance has been fixed at 100 µm reaching a current density of 0,6 A/cm^2. This result is really interesting since it makes this cathode suitable for electron guns of linear vacuum tubes.

We then assembled the carbon nanotubes cathode with an extracting grid in a compact electron source. In this configuration we achieved an outgoing current density of about 45 mA/cm^2 that is still too low in order to employ the electron source for a vacuum tube electron gun, however this represents one first example of a CNTs electron source realized with a low cost assembly.

With some improvement, such as the use of thinner mica spacer and extracting grid with higher transparency, we are confident to increase the overall current density of the electron source up to some hundreds of mA/cm^2. Those values are employable in electron guns for vacuum tubes.

#076 - Magnetization reversal in nanomagnetic switches: energy dissipation and spin dynamics

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It is well known that bistable or multistable nanomagnetic switches can be used to store information, associating each logic state to a different equilibrium orientation of the magnetization [1]. In this context, the question of the energy required to change the logic state of one bit, for instance reversing the nanodot magnetization, and the role played by the excited spin waves during this process are of great current interest to explore the lower energy limits of future devices for Information and Communication Technologies [2]. Here, the dissipated energy and the spin dynamics during magnetization reversal in realistic bistable magnetic switches, consisting of rectangular nanodots with either micrometric or nanometric lateral dimensions, are analysed by micromagnetic simulations. Two different switching strategies are considered and the relative results compared: i) the irreversible magnetization reversal obtained by the application of an external field along the easy axis, in the opposite direction with respect to the initial magnetization orientation and ii) the precessional switching obtained applying a short pulse of field, oriented perpendicular to the initial magnetization direction.

In the second part of this presentation, we analyse the energy cost of a "Landauer erasure" process [3] at different temperatures T, from 0 K to 400 K, for the same kind of realistic nanomagnetic switches considered above. Following the quasi-reversible (adiabatic) switching, resulting from driving the magnetization to reverse across the hard axis by a proper quasistatic sequence of external fields, it is shown that the minimum expected value of $k_B T \ln(2)$, known as "Landauer limit" [4], is recovered by micromagnetic simulations, independently from the fact that simulations start from a well-defined initial state or not. The only condition to achieve the correct Landauer limit is that the adopted erasure protocol includes a proper time interval where the probability distribution of the nanodot magnetization has the same amplitude in the two possible states.

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#077 - Probabilistic aspects of magnetization relaxation in nanomagnets

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Claudio Serpico (Università degli Studi Federico II, Napoli), Isaak D. Mayergoyz (University of Maryland, College Park, USA)

A single-domain nanomagnet is a basic example of system where relaxation from high to low energy is probabilistic in nature even when thermal fluctuations are neglected. The reason is the presence of multiple stable states combined with extreme sensitivity to initial conditions. It is demonstrated that for this system the probability of relaxing from high energies to one of the stable magnetization orientations can be tuned to whatever desired value between 0 and 1 by applying a small transverse magnetic field of appropriate amplitude. In particular, exact analytical predictions are derived for the conditions under which the probability of reaching one of the stable states becomes exactly 0 or 1. Under these conditions, magnetization relaxation is totally insensitive to initial conditions and the final state can be predicted with certainty, a feature that could be exploited to devise novel magnetization switching strategies or novel methods for the measurement of the magnetization damping constant.

#078 - Viewing magnetic noise through windows: determination of critical exponents in the domain wall dynamics

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In imaging experiments of Barkhausen noise in thin films, magnetic avalanches at the boundaries present challenges to analysis. Large avalanches are removed from the distribution, and the portion inside the viewing window may sometimes be treated as being smaller avalanches. This often leads to the incorrect determination of the distributions, and as a consequence, to a wrong estimation of the critical exponents.

Our previous theoretical analysis proposed to solve this problem by using new area distributions, which correctly take into account the effect of the boundaries. Here we apply this analysis to experimental domain wall dynamics in a set of films of NiO(t_NiO)/Fe(30 nm) with t_NiO = 0, 30, 80, 100, and 150 nm deposited on glass substrates, By varying the thickness, we vary the pinning properties of the domain wall dynamics in Fe.

The estimated exponents are not easily explained by the existing models, as they are not able to take into account the complexity arising from the long-range dipolar interactions occuring during the motion of zig-zag walls.

#079 - Disentanglement of spin and charge dynamics by means of time-resolved magneto-optical Kerr spectroscopy

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Time-resolved magneto-optical Kerr effect (TR-MOKE) is a well-established technique to study the ultrafast spin dynamics in magnetic materials. The MOKE signal is a complex quantity and hence it can be divided into real (rotation) and imaginary (ellipticity) parts. Kerr rotantion and ellipticity should be both proportional to the magnetization but this may not be true after an intense optical excitation [1]. Our experimental results on CrO_2 show that the interpretation of the MOKE signal is far from being straightforward and we propose a new method to extrapolate the genuine magnetization dynamics.

We have measured TR-MOKE on a 300 nm thick CrO_2 film grown by CVD on TiO_2 [2]. CrO_2 is a tetragonal ferromagnetic oxide and its conduction band features a high spin polarization due to its half-metallicity. When the optically induced reflectivity change exceeds 10%, the Kerr rotation and ellipticity differ from each other for delays as long as 50 ps. Understanding the physical origin of this discrepancy is fundamental in order to describe the true magnetization dynamics.

It is well known that MOKE effect takes its origin from off-diagonal coefficients of the dielectric tensor (ε_{xy}) and that analytical formulas of MOKE rotation and ellipticity depend on both magnetic contributions, related to ε_{xy}, and on optical contributions, related to diagonal terms of the dielectric tensor. It will be shown that thanks to the simultaneous measurement of Kerr rotations and ellipticities, we are able to quantitatively extrapolate the time evolution of the diagonal and off-diagonal terms of the dielectric tensor and disentangle the charge contribution to the MOKE signal from the pure magnetic contribution.

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#080 - Effective description of magnonic mode dynamics in 2D ferromagnetic antidot lattices

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The effective properties of two-dimensional (2D) square arrays of antidots are studied according to micromagnetic and analytical calculations. Micromagnetic calculations were performed by using the Hamiltonian-based Dynamical Matrix Method extended to periodic systems. The nanometric systems are composed by periodic square arrays of circular antidots (holes) etched into a Permalloy ferromagnetic film. In the calculations the diameter d of the holes varies between 10 nm and 120 nm, the array periodicity is $a = 800$ nm and the thickness is $L = 22$ nm. The external field is applied in the plane of the system and perpendicularly to the Bloch wave vector. From the inspection of spatial profiles of collective modes it is possible to identify a characteristic wavelength which is commensurable with the periodicity a of the system [1]. Since collective modes are mainly affected by the finite size of the holes rather than the periodicity and since the characteristic wavelength is much larger than d, the dynamics is described in terms of effective properties and an effective medium approximation is used. In this way the characteristic wavelength can be regarded as an effective wavelength λ_{eff} related to the scattering from the antidots of the given collective mode and the 2D arrays of antidots behave as 2D metamaterials with holes acting as scattering point defects [2]. It is shown that the effective wavelength, defined for each spin-wave mode of the spectrum, is not necessarily equal to the Bloch wavelength and a general relation between the two wavelength is established. In the cases studied the ratio $d / \lambda_{\text{eff}} \ll 1$ for the whole range of Bloch wave vectors investigated. This condition would not be always fulfilled by replacing λ_{eff} with the Bloch wavelength. Correspondingly, also a small wave vector is introduced and its relation with the Bloch wave vector is found. An effective rule involving the small wave vector and the dynamic magnetization is derived and its relation with the Bloch rule typical of periodic systems is established. A quantitative estimation of the effective ellipticity, expressed as the ratio between the in-plane and the out-of-plane component of the dynamic magnetization, for the most relevant mode of the spectrum is also given and is compared to that of the resonant Kittel mode of the continuous film.

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#081 - Magneto-elastic effects in isotropic ferromagnetic solids using phase field crystal approach

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Magnetic hardness (coercivity) is an important property of ferromagnetic materials that characterizes their hysteresis behaviour and applications. Being an essential component of many electronic devices, magnetic materials are at the root of progress in electrical engineering, electronics and material science.

In this work we studied the inter-relation between morphological structure and magnetic properties, specifically the dependence of coercivity on the grain size in isotropic ferromagnetic solids. We constructed a minimal free energy functional (Magnetic PFC model) to incorporate elastic and magnetic properties of isotropic ferromagnetic solids. The free energy is an extension of the phase-field crystal free energy functional with additional terms to include the paramagnetic to ferromagnetic phase transition and

magnetostriction effects. The phase diagram of the model was calculated. The equilibrium phases include liquid, ferromagnetic hexagonal solid and non- magnetic solid phases. Using amplitude expansion method, we calculated the free energy in terms of the strain tensor elements which allowed us to study the magnetostriction effect, hysteresis properties and the effect of the grain boundary on coercivity. In particular we derived a relation for the dependence of coercivity on the grain misorientation angle in the isotropic limit.

Numerical simulations were performed to further study the properties of the model. The relation between the grain size and the coercive force was analyzed and we found a qualitative agreement with the experiments on soft magnetic nanocrystalline materials.

#082 - Spin dynamics in magneto-plasmonic nanostructures

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The aim of the present work is to study the spin dynamics both in γ-Fe_2O_3 magnetic nanoparticles and in Au-γ-Fe_2O_3 hybrid nanoparticles (both dimers and coreshells) by means of ^{1}H-NMR. Nuclear relaxation rates ($1/T_1$ and $1/T_2$) and spectra have been measured on powders samples as a function of temperature, covering the range $1.5 \div 300$ K, for two different magnetic fields, H=0.65 Telsa and H=1.65 Tesla. The spin-lattice relaxation rate $1/T_1$ as a function of temperature shows three maxima at high (T~250K), intermediate (T~120K) and low (T~10K) temperature; these anomalies are damped and shifted to higher temperatures with magnetic field increasing.

We can explain this behaviour by taking into account three different contributions to the spectral spin density, each one following the Bloemberger-Purcell-Pound (BPP) equation and characterized by a specific correlation time (τ_c). Indeed, we hypothesize that: the peak at high temperatures is associated with the re-orientational motion (τ_c^{rot}) of CH_3 and CH_2 groups in the organic coating, similarly to previous results in literature; the peak observed at intermediate temperatures is related to the superparamagnetic blocking temperature T_B, i.e. to the Néel reversal of the magnetization (τ_c^{SPM}); finally, the peak low temperature peak, despite the still unclear origin, could be related to the surface spins dynamics (τ_c^{SSD}).

#083 - Superspin glass behaviour in MnFe$_2$O$_4$ nanoparticles: blocking temperature in magnetization and Mossbauer time scale

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Manganese ferrite nanopowders have been synthesized by coprecipitation of Fe_3^+ and Mn_2^+ from water-in-toluene reverse micelle system and subsequent thermal treatment at 320°C. Mean crystallite size obtained by XRD analysis is ~ 2 nm, whereas the value obtained by powder specific area (278 m^2/g) is about 4 nm. This suggests that the particles consist of a few aggregated crystallites. A superspin glass (SSG) behaviour is exhibited by Field cooled (FC) and Zero Field Cooled (ZFC) magnetization curves, both showing a maximum. The maximum of the ZFC curve is at T = 40 K (T_{max}). The freezing temperature detected by Mössbauer spectroscopy is close to Tmax, despite the significantly different time scales, supporting the existence of a collective magnetic state. The SSG behavior is confirmed by memory experiments, carried out according to the ZFC and TRM protocols, below T_{max}. The presence of strong interparticle interactions is confirmed by the analysis of remanence measurements by the Henkel Plot at 5 K.

#084 - Study of spin dynamics in the molecular antiferromagnetic nanomagnet Ni$_7$ by means of 1H NMR

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The wide interest of the scientific community in the molecular nanomagnets induced us to study several examples of the antiferromagnetic (AF) systems because of their magnetic properties related to the quantum behaviour at low temperature. In this report a 1H-NMR study of the Ni$_7$ (Fig. 1) molecular cluster, is reported [1]. The Ni$_7$ nanomagnet represents an ideal model system for investigating the effects of geometrical frustration in magnetic interactions as already demonstrated by a theoretical investigation [2].

The 1H NMR nuclear spin-lattice relaxation rate 1/T1 was studied as a function of temperature (1.5<T<300K) at applied magnetic fields H = 0.5 and 1.5 Tesla. The nuclear spin-lattice relaxation rate 1/T1 exhibits a maximum (at T<50K) that decreases and displaces toward higher temperatures by increasing the applied field. This peak is typical of most molecular nanomagnets [3], and its presence is qualitatively explained in terms of the relaxation of the magnetization due to spin-phonon interactions [2,4,5]. The presented data are of crucial importance to investigate the role of spin frustration in the magnetization dynamics [2].
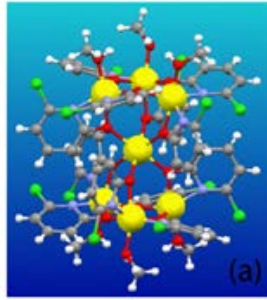
Fig. 1 The structure of Ni$_7$, where the yellow spheres represent the Ni ions (reprinted from ref. 2).

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#085 - 1D nano-ribbons and 2D sheet silicene: from single layer to multilayer

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Silicene, a single layer of silicon atoms densely packed in a honeycomb graphene-like structure, has generated actually very huge interest worldwide [1-3].

First, it has been synthesised in the form of isolated nano-ribbons (SiNRs) 1.6 nm in width [4], 1D $5\times2/5\times4$ grating with a pitch of just 2 nm [5], as well as perfectly aligned 1D multilayer of silicene with a very high aspect ratio, on the anisotropic Ag(110) surface [6]. Subsequently, the discovery of 2D sheet 4×4 silicene grown on Ag(111) has been obtained [1].

The electronic structures of the SiNRs by angle-resolved photoemission (ARPES) shows that they are 1D materials [4, 5], whereas the dispersion of the bands allows to identify states corresponding to the 1D projection of the π and π^* Dirac cones in silicene [5] similar to graphene. The presence of threefold Si-Si σ bonds [7] and the very low reactivity to molecular oxygen of the $5\times2/5\times4$ grating further compares favourably with graphene and the sp2-like hybridization of the Si-Si bonds of the SiNRs [8]. The multilayer epitaxial sheets grown on the Ag(111) surface [6, 9] exhibit in ARPES features which display circular horizontal cross-sections in precise positions in momentum space; they can be attributed to π and π^* cones, which confirms the presence of Dirac fermions with a very high Fermi velocity [6, 9].

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#086 - Silicene on Si₃N₄/Si(111) surface; a DFT study

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Silicene is the Si-based analogue of graphene, that is a single layer of silicon atoms arranged in a two-dimensional honeycomb lattice [1]. Silicene retains some of the interesting features of graphene, like, e.g., the linearity of the electronic band dispersion in the vicinity of the K point in the surface Brillouin zone. Silicene has, however, a big advantage; being a Si atoms arrangement it is conceivable to be integrate in classical semiconductor circuits.

Silicene is normally deposited on a substrate, since it is not that easy to esfoliate. Usually, metals like Ag are used for this purpose. We propose here [2] Si_3N_4/Si(111) as a possible substrate for Silicene deposition. As a matter of fact, Si_3N_4 is already used in Si-based devices for its strength, hardness, resistance to corrosion and high decomposition temperature. Moreover, Si_3N_4 and Si (111) surface share hexagonal symmetry as well as a lattice parameter mismatch lower than 1% (taking twice the Si-surface cell).

In the present work we have described the components of the system by means of Density Functional Theory calculations as implemented in the Quantum-Espresso suite of programs [3]. First we validated our description against literature data [4,5], obtaining good agreement.

Second we investigated several possibilities of arrangement of the Si layer on the Si(111)/ Si_3N_4 substrate, and calculated their relative stabilities. Some phonon calculations have been performed to compare with experimental results.

Our dispersion graphs for electronic bands show that it is possible indeed to retain linear dispersion in the neighborhood of the K point of the surface Brillouin zone by avoiding too strong a coupling between substrate and silicene. One of the possibilities is given by hydrogenation of the Si_3N_4 surface. Good experimental data are awaited for comparison on this fundamental point.

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#087 - Structure and electronic properties of self-assembled interlayers at the polymer/metaloxide interface

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Hybrid systems formed by organic conductive polymers and inorganic materials have a great technological potential in biophysics, optoelectronics and energy harvesting.

The properties of the hybrid systems are strongly affected by the control of the organic-inorganic interface and the possibility to tailor the interactions at the molecular level.

This is the case of polymer/metaloxide interfaces for photovoltaics. Despite the possibility of combining in the same system the

processability and good absorption properties of organic polymers with high transport properties and durability of inorganic crystals, hybrid systems have not yet demonstrated high photovoltaic efficiency.

Here we discuss the a novel strategy that consists in engineering the interface by self-assembled molecular interlayers [1] in order to selectively affect the interactions of the donor and acceptor components and tailor the properties of the interface.

We adopt a combination of molecular dynamics and electronic structure calculations to explain the observed properties of polymer/metaloxide interfaces [2,3] in presence of specific molecular interlayers such as metal-organic macrocyclic complexes (e.g. ZnPc's[4]) or pyridine derivatives [1,5].

Present multi-scale approach makes possible to take into account electronic effects (band alignment, charge density displacements) and thermodynamical properties (order, adhesion energy, molecular mobility) thus clarifying the role of the interlayer on the interface properties [4,5].

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#088 - Magnetic properties of self-organized Cr oxide monolayers on Fe(001)

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Thin chromium layers have been extensively studied in recent years due to their application as anti-ferromagnetic spacers in Giant MagnetoResistive (GMR) devices [1].

In the attempt to better understand this kind of systems, the growth mechanism of Cr thin films onto Fe(001) substrates has been widely investigated [2,3]. The motivations for which these studies are interesting are to be sought in the bidimensional nature of the Cr film, which presents different morphological and magnetic characteristics from those of the bulk.

The growth of Cr on Fe is the topic of many literature works; among the others, the work by Davies and coworkers [4] focuses on the morphological features and chemical reactions at the Cr/Fe interface, showing that, if the growth is performed under layer-by-layer conditions, a Cr-Fe alloy forms on the top of the iron surface.

On the contrary, we demonstrated [5] that a sharp Cr/Fe interface can be obtained if the Fe substrate has been previously passivated by oxygen. In this way, a Fe-p(1x1)O surface is achieved, and a layer-by-layer growth for Cr is possible.

We recently showed how such this system behaves when the growth is performed at 400°C at submonolayer coverages by means of Scanning Tunneling Microscopy (STM) and Low Energy Electron Diffraction (LEED) [6]: a transition from the c(4x2) phase to the ($\sqrt{5}x\sqrt{5}$)R27° one is observed, experimental data being supported by Density Functional Theory (DFT) calculations.

Here we report on the magnetic properties of Cr thin films deposited on Fe-p(1x1)O substrates in the submonolayer regime at 400°C and room temperature: X-ray Magnetic Circular Dichroism (XMCD) and Resonant PhotoEmission Spectroscopy (RPES) were employed to this purpose. All the experiments were performed at the beamline BACH of the Italian Synchrotron Elettra in Trieste. The results show an antiparallel alignment of Cr magnetic momenta with respect to the Fe substrate, even for the submonolayer-thick Cr film. These outcomes are supported by first-principles DFT calculations.

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#089 - Glutamic acid at Ag surfaces: self-assembly in the non-zwitterionic form

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The understanding of the interactions between biomolecules and inorganic surfaces is mandatory for all those applications in which this interaction wants to be either exploited (biomaterials, nanoelectronics, hybrid material design) or avoided (fouling, hygiene). Amino acids are the protagonists of this kind of fundamental studies, since they are the basic constituents of peptides and proteins and are small enough to be assumed as a prototype for the adsorption of bio-molecules at surfaces. In most cases they adsorb in the zwitterionic form, while anionic adsorption was sometimes detected.

We have recently investigated the interaction of (S)-Glutamic Acid (Glu) with LMI Ag surfaces in the temperature range 250 K<T<400 K by experimental and theoretical methods. Our study shows that Glu molecules adsorb always in the non-zwitterionic form [1-4], at variance with the majority of cases reported in literature and with what expected for analogy with other amino acids adsorbed on Ag(111) [5]. Moreover, they self-assemble in different geometries depending on the substrate and on the deposition temperature.

On Ag(100) four different structures have been identified . For two of them (namely the "square" and the "flower" structures, both forming at 350 K) a careful combination of STM, HREELS and XPS results and of ab-initio Density Functional Theory (DFT) calculations allowed to unravel the details of the self-assembled layer and to understand the driving mechanisms of the self-assembly process. The "square" geometry consists of Glu molecules in the neutral form, while the "flower" one is made by 50% neutral units and 50% of anions (forming the tetramers). The interaction of the self-assembled layer with the poorly reactive Ag substrate is only due to weak van der Waals forces in the former case, to chemisorption when deprotonation occurs. The role of H-bonds, involving mainly carboxyl groups, is fundamental for both structures. Indeed we proved that for the "square" geometry the formation of a OCOH—OCOH—OCOH—OCOH— cycle at the vertex of the squares is the driving mechanism for self-assembling.

An empirical model based on statistical analysis of high resolution STM images is proposed for the other layers.

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#090 - Nanoporous metals - structural and catalytic properties via computational simulations

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Nanoporous metals, i.e., metallic structures whose framework exhibits continuously connected cavities (pores) of nanoscale size, usually obtained by electrochemical leaching an alloy of the target metal with a more electropositive element, have attracted an explosive interest in the last 10 years due to their unique properties leading to applications in catalysis, sensors, and opto-electronic devices. Despite an intense experimental effort, lack of fundamental knowledge still remains on these systems concerning their geometric features and the relationships between these features and the corresponding properties, hindering further development. In this work we achieve for the first time knowledge and understanding on the atomistic structure of nanoporous systems via first-principles-based theory and simulations, focusing on the prototypical case of nanoporous platinum obtained by dealloying of Ni-Pt nanoparticles and its specific, experimentally proven superior catalytic activity in the oxygen reduction reaction (ORR) which is the rate determining step in low-temperature hydrogen fuel cells for sustainable and energy-efficient electrical power. A computational protocol is presented consisting of the following steps: (i) prepare Ni-Pt nanoparticle models of realistic size and shape and in a range of compositions using a Pt/Ni first-principles-based reactive force field (Reax); (ii) simulate the de-alloying process via dynamical simulations in the presence of a tangential force leading to extraction of the electropositive element (Ni); (iii) analyze the resulting structures in terms of number of internal and external surface sites, their local coordination environment, corresponding stress fields, and percolation characteristics of the overall nanostructure; (iv) investigate the catalytic properties of the system via a Reactive Global Optimization (RGO) approach; (v) correlate the catalytic activity to the geometric and electronic state of surface exploiting the previous analysis of coordination environment and stress fields – compare/contrast with non-porous systems. As a result, the relationship between structure and catalytic function and the origin of enhanced catalytic performance in nanoporous platinum are unveiled, with the final goal of designing platinum systems with optimal catalytic activity. It turns out that nanoporous platinum exhibits a specific local coordination environment at both the internal and external surfaces which selectively quenches the energy barriers of the ORR. A direct connection with amorphous systems is shown. Impact on the general theme of nanoporous metals and their science and technology is finally outlined.

#091 - Photoionization study of water clusters

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Water molecules play a very important role in many fields of planetary life, namely, in atmospheric, biological and chemical processes. Water clusters are multimers of water molecules held together by extensive hydrogen bond networks. They are formed by condensation of water vapor in the supersonic beam as it passes from the atmospheric to low pressure region of the source through an orifice.

Recently, particular attention has been focused on studying water clusters, which exhibit many features of condensed phase, but have finite size. Whereas a huge number of papers have been published on photoionization of mixed clusters of water with alcohols or aromatic molecules few is known about photoionization of neat water clusters.

The present work presents the results of the application of electron impact and laser ionization TOF-MS on water clusters up to 160 molecules in order to have information on the electronic states of clusters of different sizes up to dimensions that can approximate the bulk phase.

Laser pulses in nanosecond and picosecond range have been applied in order to test the possibility of extending the mass detection much over the previous published papers.

A comparison between two configurations of TOF-MS detector, linear and reflectron, in water clusters spectral analysis is also reported in order to show the advantages of both for obtaining more complete information.

A study of signal intensities of water clusters formed by using nanosecond and picosecond laser ionization vs laser pulse fluence concludes the work.

#092 - Homoepitaxy on Si(111) vicinal surface: spirals and pyramids - in situ reflection electron microscopy

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Improved reflection electron microscopy technique (LODREM) is used to demonstrate in situ two of the basic mechanisms for crystal growth – spiral and layer by layer. Perfectly controlled thermodynamic conditions (super or under saturation) around the sample allow us to study in details growth spirals at elevated temperatures and growth pyramids on reconstructed Si(111)-(7×7) surface. Detailed study of the dependence between the distance of the spiral monatomic steps and the deposition rate shows that the scaling exponent differs from that predicted by the classical Burton-Cabrera-Frank theory. The role of the back-stress effect and the step permeability on this dependence is discussed. When the terrace width on a vicinal surface exceeds certain critical value, the step flow growth mode is switched to a 2D island growth. These islands are precursors for appearing of a periodic pattern of pyramids onto the vicinal surface. Real time movies reveal the process of this periodic pattern formation. The dependence between the critical terrace width for 2D island growth and the temperature is used to extract information about the activation energy for 2D nucleation and the Ehrlich–Schwoebel barrier.

#093 - Pt-decorated CdSe/CdS octapod nanocrystals for photocatalysis

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Solution-processed colloidal nanocrystals are considered promising materials for photocatalysis, as control over topology, shape and size of nanocrystals offers the ability to design self-standing nanometric reactors [1-3]. Particular attention has been devoted to nanocrystals comprising epitaxial interfaces between semiconductors able to absorb solar light and noble metals able to catalyze chemical reactions. Nanocrystals based on metal chalcogenide semiconductors, like CdSe and CdS, decorated with noble metals like Au and Pt have been successfully demonstrated in recent experiments to reduce water into molecular hydrogen upon illumination with solar light [4-8]. Achieving efficient photocatalytic water splitting will however require several further steps in materials development, including the simultaneous presence of an oxidizing electrode and the ability to store several photoexcited charges inside the same nanocrystals to activate multi-electron reactions.

With this aim, we tested as a novel platform for photocatalysis octapod shaped CdSe/CdS nanocrystals [9-13]. Taking advantage of the different chemical reactivity of the various crystal planes, we were able to controllably decorate the nanocrystals with Pt nanoclusters at selected locations. We measured the optical properties of such heterostructured nanocrystals, both with cw and ultrafast spectroscopy techniques. Our results demonstrate charge separation and storage of multiple photoexcited electrons in the Pt tips. A rational base is provided for the development of branched nanocrystals for photocatalysis, where each branch could host a different metal tips to catalyze both reduction and oxidation within the same nanocrystal, to connect nanocrystals among themselves or even support them over a substrate.

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#094 - ARPES in cuprates and iron-based superconductors

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I will overview our recent results on iron-based and cuprates superconductors obtained using Angle-resolved Photoemission Spectroscopy. Our setup allows carrying out the experiments at extremely low temperatures fully controlling polarization of incoming light as well as its photon energy. Such approach allows us to unravel the electronic structure of complicated many-band materials and determine their Fermi surfaces. Knowing the Fermi momenta with a high precision we then determine the superconducting gap thus gaining the knowledge about the structure and symmetry of the order parameter. Systematic ARPES studies of many families of iron-based superconductors clearly point to the key role of band structure anomalies located near the Fermi level in the formation of the superconducting state.

#095 - Superconductivity in actinide compounds

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Most of the $5f$ heavy-electron superconductors are materials close to a magnetic instability where spin fluctuations are supposed to provide the mediating bosons responsible for Cooper pairing of itinerant 5f-electrons. In several uranium heavy-fermion compounds superconductivity coexists with antiferromagnetic order, the gap function is highly anisotropic, and the critical temperature Tc lies in the sub-kelvin range [1]. On the other hand, $PuCoGa_5$, $PuRhGa_5$, $PuCoIn_5$, and $NpPd_5Al_2$, the only four known superconductors containing a transuranium element, have a Tc that is considerably larger, namely 18.5 K [2], 9 K [3], 2.1 K [4] and 4.9 K [5], respectively. The nature of the electron pairing mechanism in these spin-singlet d-wave superconductors is still controversial. Electronic structure calculations combining the local-density approximation with an exact diagonalization of the Anderson impurity model show an intermediate $5f5$-$5f6$-valence ground state and delocalization of the $5f\,5$ multiplet of the Pu atom $5f$ shell in $PuCoIn_5$ and $PuCoGa_5$. The $5f$ local magnetic moment is compensated by a moment formed in the surrounding cloud of conduction electrons. For $PuCoGa_5$ the compensation is complete, and the Anderson impurity ground state is a singlet. For $PuCoIn_5$ the compensation is partial, and the Pu ground state is magnetic. We suggest that the unconventional d-wave superconductivity is likely mediated by the 5f-state antiferromagnetic fluctuations in $PuCoIn_5$ and by spin fluctuations associated to valence instabilities in $PuCoGa_5$ [6, 7]. For $NpPd_5Al_2$, a two-channel Kondo mechanism leading to the formation of a condensate of composite pairs between local moments and charge carriers has been proposed [8]. The results of key experiments probing the superconductive and the normal state properties of these exotic materials will be presented and discussed against theoretical predictions.

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#096 - Hall effect in pnictides

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The multiband character of pnictide systems complicates the analysis of transport experiments data, sincein these systems the contribution of carriers having hole and electron character is unavoidably mixed. The experiments on Hall transport highlighted several anomalies both concerning the order of magnitude of the Hall coefficient R_H and its temperature/doping dependence. For example, within a semiclassical Boltzmann-like approach, R_H is expected to be almost zero in slightly doped compounds, while from experiments it is found to have a large absolute value with a strong temperature dependence.
We present a theoretical investigation of Hall transport taking into account the multiband character of pnictides.
The analysis of an effective two-band model with dominant interband interaction, reveals an unconventional scenario, beyond the Boltzmann theory, where the quasiparticle currents dressed by vertex corrections acquire the character of the majority carriers. This leads to a larger (positive or negative) Hall coefficient than what expected on the basis of the carrier balance, with a marked temperature dependence.
Moreover in order to deeply understand the orbitals role in transport phenomena, we consider the analysis of Hall transport within a more microscopic multiorbital language.

#097 - The onset of magnetism in optimally electron-doped $LnFe_1$-xRuxAsO$_1$-yFy (Ln = La, Nd or Sm) superconductors around x = 1/4

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From µSR measurements it is shown that the appearance of static magnetism, nanoscopically coexisting with superconductivity, is a general feature of optimally electron-doped $LnFe_{1-x}Ru_xAsO_{1-y}F_y$ superconductor, with Ln a lanthanide ion. The magnetic ordering temperature TN and the magnitude of the internal field display a dome-like x-dependence, peaked around x = 1/4, with higher values for those materials characterized by a larger As z lattice parameter. Remarkably, the latter are also those with the highest superconducting transition temperature (Tc) for x = 0. The reduction of Tc(x) is found to be signicant in the x region of the phase diagram where the static magnetism develops. Upon increasing the Ru content superconductivity eventually disappears only at x approaching 0.6. The experimental findings are discussed in the framework of the possible pairing mechanisms.

#098 - Electronic structure of iron-chalcogenide thin films

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The discovery of high-temperature superconductivity in iron pnictides (FePn) raised a strong interest in searching for new superconducting materials which contain Fe and share common structural features with FePn superconductors.
In addition, perspectives of suitable applications boosted the interest on characteristics and properties of both the normal and the superconducting (SC) state of these compounds. However, due to the complex nature of the structural and magnetic interactions in these compounds, most part of theoretical issues are, up today, still under a heated debate.
Recently, the successful growth of one-monolayer FeSe on $SrTiO_3(001)$ surface and the subsequent dramatic enhancement of superconducting critical temperature at 55-65K [1], posed new questions, unanswered at the moment, on the origin of the superconducting phase in iron-based materials. A notable experimental evidence is the presence of only electron-like Fermi surfaces, without hole-like gamma-centered Fermi surface (always present in all the other, bulk, iron-based superconductor). How superconductivity is sustained with such a Fermi surface is an open issue.
In this talk we present a theoretical and computational study of reduced dimensions and their effects on structural, electronic and magnetic properties of fe-chalcogenides thin films (monolayer, bilayer and bulk limit) by means of first-principles density Functional Theory.
We show how surface has strong influence on the electronic dispersion due to band-folding effect and we successfully compare the electronic band structure with recent ARPES spectra obtained in FeSe thin films [3]. We discuss possible origin of Fermi surface closure at Gamma point in the monolayer limit considering possible magnetic phase and charge doping due to the substrate.
We extend the prediction to other Fe-Chalcogenide monolayers, namely FeTe and $FeSe_xTe_{1-x}$ discussing the relevant differences with respect to FeSe case in view of possible new two dimensional superconducting phases.

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#099 - Glassy transition in the vortex lattice of $Ba(Fe_{0.93}Rh_{0.07})_2As_2$ superconductor probed by NMR and Ac-susceptibility

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The iron-pnictide superconductors of the 122 family ($Ba_2(Fe_{1-x}TM_x)_2As_2$, TM = transition metal) have attracted great attention both for their remarkably high critical fields ($Hc_2 \approx 60$ T), and for the high quality of the single crystals, despite the low transition temperatures ($T_{cmax} = 38$ K). However, once a current is injected, flux dynamics leads to dissipation effects which can prevent any efficient application. Accordingly, the understanding of the pinning effects is of major relevance. It is then of significant importance to characterize the dynamical and dissipative properties of the vortex lattice, such as the correlation times for the vortex motions τ_c, the pinning activation barrier U, their dependence on the magnetic field H and temperature T, as well as the phase transitions which may occur in the mixed phase, across the phase diagram. When fields of some Tesla are applied, the time-scales of the vortex dynamics match with the nuclear magnetic resonance (NMR) and ac-susceptibility time-scales. These two experimental tools are excellent to study the pinning effect, and their joint employ provides complementary information on the vortex dynamics. In both cases the vortex lattice (VL) excitations are probed in the radio-frequency range but, while ac-susceptibility is sensitive to dissipative/dispersive mechanisms taking place at wave-vector $q \to 0$, NMR is sensitive to the q-integrated dynamics.
In this work, measurements of the real χ' and imaginary part χ'' of the ac-susceptibility are presented and discussed together with 75As nuclear spin-lattice relaxation rate $1/T1$, in a single crystal of $Ba(Fe_{0.93}Rh_{0.07})_2As_2$ superconductor. The vortex correlation times $\tau_c(H,T)$ are extracted both from the peaks in $1/T_1$ and χ'', and their dependence on the T and H is analyzed.
Surprisingly, the temperature dependence of the correlation time agrees with a Vogel-Fulcher (VF) behavior, rather than with an Arrhenius law, as early found in the cuprates, and shows an activation barrier U~130 K, weakly dependent on the magnetic field, in contrast with former observations on the 1111 compounds. In addition, the VF character of these systems displays a crossover conceivable with a vortex glass transition, instead of a pure vortex solid lattice.
Moreover, the pinning barrier shows a weak dependence on the magnetic field which can heuristically be justified within a fragile glass scenario. Finally, the glass freezing temperatures, close to the VF temperature T_0, obtained by the two techniques, merge together onto the de Almeida-Thouless line, typical of glass-forming systems.

In conclusion, NMR and ac-susceptibility allow to characterize the phase diagram of the mixed state, to determine the melting/freezing line of the vortices and the nature of the frozen state.

#100 - Hard X-ray measurements on $Nd_{2-x}Ce_xCuO_4$+delta films

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We have studied the Cu 2p core levels by x-ray photoemission spectra of as-grown $Nd_{2-x}Ce_xCuO_{4+\delta}$ samples. The comparison in the spectrum features, from the thinner film to the single crystal, has pointed out a different behavior of the Cu $2p_{3/2}$ $3d^{10}$ peak with results not related to the superconductivity. The confirm of the presence of the satellite peak discovered by Taguchi et al. [1] in the $Nd_{2-x}Ce_xCuO_{4+\delta}$ single crystal hard x-ray photoemission Cu $2p_{3/2}$ $3d^{10}$ spectrum is pointed out by all the acquired spectra on our samples, films and single crystals.

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#101 - Field-effect manipulation of single-electron systems

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The metal-seeded growth of semiconductor nanowires (NWs) is a promising technique for the fabrication of high-perfection self-assembled nanostructures, with innovative device applications in nanoelectronics [1], optoelectronics [2] and energy harvesting [3]. In particular, InAs/InP NW-based singleelectron devices have a great potential and allow an extreme and reliable control of electron filling down to the last free electron, even if energy spectrum and coupling are usually harder to tune. Here we demonstrate an innovative implementation where we achieve an easy manipulation of the orbital energies in an InAs/InP quantum dot (QD) and a dramatic modification of its energy spectrum. At present our technique can be used to: (i) enhance the device working temperature up to about ~77 K [4]; (ii) electrostatically tune the spin configuration of the QD and induce controllable singlet-triplet spin transitions [5]. The device architecture is shown in Fig.1. Energy spectrum warping is achieved through a transverse electric field induced using twin local gates (lg1 and lg2). Due to the lack of surface depletion in InAs, the QD potential landscape and energy spectrum are strongly affected by such transverse field. This is in contrast to usual QDs defined by a smooth and approximately harmonic confinement potential. We demonstrate that the Coulomb gaps in our device can be tuned continuously from virtually zero up to ~75 meV. In this configuration, a strong modulation of the device conductivity as a function of the electron filling is well visible up to 77 K. The same technique can also be used to induce a level degeneracy in the QD. In this case, we show that strong exchange-driven spin transitions can be obtained and controlled by field-effect up to over 20 K. As all the described manipulation techniques are based on bare field-effect, they open a new window of opportunity for the time-resolved investigation of few-electron QD systems based on InAs/InP NWs. Potential applicative impacts and research perspectives will be discussed.

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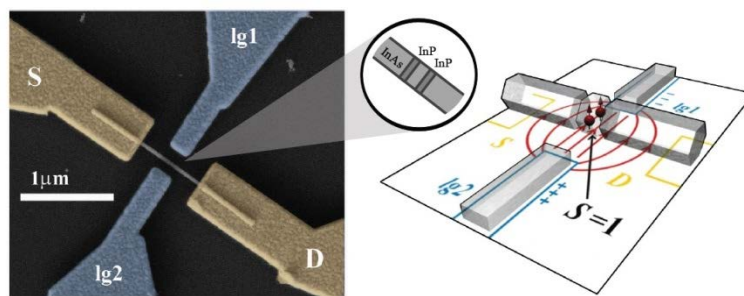
Fig.1 – Scanning electron micrograph (left) and general sketch (right) of the device structure. A multipole gating technique allows the electrostatic control of the spin configuration of InAs/InP few-electron systems up to 20 K. Image from [5].

#102 - Near infrared emitting silica nanoparticle: O_2 diffusion properties and excited state relaxation

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The experimental studies on the Near Infrared (NIR) emission properties of high purity silica (a-SiO$_2$) nanoparticles opportunely functionalized by O_2 molecules are reviewed. The investigated nanoparticles size ranges from 7 up to 40 nm and they feature NIR emission peaked at 1272 nm arising from embedded molecules. This emission can be excited both in the NIR (from 1060 up to 1075 nm) and in the visible (at 765 nm and 690 nm) ranges with lifetime in the timescale of 0.5 s, giving the emitters good features for probe applications and dynamic studies. The obtained particles are soluble in water, radiation resistant and surface functionalizable. Furthermore, not changing the properties of the host silica material, these emitters are highly biocompatible and perspectively useful for in vivo applications. The basic physical-chemical properties of the dynamics of diffusion of O_2 in the silica nanoparticles were investigated as a function of temperature, pressure and particles size enabling to determine characteristic thermodynamics parameters of the involved process. The photoluminescence of the excited singlet state was studied as a function of temperature down to 10 K and characteristic relaxation mechanisms of O_2 embedded in the solid matrix were highlighted.

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#103 - Electro-refractive effect in Ge/SiGe multiple quantum wells

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Ge/SiGe multiple quantum wells (MQW) has received a great attention in the context of silicon photonics for the realization of efficient electro-absorption (EA) modulators based on the quantum confined stark effect (QCSE). QCSE causes strong variations in the absorption spectrum, which are associated to a change of the refractive index at a given wavelength, as stated by Kramers-Kronig relations. Large changes in the refractive index would make Ge/SiGe MQW attractive for the realization of electro-optic devices such as Mach-Zender phase modulators. In order to characterize the electro refractive effect in germanium quantum wells , 20 MQW (10 nm Ge/15 nm Si0.15Ge0.85) were grown on a Si0.1Ge0.9 virtual substrate by low-energy-plasma-enhanced-chemical-vapor-deposition (LEPECVD).The sample was then processed in 64 μm long slab waveguides by standard optical lithography and dry etching. The electro-refractive effect was characterized by the measurement of the shift of Fabry-Perot fringes in the transmission spectra of the device for different applied voltages. A refractive index variation up to 1.3 x 10-3 was measured with an applied electric field of 88 kV/cm at 0.84 eV, with a VπLπ figure of merit of 0.46 Vcm. The device performances are promising for the realization of Mach Zender modulators in the Ge-Si material system, with several potential advantages over the EA modulators such as the improved thermal stability and the extended operative wavelengths.

#104 - SiGe stressors for tensile strain in Ge films by e-beam lithography top-down approach

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Information and communication technologies (ICT) eagerly need novel approaches, or even paradigm shifts, to continue the improvement of the performance and the scaling down of silicon metal oxide semiconductor field effect transistors (MOSFETs). The mobility enhancement can be achieved by altering the properties of silicon through strain-induced manipulation of the band structure, which modifies the effective masses and phonon scattering within the channel. Uniaxial strain obtained using local stressors has become part of mainstream Si-based technology over the past few years, since uniaxial strain in Si improves its figures of merit in terms of microelectronic applications [1].

Tensile strain in germanium reduces the separation between the indirect (L) and direct (Γ) conduction band minima. The application of 2% biaxial strain to a Ge(001) layer is expected to lower the direct gap below that of the indirect gap, and a similar result is expected for 4% uniaxial strain applied along [100]. A direct-gap semiconductor which is fully compatible with Si-based technology would greatly facilitate full integration of electronics and optoelectronics [2].

In this work, top-down structures obtained by nanolithography will be used as stressors for the creation of high deformation fields [3,4]. A strained Si1-xGex film will be grown on Ge relaxed buffer on Si(001) substrates by low-energy plasma-enhanced chemical vapor deposition and characterized by x-ray diffraction to verify the composition and strain state of as-grown heterolayers. Nanostructures, in the form of long ridges in order to induce uniaxial strain in Ge film, will be defined by electron-beam lithography and reactive ion etching. Micro-Raman spectroscopy will be used to obtain complementary information on the composition and strain state within nanostructures on the micron scale. The nanostructures will be designed with the help of FEM modeling [5]. The same modeling will also be used to interpret both micro-Raman and x-ray diffraction results, in the latter case by constructing kinematical simulations of the diffraction pattern using the displacement field produced by the FEM.

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#105 - Proximity gettering of slow diffuser contaminants

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The most commonly used gettering techniques are not effective for slow diffuser contaminants, for instance molybdenum and tungsten, because getter sites are usually too far from the device regions. These contaminants may be gettered only by a sort of "proximity gettering", such that the gettering regions are located at a shorter distance from the device than the metal diffusion length during the thermal treatments involved in device process. In addition, even if this condition is met, it is not clear if gettering would be

effective for these metals. For instance, molybdenum is reported not to be gettered at all even in the region close to the gettering layer. On the other hand, these elements are reported to be very harmful for devices, so effective gettering techniques are needed for these elements too.   In this paper, we test proximity gettering layers obtained by carbon or silicon implantation for their efficiency in molybdenum and tungsten gettering. The samples were intentionally contaminated by molybdenum and tungsten contaminated solutions (10, 100 and 1000 ppb) and thermally treated (1100 C, 3 min) to diffuse the contaminant in silicon. Then a gettering layer was formed byimplantation of carbon or silicon. The wafers were then annealed to re-crystallize the implanted region and nucleate getter sites, and received a final annealing at 800°C for 10 min to enhance the segregation of metal impurities into the gettering region. DLTS was used to measure the electrically active concentration in the silicon volume. The gettering efficiency was estimated by comparing gettered and not gettered wafers. A relevant reduction of the contaminant concentration was obtained by carbon implantation in 100 ppb contaminated samples, on the contrary the contaminant concentration was not significantly modified in 10 ppb contaminated samples Opposite to what observed for carbon implantation, no gettering at all is obtained by silicon implantation. TEM analyses showed defects in silicon-implanted wafers, and no defects in carbon-implanted wafers. This result shows that crystal defects do not play the most important role in gettering these elements. A similar conclusion was reached in the past by comparing the gettering efficiency of layers heavily doped with various dopant elements. Also in that case, the gettering efficiency was not related to extended defects. In both cases gettering is obtained by doping with an impurity having smaller tetrahedral radius than the silicon radius, so gettering can be partially due to the tensile strain region surrounding the impurity. Both molybdenum and tungsten gettering are found to be less effective at low concentration. A similar effect was previously observed for iron. Our data suggest that this property is common to other impurities. Finally, in-depth profiles suggest that gettering of slow diffusers is limited by impurity diffusion to getter sites.

#106 - Dislocation engineering in SiGe epilayers on pre-patterned Si substrates

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The possibility to use thick Si-rich SiGe epilayers for the SiGe technology, for example in photodetectors, is hindered by the nucleation of misfit dislocations. In the present work we exploit a suitable pit-patterning of a Si(001) substrate to influence the nucleation and the propagation of dislocations during epitaxial deposition of $Si_{1-x}Ge_x$ alloys, preferentially gettering misfit segments along pit rows.
The {111}-faceted pits, hundreds of nm large, are created on Si substrates covered with a SiN_x mask. Electron beam lithography was used to realize pit arrays aligned along <110> spaced by 1.0-10.0μm. This pattern is transferred to the SiN_x layer by reactive ion etching to define a hard mask, which is used for anisotropic wet-chemical etching of the Si substrate and then removed. The samples are chemically cleaned and a layer of $Si_{1-x}Ge_x$ (x~10-30%; thickness~150-250 nm) is epitaxially deposited.
The structures have been characterized by X-ray diffraction, scanning electron microscopy and atomic force microscopy. AFM images show that under the right conditions, the distribution of surface crosshatch lines, which indicate the presences of dislocations bunches, can be controlled by the pit pattern. The effect continues for ~20μm outside the patterned region.
The strain within the pattern has been characterized by μRaman spectroscopy. The strain distribution is inhomogeneous due to the dislocation bunches created along pit rows, with higher levels of compressive strain in the dislocation-free region.

#107 - X-ray nanodiffraction in lithographically-defined semiconductor structures

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The continued progress of computing technologies continually requires new concepts which improve the performance, efficiency, and scalability of Si-based devices. Uniaxial strain obtained using local stressors [1] has become part of mainstream Si-based technology over the past few years, since uniaxial strain in Si improves its figures of merit in terms of microelectronic applications. In this work, top?down structures obtained by nanolithography will be used as stressors for the creation of high deformation fields. Exploiting the fact that the Ge lattice parameter is 4.17% larger than that of Si, carefully shaped SiGe nanostructures can be used to locally induce uniaxial strain in Si. Nanofocused x-ray beams based on refractive or diffractive optics have recently become available at synchrotron light sources, allowing the distribution of strain within individual nanostructures to be measured directly [2].
Si-capped SiGe layers have been grown epitaxially on Si(001) substrates by low-energy plasma?enhanced chemical vapour deposition, and laboratory x-ray diffraction verified that the SiGe layers were fully strained. Nanostructures, in the form of long ridges [3, 4], were defined by electron-beam lithography and reactive ion etching. Since the ridges are free to expand laterally, the misfit strain is able to partially elastically relax, inducing uniaxial compressive strain in the silicon substrate and tensile strain in the silicon cap. The focused x-ray beam is scanned over the nanostructure in ~100 nm steps, so that a spatial picture of the elastic relaxation process is obtained.
The diffraction results are compared to simulations of kinetic diffraction of finite-element method models, and results from micro-Raman spectroscopy.

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#108 - Fabrication of SiGe rings and holes on Si(001) and Si(111) by flash annealing

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Recent advancements in the fabrication and self-assembly of strained epitaxial thin films have allowed for the realization of a variety of semiconductor nanostructural assemblies, such as quantum dots and more complex ring-like and hole clusters [1]. Due to their peculiar geometry, nanoholes and rings exhibit unique electronic and optical properties and are envisaged for potential application in future generation devices [2]. So far, such nanostructures have been fabricated mainly by using droplet epitaxy or by partial capping of strained islands. In particular, previous results have shown that SiGe rings can only be formed via material redistribution/shape transformation of islands by a process activated by Si capping and driven by strain energy relief. It is a widespread assumption that SiGe islands could not be transformed into nanoholes and rings by annealing treatments only and without Si capping [3].
In this study we present the results about the development of a procedure based on annealing treatments able to produce nanoholes and ring-like morphologies in Ge/Si(001) epitaxy. Compositional analysis by Raman and X-ray photoelectron spectroscopy (XPS) indicates that rings are markedly enriched in Si with respect to the parent islands, suggesting that the evolution path from SiGe islands to rings is driven by the partial dissolution of Ge during high-temperature annealing. Similar nanoholes and ring-like morphologies have been obtained on Ge/Si(111) systems also.

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#109 - The NFFA nanoscience data repository

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The ultimate goal of data archiving is to make it possible and likely a more extensive and complete use of the data itself. The nanoscience community could enormously benefit from effective archiving, i.e. from open-access scientific Data Repositories (DR) that could support sample/material preparation protocols with absolute metrology, and adequate metadata for the characterization and scientific investigations. In many aspects nanoscience poses an extreme challenge due to the abundance of inhomogeneous information to be archived, and the need of advanced data management methods and services. On the other hand advanced automatization of the full data set can be pursued minimizing the operator's role in the fulfillment of metadata.
The EU NFFA project (www.nffa.eu), coordinated by IOM-CNR, addresses the creation of the first Data Repository (DR) in nanoscience, as a key element of the distributed research infrastructure on Nano Foundries and Fine Analysis centres.
Suitable data formats for transferability, analysis, archiving, and interoperability have been investigated with reference with the current efforts (EUDAT and Pandata, I-CAT for instance)[1], and a new engineering is addressed for the link to metadata to complete the relevant information on the protocols followed in the sample definition and in the measurements. The aim is enabling the full reproducibility of preparations and experiments in order to exploit truly complementary data as obtained with different methods on true replica samples and sample environment conditions.
We present here the DR-prototype developed with the NFFA project in strict collaboration with Sincrotrone Trieste S.C.p.A., official subcontractor of the project. Such prototype that has been connected to three different experimental facilities: a scanning electron microscope (SEM) instrument, a synchrotron radiation beamline for spectroscopy, and an open package for first principle simulation (Quantum Espresso) being representative facilities of a NFFA Centre.
The ongoing activity is now focused on expanding and improving the prototype making it more robust and making it available for real case scenario where the workflow of production experiments and associated simulations can be fully recorded with associated data and metadata in order to guarantee the full reproducibility of procedures as mentioned above.

[1] Design of NFFA Data Repository and access criteria. Deliverable 4.9 NFFA project; available at http://www.nffa.eu/UserFiles/file/Deliverable4-9DataRepository.pdf

#110 - Atmospheric composition models: a personal review of some key problems and approaches to solution

Francesco Tampieri (I) – CNR- Istituto di Scienze dell'Atmosfera e del Clima, Bologna

Atmospheric composition models results from the evolution and merging of atmospheric circulation models and air quality models. As any model is a partial description of the real world, it is optimised to give better results in limited and specialized ranges of application. From the point of view of the present talk, this is made using appropriate parameterisation of physical processes. Thus it is interesting to analyse the new problems and parameterisations necessary to the combined approach, the relation with the new data that are available from time to time, and some perspectives for the future.

#111 - Integrated aerosol observing system

Aldo Amodeo (I) – CNR- Istituto di Metodologie per l'Analisi Ambientale, Tito (Potenza)

Aerosol impact on climate is one of the most uncertain aspects of climate change, and impact of aerosols on human health is a growing matter of concern, particularly in urban areas.
There is a need to develop an integrated approach of characterizing particles by including ground-level and airborne in-situ measurements, ground-based remote sensing, and space-borne observations in combination with advanced modelling.
The main goal is to establish an integrated observing system that should foster aerosol-related process studies, validation of satellite sensors, model development and evaluation, assimilation of aerosol data into operational models, and build a comprehensive aerosol climatology on a global scale.
ACTRIS (Aerosols, Clouds and Trace gases Research InfraStructure Network) is an outstanding research infrastructure launched in 2011 and will, for the first time, provide coordinated observations of the major atmospheric variables. ACTRIS aims at integrating European ground-based stations equipped with advanced atmospheric probing instrumentation for aerosols, clouds and short-lived gas-phase species. ACTRIS will have the essential role to support building of new knowledge as well as policy issues on climate change, air quality and long-range transport of pollutants.
ACTRIS represents an unprecedented effort towards integration of a distributed network of ground-based stations, covering most climatic regions of Europe, and responding to a strong demand from the atmospheric research community. ACTRIS will be a step towards better integration of aerosol, cloud and trace gases communities in Europe necessary to match the integration of high-quality long-term observations of aerosol, clouds and short-lived gas-phase species and for assessing their impact on climate and environment. ACTRIS outcomes will be used for supporting decisions in a wide range of policy areas, including air quality but also health, international protocols and research requirements.
At international level ACTRIS operates in strong cooperation with the Global Atmospheric Watch Program of the WMO, the ARM Climate Research Program and all the relevant research networks as (i.e. AERONET, GALION, NDACC, etc.) for the establishment of the ground-based component of the Global Earth Observation System of Systems.

#112 - Validation of water vapour, carbon dioxide and ozone spectroscopic parameters in the infrared region between 5 and 27 micron

Guido Masiello – Università della Basilicata, Potenza

Carmine Serio, Francesco Esposito (Università della Basilicata, Potenza), Giulia Pavese (CNR – IMAA, Potenza), Giuseppe Grieco, Giuliano Liuzzi, Pietro Milillo, Sara Venafra (Università della Basilicata, Potenza)

During the 2007 ECOWAR (Earth COoling by Water vapour Radiation) field campaign, two moderate spectral resolution Fourier Transform Spectrometers, REFIR (Radiation Explorer in the Far InfraRed) and I-BEST (Interferometer for Basic observation of Emitted Spectral Radiance of the Troposphere) were deployed to sense the water vapour rotational band in the range 260–590 cm-1. These measurements allowed us to revise and improve the current version of the water vapour foreign continuum semi empirical model MT_CKD (version 2.1). After 2007 RHUBC-I (Radiative Heating in Under explored Bands) polar arctic campaigns, MT_CKD authors have proposed and developed a new approach to the problem of water vapour continuum, which includes also a modification of the line half-width parameters in addition to the definition of an appropriate foreign and self-continuum absorption. Although the detailed formulation of this new scheme has not yet appeared in the peer reviewed literature, it has been incorporated within the LBLRTM (Line by Line Radiative Transfer Model) version 12 (see, e.g., the url http://rtweb.aer.com/), as MT_CKD module, version 2.5.2. In this work we show that the current module for the water vapour continuum (released in 2010) performs quite good over the previous version (2.1, released in 2007) and removes the large misfit which affected the micro window at 403 cm^{-1}. Even if it has been implemented with a new water vapour line absorption compilation, in which the half-widths have been properly adjusted, the current continuum module does not perform much better than the previous ECOWAR - adjusted version. Our conclusion is that our ECOWAR dataset definitely validates the current MT CKD 2.5.2 model parameterization, but indicates the need to strengthen the parameterization in the range 360 to 600 cm^{-1} and in general in window channels. In addition, the high quality of the observations also have allowed us to gain insight into understanding the quality of recent new compilation of lines and related treatment for the ν_2 CO_2 band and the O_3 band at 9.6 μm. Comparisons between forward calculations of atmospheric transmission spectra and spectral radiances demonstrate that the ozone absorption is very accurately reproduced and, although to a less extent, this is also the case of CO_2 absorption in the long wave ν_2 band.

#113 - Aerosol typing over Beijing using a scanning Raman Lidar with enhanced dynamics

Gianluca Pisani – China - Italy Joint Research Center for Laser Remote Sensing, Napoli

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Studies on atmospheric aerosol are required mainly to carry out information on the air pollution and its effects on human health. In the last years, the increasing urbanization and industrialization of the Asia region made China acted as one of the countries more affected by atmospheric anthropogenic particles. This, in part, is due to the fact that the Gobi desert, located in the Northern part of the country, acts as a natural particle source in the region. Thus, the combination of both anthropogenic and mineral particles strongly affects the air quality over the city of Beijing, in particular, in the lower troposphere. Hence, in order to improve the effectiveness of the solutions to be carried out by environmental agencies, more detailed characterization of the atmospheric aerosol load is primarily needed.

In this context, the Aerosol Multi-wavelength Polarization Lidar Experiment (AMPLE) has been designed, developed and installed in urban area of Beijing, in the framework of the China-Italy Joint Research Center for Laser Remote Sensing, a research center recently constituted by CNISM and BRIT. The apparatus is based on high repetition rate laser transmitter to perform measurements of the aerosol extinction and backscatter coefficients, and particle linear depolarization ratio at 355 nm and 532 nm even for optical dense aerosol layers. Moreover, the scanning capability of this lidar device allows improving the monitor of the aerosol volume distribution. Preliminary results show how the contribution to the total aerosol load of natural and anthropogenic particles can be discriminated through lidar measurements.

#114 - Improving the monitoring of Etna's volcanic ash plumes using a new scanning Lidar

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Since 2011 several lava fountains episodes have occurred at Etna. The volcanic activity produces eruption columns that may reach up to 10 km a.s.l. and eject to the atmosphere large amounts of volcanic ash. Volcanic ash particles dispersed in the atmosphere are dangerous to aviation operations and should be continuously monitored. In particular, the spatial distribution of volcanic ash and the estimation of the mass concentration in air are an essential information to forecast the volcanic ash plume evolution. For this reason, a new lidar with scanning capability has been recently realized by CNISM (Consorzio Nazionale Interuniversitario per le Scienze fisiche e della Materia) and funded by the VAMOS SEGURO project (www.ct.ingc.it/vamosseguro). The Lidar laser transmitter works at 355 nm, the laser power is 0.6 W, the laser beam divergence is 0.3 mrad, the pulse width is 1 ns, and the laser repetition rate is 1 kHz. The lidar may also be easily transported to three different locations: Montedoro (CL), Serra La Nave Observatory, only 7 km away from the Etna summit craters, and to INAF - Catania Astrophysical Observatory, about 7 km from the International airport Fontanarossa. Zenithal Lidar measurements have been routinely carried out during days without eruptive activity. When lava fountain events occurred the Lidar beam was directed toward the volcanic plume with the aim to investigate physical properties of volcanic aerosols. In this work, preliminary results of data collected during the first months of 2013 are investigated. Reported measurements show how a scanning Lidar used near an active volcano is useful for analyzing both the background of atmospheric aerosols and some features of volcanic ash dispersion.

#115 - Long term observations of desert dust at CIAO, the atmospheric observatory of Potenza

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At the Istituto di Metodologie per l'Analisi Ambientale of the Italian National Research Council (CNR-IMAA) an advanced atmospheric observatory, named CIAO, is operative. CIAO is equipped with the state-of-the-art instruments for the ground-based remote sensing of aerosol, water vapour and clouds including active and passive sensors (like lidars, ceilometers, radiometers and radar). CIAO main scientific objective is the long term measurements for aerosols and clouds climatology and allows to carry out aerosol studies exploiting the synergy among several instruments and techniques. Sited in the central part of the Mediterranean region, this site is particularly appealing for the Saharan dust study. Systematic lidar observations have been performing within EARLINET since its beginning on May 2000. In particular a suitable observing methodology has been established within the network for Saharan dust monitoring over Europe. Based on this schedule, one of the largest database of vertical profiles of Saharan dust optical properties from ground-based instruments has been collected at CIAO. This extended database permits the identification of case studies and Saharan dust climatological studies. Case studies provide an opportunity to investigate, for example, dust modification processes during transport from the source region, mixing with other aerosol types, and dust/cloud interactions. The comparison with CALIOP, the first satellite borne lidar for aerosol study, data permitted the identification of potential improvements in the CALIOP retrieval.

The 12-year Saharan dust observations database permits climatological study of the occurrence in Southern Italy of desert dust, of the altitude they are observed and of their optical properties. In addition, lidar measurements used in conjunction with transport models allowed the identification of source region of the observed Saharan dust particles. Finally, a quantitative evaluation of the DREAM dust-modeled profiles was carried long term database of dust profiles collected at CIAO.

#116 - Inkjet printed organic photodetector with high quantum yield for large area X-ray imager

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The combination of good optoelectronic properties, of the possibility to cover different substrates by means of solution-based techniques and of the low thermal budget involved in the fabrication have definitely consolidated the interest toward organic semiconductors and made this technology attractive for many innovative optoelectronic applications. Here we focus on Organic-based Photodetectors (OPD)[1] suited for a pixellated digital imager that can be coupled to a CsI:Tl scintillator to address X-ray applications, such as industrial quality control, homeland security or biomedical X-ray imaging. Aiming at integrating a photodiode and an addressing transistor into a single pixel, we choose drop-on-demand Inkjet printing as patterning technique [2] .

The OPD has a vertical topology with the photoactive layer (a blend of P3HT-PC61BM) sandwiched between two conductive stripes (silver-based ink at the bottom and PEDOT:PSS for the semi-transparent top electrode) over a polymeric PEN substrate. Ink-jet printing processes have been optimized to obtain controlled stripes 120 µm large, about 80 nm thick, with scallop-free edges. The device active area was defined by the overlap between the PEDOT:PSS and the silver strips, which are mutually orthogonal. We measured an External Quantum Efficiency in excess of 60 % over a broad wavelength range up to ~ 600 nm.

From the experimental measurements of EQE and photocurrent fall time as a function of the optical impinging power we extracted the mobility of carriers (0.5×10-3 - 1×10^{-3} cm^{2}V^{-1}s^{-1}) and the characteristic temperature of the DOS (TC = 872 K) [3]. This latter is about 50 % larger than what reported in the literature for spin-coated devices, indicating a higher degree of disorder connected with the different manufacturing process.

In view of X-ray applications, we performed X-ray stability tests (15 min of direct irradiation at 30 keV, 1 mA) of spin-coated OPD and we did not record any sizeable deterioration. In addition, OPD coupled to a scintillator was tested by impinging with an X-ray flux (30 keV, 100 µA), recording a photocurrent of 150 pA over 50 pA dark current floor, a promising starting point towards the development of organic X-ray indirect imagers [4].

Our results demonstrate that OPD with dimensions and performances suitable for their integration in pixels can be obtained by means of a cost-effective, additive and scalable printing technique such as inkjet printing.

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#117 - High fluorescence of thioflavin T confined in mesoporous silica xerogels

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Trapping of organic molecules and dyes within nanoporous matrices is of great interest for the potential creation of new materials with tailored features and thus different possible applications ranging from nanomedicine to material science. The understanding of the physical basis of entrapment and of the spectral properties of the guest molecules within the host matrix is an essential prerequisite for the design and control of the properties of these materials. In this work we show that a mesoporous silica xerogel can efficiently trap the dye thioflavin T (ThT, a molecule used as marker of amyloid fibrils and with potential drug benefits) sequestering it from an aqueous solution and producing an highly fluorescent material. The study of spectroscopical properties of this system and the comparison with fluorescence of an uncharged analog of ThT give indications about the mechanism responsible for the fluorescence switching-on of ThT molecules during their uptaking into the glass. Diffusion and nanocapillarity are responsible for ThT absorption whereas electrostatic interaction between positive ThT molecules and negative dangling SiO groups covering the pore surfaces causes the immobilization of ThT molecules inside the pores and the enhancement of its fluorescence, in line with the molecular rotor model proposed for this dye. We show also that entrapment efficiency and kinetics can be tuned by varying the electrostatic properties of the dye and/or of the matrix.

#118 - Exploiting the stable alignment of tautomers at RT in porphyrin single layers

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As pointed out by the International Technology Roadmap, the semiconductor industry is approaching a "red brick wall". The incessant miniaturization of devices necessary to increase the available computer power imposes that current devices have long surpassed the areal power density of a hot-plate, are not far away from the values for a nuclear reactor, and somewhere around the middle of the next decade will surpass the surface of the sun [see, for example, the web site: http://www.roadmappingtechnology.com]. Molecular-scale electronics might overcome this difficulty and provides the ultimate miniaturization. Despite simplest devices, like diodes, have been convincingly demonstrated in the lab, pure organic molecular logic

gates represent an apparent insurmountable bottleneck to date. Generally speaking, a logic gate consists of an array of configurable switches [1], which are organic molecules in organic molecular-scale electronics. Recently, a new type of molecular device has been proposed where the switching characteristic is mediated by the bistability in the position of the two hydrogen atoms (tautomerization) in the inner cavity of naphthalocyanines and porphyrins [2, 3]. Unfortunately, such an isomerization apparently can be only exploited at very low temperatures (about 6 K) and limited to individual molecules, while logic gates require an array of configurable molecular switches. These facts represent a severe drawback in the possibility of applications in marketable organic molecular electronics.

Here, we provide full evidence that 2-D layers of metal-free tetraphenylporphyrins (H_2TPP) show frozen tautomerization even at room temperature, with the H atoms aligned along a direction settled *a priori*, if a proper new strategy is followed to grow 2-D layers. On this basis, we describe how to exploit uniaxially oriented H_2TPP tautomers in a first elementary logic device.

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#119 - Photoluminescence enhancement and lasing from conjugated polymer in a full plastic microcavity

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A full polymer high quality laser microcavity structure has been realized. A couple of Distributed Bragg Reflectors (DBR), which works as mirrors in the microcavity structure are prepared by spin coating of polyvinylcarbazole and cellulose acetate orthogonal solutions. The active layer, embed between the dielectric mirrors, consists of a highly fluorescent conjugated polymer poly(9,9-dioctylfluorenyl-2,7-diyl-co-1,4-benzo-(2,1'-3)-thiadiazole) (F8BT) spun film. The microcavity strongly affects F8BT spontaneous emission, leading to a deep modification of PL spectra. High quality factor is achieved, reaching for best samples a values over 130. To achieve lasing from this kind structure the cavity mode is tuned on the peak of the Amplified Spontaneous Emission spectrum of the polymer. Under femtosecond optical pumping laser emission is obtained with a surprising low lasing threshold (<20 J/cm^2) for a full plastic DBR optical cavity. This result opens a simple and cheap way to obtain a new class of flexible polymer lasers.

#120 - Chiroptical techniques, CD and CPL, for investigating soft matter and organic - based conducting materials

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All sorts of materials found in a living organism are chiral, namely they possess either a left-handed or right-handed configuration; they also belong to the more general category of the so called soft matter, which, as a consequence, contains a significant percentage of chiral materials. But there are also several chiral systems which are studied in Material Science, namely the ones which are obtained from Organic Chemistry methods.

Structural properties of both categories of the above materials are investigated by Chiroptical Methods, the most important ones being Circular Dichroism (CD), which consists in the different absorption of left and right circularly polarized light. In this note we present three examples of such studies, two of them useful for soft matter investigations and one for material science. In the first study we deal with the supramolecular gel aggregation of D- and L-amino acid based peptides; as the second example we report on the investigation by VCD (vibrational circular dichroism, i.e. CD in the IR range) of foldamer molecules [1], namely ad hoc synthesized molecules allowing to monitor peptide and protein folding. Finally we will report on structural and optical properties of helicenes [2,3], which are ortho-fused benzenes, exhibiting conduction and strong second-order non linear response. On the latter materials we have also successfully experimented CPL (Circularly Polarized Luminescence).

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#121 - Structure and crystallinity of polymer/metal oxide hybrid interfaces at the molecular scale

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Hybrid interfaces formed by conductive polymers and inorganic crystalline susbstrates are used in a wide range of applications such as photonics, sensors, diagnostics and solar cells. In particular, polymer/metaloxides hybrid layers are extensively studied for low cost photovoltaics.   For example, systems formed by poly(3-hexylthiophene) (P3HT) and ZnO, allow, in principle, to combine the tunable optical properties of the polymer with the excellent transport properties of ZnO [2, 3]. The poor efficiency obtained until

now in hybrid P3HT/ZnO solar cell (~ 2% [4]) requires, among the other factors, an in-depth investigation of the organization of the polymer at the interface.

The assembling and molecular organization of the polymer plays a key role on the overall properties of the interfaces and it critically depends on the synthesis conditions [1] and on the specific nature and crystal structure of the metal oxide used as a substrate. Here, by means of large scale model potential molecular dynamics simulations, we study the structure and the crystallinity of the P3HT/ZnO interface at low and room temperature.

We investigate the structure and morphology of interfaces generated by adopting different boundary conditions and by taking into account the effect of the polymer deposition rates, representing the possible experimental regimes.

We calculate the energetics of the different interfaces and we characterize the polymer crystallinity close to the substrate, by analyzing the global structure factor. The polymer order results to be highly affected by the interaction with ZnO with strong implications on the transport properties of the P3HT/ZnO interface, that are estimated by an effective approximation of the electronic transfer integral between molecules.

The effect of molecular interlayers between the polymer and the substrate and the case of different metal oxides (such as titania) is also discussed in comparison with ZnO.

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#122 - P3HT and PBTTT: a comparative molecular dynamics study inspired by OTFT fabrication techniques

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Organic Thin Film Transistors (OTFT) are metal-insulator-semiconductor field-effect transistors in which the semiconductor is a conjugated organic material. They are the subject of intense industrial research because their fabrication process is less expensive when compared with inorganic TFTs. The most used organic material for their construction consists in two semiconductor polymers, namely poly(3-hexylthiophene) (P3HT) and poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophene) (PBTTT). Despite the large amount of experimental efforts in the characterization of the electronic properties of these devices, several questions regarding their morphological arrangement and the interface with biologic material (phospholipid bilayer) remain wide open. We have recently approached this field of research by applying Molecular Dynamics simulations to investigate bulk and interface properties of these two polymers. Our simulations were inspired by OTFT fabrication techniques: in particular, we have characterized the effects produced by the annealing process, widely used to enhance the charge transport properties of these devices, and by the presence of residual solvent molecules after the spin coating deposition procedure.

We will present the results obtained in bulk and at the interfaces polymer/vacuum, polymer/SiO$_2$ and polymer/phospholipidic membrane, discuss their relevance in the phenomenological context and highlight a roadmap for future plans of research.

#123 - Reliable extraction of the density of states in organic semiconductors

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Organic electronics has advanced exponentially in the last twenty years [1]. Several commercial applications have already appeared on the market, such as those based on organic light emitting diodes, and more are on the way in the field of photovoltaics [2], photodetection [3] and photonics [4] ,[large-area electronics [5], bioelectronics [6] . However, in spite of the extensive studies so far, the fundamental properties of these materials are still not fully understood. In particular, the description of the Density of States (DOS), which is of fundamental importance to rationalize materials optoelectronic properties, is non-trivial in organic semiconductors [7]. On the one hand, structural and energetic disorder result in a distribution of energy states, hence DOS quantitative predictions by means of microscopic simulations are challenging [8] . On the other hand, many experimental approaches proposed so far require a model for charge carrier mobility as well [7,9,10] , resulting in the entanglement of DOS and transport properties which is inconvenient, as transport models for organic semiconductors are still a subject of debate themselves. We tackle this problem by means of Capacitance-Voltage (CV) measurements on Metal-Insulator-Semiconductor (MIS) capacitors. To disentangle DOS from transport phenomena, measurements are performed in quasi-static regime so that carrier mobility does not affect the measured capacitance. To quantitatively extract the DOS, experimental CV curves are fitted against numerically simulated ones, obtained by solving the static, non-linear Poisson equation. We find that CV curves are highly sensitive to the distribution of energy states, hence confirming they are an effective tool to extract the DOS. We consider two prototypical high-mobility polymers, n-type P(NDI2OD-T2) and p-type PBTTT, and show that thanks to the DOSs extracted with our technique, we are able to reproduce with high accuracy the measured transfer characteristic curves of thin film transistors in the whole range of operation, from

subthreshold up to strong accumulation, without introducing additional fitting parameters (apart from a multiplicative coefficient), thus proving the validity and effectiveness of our approach.

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#131-Recognizing of the antiferromagnetic islands and individual localized electrons in new (DOEO)4[HgBr$_4$]·TCE organic semiconductors

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Strong electron-electron correlation and their contribution to the magnetic properties of the new (DOEO)4[HgBr$_4$]·TCE organic were observed. Two critical temperatures 140 K and 70 K were revealed by electron spin resonance (ESR) spectroscopy. Difference of the angular dependencies of centres (corresponding by two separated ESR lines) is fingertip of the contributions of two independent magnetic species to the total magnetisation.

Unusual magnetic behaviour was observed by the SQUID measured field dependence of the magnetization. It was established that field is combination of the straight line corresponding to antiferromagnet contribution (islands) and Brilloin function corresponding to paramagnetic individual centers. Concentration of the charge carriers and paramagnetic structural defects are very low to explain this result by long-range antiferromagnetic ordering. Small islands of the localized electrons become antiferromagnetic at low temperatures (2 K) providing linear field dependence. The rest (non localized) charge carriers possess standard Brilloin field dependence. Transition to the unusual low temperature state was accompanied by splitting of the XPS and HAXPES lines confirming complicated magnetic state of the crystals.

#124 - 10 years of high resolution RIXS of high Tc superconductors: orbital, spin and charge excitations uncovered

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In the last 10 years high resolution resonant inelastic x-ray scattering (RIXS) in the soft x-rays has emerged as the most innovative and informative spectroscopic technique for the study of the orbital, spin and charge excitations in high Tc cuprate superconductors. This exceptional development has been made possible by the AXES and SAXES instruments operational at the European Sybchrotron Radiation facility (Grenoble) and Swiss Light Source at the PSI (Switzerland) respectively, both designed and built at the Dipartimento di Fisica of the Politecnico di Milano. We will briefly review the main results obtained. Those include the accurate determination of dd excitations in undoped parent compounds (orbital excitations), the persistence upon doping of high energy (para-)magnon excitations in the superconducting regime (spin excitations) and the existence of charge density spatial modulations with stripe-like patterning in the underdoped regime (charge ordering).

#125 - Intrinsic charge instability in oxide heterostructures with Rashba spin-orbit

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The peculiar "tailish" resistance of the $LaAlO_3/SrTiO_3$ or $LaTiO_3/SrTiO_3$ (LXO/STO) heterostructures is due to the occurrence of a low-dimensional (e.g., filamentary or fractal) structure of the superconducting cluster with small long-distance connectivity embedded in the two-dimensional system [1,2]. To explain the systematic occurrence of such mesoscopically disordered regions, we model the electron gas at the interface of superconducting oxide heterostructures considering a twodimensional electron gas in the presence of a sizable Rashba spin-orbit coupling (RSOC). Under simple general assumptions, we show that an electronic phase separation occurs for realistic values of the RSOC and of the band parameters [3]. This could provide an intrinsic mechanism for the recently observed inhomogenous phases at the LAO/STO or LTO/STO interfaces and could open the way to new mechanisms useful for spintronics [4]. This also allows to interpret the recently discovered unconventional quantum critical behaviour of LTO/STO [5]. We investigate the effects of temperature and magnetic field on the charge instability finding a novel type of quantum critical point related to the vanishing of the critical temperature of the electronic phase separation [6].

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#126 - Entanglement entropy and macroscopic quantum states with dipolar bosons in a triple-well potential

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We study interacting dipolar (atomic) bosons in a triple-well potential within a ring geometry. This system is shown to be equivalent to a three-site Bose-Hubbard model. We analyze the ground state of dipolar bosons by varying the effective on-site interaction. This analysis is performed both numerically and analytically by using suitable coherent-state representations of the ground state. The latter exhibits a variety of forms ranging from the su(3) coherent state in the delocalization regimes to a macroscopic cat-like state with fully localized populations, passing for a coexistence regime where the ground state displays a mixed character. We characterize the quantum correlations of the ground state from the bi-partition perspective. We calculate both numerically and analytically (within the previous coherent-state representation) the single-site entanglement entropy which, among various interesting properties, exhibits a maximum value in correspondence to the transition from the cat-like to the coexistence regime. In the latter case, we show that the ground-state mixed form corresponds, semiclassically, to an energy exhibiting two almost-degenerate minima.

#127 - Electronic and magnetic properties of magnetically doped topological insulators

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The topologically protected surface spin environment in topological insulators favors the long range spin coherence and fault-tolerant information storage [1], rendering them particularly suitable for novel spintronic devices [2]. The inclusion of 3d-metal impurities (i.e. Mn) in Bi_2Te_3 topological insulator (TI) results in bulk ferromagnetism [3]. The ferromagnetic ordering temperature of 13 K is however well below practical operating conditions. We demonstrated that the long range ferromagnetism at ambient temperature can be induced in $Bi_{2-x}Mn_xTe_3$ by the magnetic proximity effect through deposited Fe overlayer films [4].

Despite the expectation of observing the magnetically induced gap at the Dirac point due to the breaking of time-reversal symmetry, we find no evidence for opening of such a gap neither in $Bi_{2-x}Mn_xTe_3$ crystals nor in $Bi_{2-x}Fe_xSe_3$ thin films.

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#128 - Spin-orbital separation beyond strictly 1D

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Recently, resonant inelastic X-ray scattering (RIXS) on the 1D spin chain system Sr_2CuO_3 has revealed an unprecedented and strong dispersion of *dd* orbital excitations. This result, observed in [1] for the first time, has been interpreted as the spin and orbital separation from the elementary electron in a 1D S=1/2 system, similarly to the spin-holon separation observed in previous angle-resolved photoemission studies of the same system [2]. In this talk we report on the Cu L_3 RIXS investigation of the two-leg ladder compound $CaCu_2O_3$, consisting of two coupled spin chains. Due to its buckled geometry, the inter-chain interaction of this system is one order of magnitude smaller than the in-chain interaction, but not negligible [3]. Therefore, $CaCu_2O_3$ is an ideal model system to study the effect of a weak inter-chain interaction, i.e. the effect of a dimensionality higher than 1D, on both the low (spin excitation) and the high (*dd* excitations) energy scale. Although the dispersion of the spinon continuum can largely be accounted for by neglecting the presence of the inter-chain interaction (as far as it concerns the energy range accessible to Cu L_3 RIXS), surprisingly the absence of a strong dispersion in the *dd* excitations emerges from the raw data. A deep analysis of these results shows indeed that the various orbital channels feel different dimensionalities, 1D or 2D, depending on their intrinsic directionality. In particular, spin-orbital separation persists in this system for the *3d*$_{xz}$ orbital, oriented along the chain direction *x*.

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#129 - Stripe dynamics in the La$_{2-x}$Sr$_x$CoO$_4$ layered cobaltates by ^{59}Co and ^{139}La NMR and μSR

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Rare-earth-based transition metal oxides display a large variety of different phenomena, including high-T_c superconductivity, magnetic order, stripe phases [1,2] and phase separations. The hole doped lanthanum cobaltates $La_{2-x}Sr_xCoO_4$ share much of such physics. They are layered, magnetic insulators, isostructural with the '214' copper oxide family $La_{2-x}Sr_xCoO_4$. The two families apparently exhibit similar magnetic properties, although the superconductive phases, which are present in the cuprates, are missing in the cobaltates. In view of their similarity, it is reasonable to argue that the study of cobaltates can provide insight also in the physics of cuprates, with particular regard to the possible interplay of magnetism and superconductivity.

In doped cobaltates, holes localize themselves on Co^{3+} in a spinless state [3], and tend to self-organize into arrays of charged stripes. As a result, the magnetic Co^{2+} ions give rise to a striped antiferromagnetic spin structure, similar to the one observed in cuprates [4], where the non-magnetic stripes behave as antiphase domain walls. Recently, inelastic neutron scattering on La5/3Sr1/3CoO4 revealed a hour-glass-shaped dispersion branch in the magnetic excitations of the system[5]. The same hour-glass dispersion was also observed in several cuprates. This suggest that the underlying excitations arise from magnetic stripes (either static or fluctuating) in all case.

We present an investigation on a series of $La_{2-x}Sr_xCoO_4$ crystals (x = 0.25-0.9) by ^{139}La and ^{59}Co NMR. The detection of a ^{59}Co signal with moderate shifts proves the low-spin (diamagnetic) state of Co^{3+}. The magnetic transition temperatures are loosely determined as $T_N \sim 40K$ from the broadening of the NMR spectra. The most remarkable finding is, however, the detection of slow dynamical excitations, ascribed to the collective motion of charge and spins across and within the stripes, their evidence is provided by the partial or total loss of the NMR signal (wipeout), due to very short and inhomogeneous T_2 relaxation times. Two wipeout regimes are detected over distinct temperature intervals. Comparison with μSR experiments assigns the higher- and lower-temperature signal minima to the thermally activated diffusion of holes and spins, respectively. A simple phenomenological diffusion model, accounting quantitatively for the signal wipeout, will be presented.

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#130 - Ferromagnetism in Cr-doped In_2O_3 revisited with hybrid-density functionals

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Cr-doped indium oxide has been reported to be a high-Curie-temperature ferromagnet whose current theoretical picture is that of a diluted magnetic system ordered via delocalized extrinsic carriers which populate spin-polarized Cr-induced levels near or within the host conduction band edge. The foremost ingredient of a theoretical discussion of magnetic coupling is an accurate description of the location of Cr-induced states relative to the bulk bands edges, whose description should of course be also accurate. These predictions are a weak and often contentious point in ab initio density-functional theory defects calculations, especially those based on semilocal functionals such as the local and gradient-corrected approximations, which underestimate the fundamental gap and may misplace the extrinsic levels within the host band structure. The picture hinted to above, indeed, was obtained on the basis of density functional-theory calculations supplemented with empirical non-local external potentials (NLEP) combined with "+U" corrections on In and Cr d-states to correct ad hoc the gap underestimate. In this paper we reconsider magnetism in Cr-doped In_2O_3 using a DFT-based theoretical approach at the cutting edge among those aimed at improving over semilocal functionals, namely hybrid density functionals. The results (for isolated Cr, as well as in combination with Sn or the oxygen vacancy) suggest that significant changes may be needed in the current picture. Spin-polarized Cr-related states turn out to be inaccessible to doping, essentially barring magnetic coupling in the form previously envisaged. As an alternative we propose that Cr-V complexes may provide an electronic structure conducive to magnetic coupling. This mechanism has the additional merit of matching the overwhelming experimental indications that ferromagnetism is invariably achieved in O-deficient conditions.

#132 - Graphene plasma-wave Terahertz photodetectors and Graphene-GaAs hybrid systems

Davide Spirito (I) – NEST, CNR - Istituto Nanoscienze e Scuola Normale Superiore, Pisa

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In this talk, I will first present some recent experimental results [1] on efficient Terahertz (THz) detection via antenna-coupled single-layer and bilayer graphene field-effect transistors (FETs). These first devices operate at room temperature and at 0.3 THz and can be used in a realistic setting, enabling large area, fast imaging of macroscopic samples. I will then discuss the main mechanism of photodetection which is exploited by the FETs in Ref. [1], i.e. the non-linear response of the two-dimensional (2D) massless Dirac fermion (MDF) fluid in the FET channel to the oscillating radiation field at the gate electrode. In the second part of the talk I will concentrate on a new hybrid double-layer fluid composed by an ordinary two-dimensional electron gas (2DEG) hosted in a GaAs heterostructure and by a graphene sheet placed on the surface of the semiconductor in close proximity to the 2DEG [2]. I'll present our ongoing efforts directed to the observation of inter-layer interaction effects via Coulomb drag experiments [3].

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#133 - Fundamental properties of Dirac plasmons in graphene

Marco Polini (I) - NEST, CNR - Istituto Nanoscienze e Scuola Normale Superiore, Pisa

In this talk I will review recent progress in the rapidly evolving field of `graphene plasmonics'. In particular, I will focus on the fundamental properties of Dirac plasmons in a doped graphene sheet, highlighting the subtle differences with plasmons in ordinary two-dimensional electron liquids.

#134 - Illuminating graphene nanosystems

Elisa Molinari (I) - University of Modena and Reggio Emilia e CNR - Istituto Nanoscienze, Modena

I will present the striking properties of graphene-based nanosystems, where the extended π–electrons of graphene can coexist with a band gap, controlled quantum states and excitations [1], and peculiar width- and edge-related phenomena [2].
Radically new electronic and optical functionalities –beyond those expected both for extended graphene and for conventional semiconductors-, are designed for these systems by ab-initio approaches within many body perturbation theory, and are now observed in a new class of atomically controlled nanoribbons [3].
I will discuss the perspectives in terms of new physical phenomena and nanodevices.

Work performed in collaboration with Andrea Ferretti, Deborah Prezzi, Alice Ruini, Daniele Varsano, and Shudong Wang.

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#135 - Transfer-free electrical insulation of epitaxial graphene from its metal substrate

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A proven route to large-scale, single-layer graphene is the epitaxial growth on transition metal surfaces; however, in contrast to epitaxial graphene on SiC, this has the disadvantage of a conductive substrate, which renders the conduction through graphene irrelevant. Then, exploiting the electronic properties requires graphene to be placed on an insulating substrate, such as SiO_2. We have demonstrated a transfer-free method to electrically insulate such epitaxial graphene from the metal it is grown on. We showed that, by a stepwise intercalation of Si and oxygen [1], it is possible to synthesize in situ a thin layer of SiO_2 which electrically decouples graphene from the substrate [2,3]. We have followed the reaction steps by high resolution core level photoemission spectroscopy and demonstrated the electrical insulation using a nanoscale multipoint probe technique.
By exposing epitaxial graphene on Ru(0001) to a flux of Si at 720 K we obtained that all the Si atoms intercalate and form a Ru silicide layer. Intercalation of oxygen at T = 630 K rapidly oxidizes the silicide producing a thin SiO_2 layer over an oxygen covered Ru surface. By following the entire process by fast-XPS measurements we established that graphene does not react with O_2 [4] and that during the decomposition of the Ru silicide oxygen binds exclusively to Si. Lateral transport measurement on the surface, using

a microscopic 12 point probe indicated that the transport is two-dimensional and is dominated by graphene. The demonstrated process to insulate graphene from the metallic substrate it is grown on relies on the tendency of almost any adsorbate to intercalate under the graphene layer that can be exploited to promote the chemical synthesis of materials below graphene. This proven concept opens many design options and might thus have wide application in graphene research and device fabrication.

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#136 - Hydrogen absorption in alkali metal fullerides

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Hydrogen storage in carbon based material is a very promising area of research, due to the light weight and large surface areas of carbon. Some theoretical works shows that metal-decorated C_{60} can absorb hydrogen up to 9.5 wt% [1,2]. Recently, the reversible hydrogen absorption in $Na_{10}C_{60}$ [3] and Li_xC_{60} [4] systems was experimentally evidenced. Highly doped alkali metal intercalated fullerides M_xC_{60} (M=Li, Na) were synthesized via solid state reaction or chemical intercalation of pure metal dissolved in liquid-ammonia. The as synthesized samples were then treated in 100-200 bar of H_2/D_2 pressure at temperatures up to 350°C to obtain the metal intercalated hydrofulleride. The characterization was carried out by in-situ neutron diffraction, X-ray diffraction (XRD), Muon Spin Resonance (µSR) and Inelastic Neutron Scattering (INS). In-situ neutron diffraction (100 bar of D_2) shows that M_xC_{60} reacts with hydrogen at 200°C, forming a fcc metal intercalated hydrofulleride and partially segregating metal hydride.
Absorption measurements shows that $Na_{10}C_{60}$ can reversibly absorb up to 3.5 wt% of H_2 at 200°C and 200 bar. During the hydrogenation Na de-intercalates and forms NaH [3]. The desorption starts at 250°C, which is considerably lower than the temperature needed for the decomposition of NaH (~ 800°C), and at the end all the Na atoms re-intercalate in the $Na_{10}C_{60}$. In comparison, $Li_{12} C_{60}$ and $Li_6 C_{60}$ can absorb, following similar mechanism, up to 4.5 and 5 wt% H_2 respectively. Inelastic Neutron Scattering on the hydrogenated samples shows the formation of C-H bending mode on C_{60} molecule. µSR investigation showed the formation of a radical state on the C_{60} anion. This radical (hydrogen bonded to C_{60}) is observed at 300 K (in both hydrogenated and non-hydrogenated sample) and its stability increases lowering the temperature, suggesting that hydrogenation could occur at low temperature if hydrogen was atomic [5].

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#137 - Graphene oxide as a convenient platform for nanotechnology and sensing applications

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Graphene oxide (GO), a chemical derivative of graphene obtained from graphite in the presence of strong acids and oxidants, is attracting today great interest as a versatile, low cost, large scale production platform for a wide range of technological applications, in many cases complementary to those where graphene is used. Here we illustrate our contribution to the study of the physical properties that make GO one of the most convincing next generation materials for nanotechnology and sensing applications.
Oxidation degree is the crucial parameter determining the physical properties of GO. A systematical study of this parameter is reported in [1], where data from X-ray photoemission spectroscopy, Raman spectroscopy, and color contrast analysis are correlated. The oxygen functional groups – whose surface density defines the oxidation degree – are used by GO to communicate with everything reaches its surface. In this work we report on the role of these groups as active sites in gas molecules detection and as scattering sites under exposure to extreme-ultraviolet (EUV) light. On the one hand, a practical, high-sensitivity, and easy to fabricate gas sensor based – for the first time – on pristine GO has been demonstrated outperforming the category of practical devices based on reduced GO [2]. On the other hand, EUV induced GO photo-reduction has been studied in the 1 – 60 nm wavelength range encouraging new strategies for both graphene nano-patterning and EUV light detection (preliminary results are reported in [3]). Our GO has been prepared via a modified Hummers method [4] starting from graphite flakes of 500 μm maximum size. Monolayers with ~ 30 μm average size (about two orders of magnitude higher than for commercial GO) and 1.1 ± 0.1 nm thickness [5] have been obtained and dispersed in water for eventual deposition. GO for gas sensing experiments has been drop-casted on standard 30 μm spaced inter-digitated Pt electrodes and tested with several gases; in particular, 20 ppb detection limit has been measured in the case of NO_2, that is the lowest detection limit ever measured for this gas with practical graphene-based sensors. The GO photo-reduction experiments have been performed exposing multi-layer GO films (~ 10 nm mean thickness) to different doses of 59 nm, 27.5 nm, and 1.97 nm wavelength radiation; the rate of de-oxygenation has been demonstrated to be proportional to the photo-absorption probability.

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#138 - Novel mismatched graphene-ferromagnetic interfaces

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The low-energy excitations in graphene depend on the interaction strength with the metal that serves as support [1, 2]. By varying the support itself or by intercalation of foreign atoms it is possible, through electron hybridization and structural modifications, to tailor graphene electronic properties [3]. Variable interaction strengths can thus provide an additional control over the properties of graphene and may open new fields of applications.

We will present the structural and electronic properties of novel mismatched systems obtained by intercalation of one-single ferromagnetic (FM=Ni, Co) layer on graphene/Ir(111). Upon intercalation the FM lattice is resized to match the Ir-Ir lattice parameter, resulting in a mismatched graphene/FM/Ir(111) system [4, 5]. By performing scanning tunneling microscopy measurements and density functional theory calculations we prove that the intercalated Ni layer strongly increases the local interaction for specific adsorption sites and induces a strong rumpling of the graphene film. Angle-resolved photoemission spectroscopy studies on graphene/FM/Ir(111) systems show a clear transition from nearly-free-standing to strongly-hybridized character of the graphene film. Finally, the implications of these results and their potential applications for graphene based devices will be discussed.

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#139 - Emergence of criticality in living systems

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In physical systems, critical phenomena are observed on fine-tuning parameters. For example, at the liquid vapor critical point, one must tune the pressure and temperature to their critical values to observe droplets of water and bubbles of gas of all sizes thoroughly interspersed among each other. Scale free behavior characterized by power laws is found at critical points.

In recent years, evidence has been mounting that biological systems (or parts, aspects or groups of them) seem to operate at the vicinity of critical points. Examples include spontaneous brain activity, gene expression patterns, cell growth, bacterial clustering, and flock dynamics. In some cases, theoretical models have suggested that such critical-like behavior leads to optimal computational capabilities, optimal transmission and storage of information, and maximal sensitivity to sensory stimuli. Nevertheless, a general mathematical framework providing deep theoretical principles behind the common behavior of these diverse systems and explaining the origin of criticality in living adaptive systems is still lacking.

We will present a mathematical framework, rooted in statistical physics and information theory, revealing a link between the emergence of criticality in biological systems and related evolutionary advantages.

#140 - Long-range interactions: results and perspectives

Stefano Ruffo (I) -Dipartimento di Fisica e Astronomia, Università di Firenze

Systems with long-range interactions, like self-gravitating systems, charged and dipolar systems, etc. can be made extensive, but are intrinsically non additive [1]. The violation of this basic property of thermodynamics is the origin of ensemble inequivalence, which in turn implies that specific heat can be negative in the microcanonical ensemble, temperature jumps can appear at microcanonical first order phase transitions, ergodicity may be broken. Realizing that such features may be present for a wide class of systems has renewed the interest in long-range interactions [2]. In this seminar, I will present a review of the recent advances on the statistical mechanics and out-of-equilibrium dynamics of systems with long-range interactions.

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#141 - Nonlinear relaxation and environmental noise in biological systems

Bernardo Spagnolo (I) - Dipartimento di Fisica e Chimica, Università di Palermo

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The interplay between environmental noise sources and nonlinearity in three different biological systems is investigated. (i) A Verhulst model perturbed by arbitrary multiplicative Lévy noise is considered as a first biological system. For Cauchy stable noise, exact results for the probability distribution of the population density and nonlinear relaxation are derived. We find a transition induced by the multiplicative Lévy noise, from a trimodal probability distribution to a bimodal probability distribution in asymptotics, and a nonmonotonic behavior of the nonlinear relaxation time as a function of the Cauchy stable noise intensity. (ii) The noise driven translocation of short polymers in crowded solutions and driven by an oscillating force is analyzed as a second biological system. The dynamics is numerically investigated by solving a Langevin equation in a two-dimensional domain. We consider a phenomenological cubic potential with a metastable state to model the polymer-pore interaction and the entropic free energy barrier characterizing the translocation process. The mean first translocation time of the center of inertia of polymers shows a nonmonotonic behavior, with a minimum, as a function of the number of the monomers. Moreover, the translocation time shows a minimum as a function of the frequency of the oscillating forcing field for all the polymer lengths investigated. This finding represents the evidence of the resonant activation phenomenon in the dynamics of polymer translocation, whose occurrence is maintained for different values of the noise intensity. (iii) The phenomena of dissonance and consonance in a simple auditory sensory model composed of three neurons are considered. Two of them, here so-called sensory neurons, are driven by noise and subthreshold periodic signals with different ratio of frequencies, and its outputs plus noise are applied synaptically to a third neuron, so-called interneuron. We propose a theoretical analysis with a probabilistic approach to investigate the interspike intervals (ISI) statistics of the spike train generated by the interneuron. We find that at the output of the interneuron, inharmonious signals give rise to blurry spike trains, while the harmonious signals produce more regular, less noisy, spike trains. The regularity is introduced as the quantity linearly connected with informational entropy. We show that consonant chords influencing the auditory system produce regular spike trains (low entropy) at the systems output, in contrast to dissonant chords, which result in irregular spike trains (high entropy). Theoretical results are compared with numerical simulations.

#142 - Non-Markovian models of blocking in concurrent and countercurrent flows

Andrea Gabrielli – CNR - Istituto dei Sistemi Complessi, Roma

Julian Talbot , Pascal Viot (Laboratoire de Physique Theorique de la Matiere Condensee (LPTMC), Universite' "Pierre et Marie Curie", Paris, France)

We investigate models in which blocking can interrupt a particulate flow process at any time. Filtration, and flow in micro or nanochannels and traffic flow are examples of such processes. We first consider concurrent flow models where particles enter a channel randomly. If at any time two particles are simultaneously present in the channel, failure occurs. The key quantities are the survival probability and the distribution of the number of particles that pass before failure. We then consider a counterflow model with two opposing Poisson streams. There is no restriction on the number of particles passing in the same direction, but blockage occurs if, at any time, two opposing particles are simultaneously present in the passage.

#143 - Dynamics of a driven dissipative quantum system

Luca Magazzù - Dipartimento di Fisica e Chimica, Università di Palermo

Davide Valenti, Bernardo Spagnolo (Dipartimento di Fisica e Chimica, Università di Palermo), Giuseppe Falci (Dipartimento di Fisica e Astronomia, Università di Catania)

We investigate the dynamics of a driven multilevel system, consisting of a particle in an asymmetric bistable potential, strongly interacting with a thermal bath according to the Caldeira-Leggett model. The populations in the discrete (position) variable representation (DVR), are obtained as solution of a Markovian approximated master equation, which is derived from a discretized path integral approach based on the Feynman-Vernon influence functional.
 By varying the environmental parameters (temperature and coupling strength) as well as the driving frequency and amplitude, we study the transient dynamics and stationary configuration of the system. In particular, we analyze the population of the metastable well. The asymptotic population of the metastable well displays a strong non-monotonicity, characterized by a maximum, as a function of the driving frequency. We find also that an increase of the coupling strength inhibits this effect of induced stability and slows down the dynamics, forcing the system towards the relaxation.

#144 - Large-deviations and condensation of fluctuations in equilibrium and off-equilibrium systems

Federico Corberi - Università di Salerno

G. Gonnella , A. Piscitelli (Universita' di Bari), M.Zannetti (Universita' di Salerno)

We present the exact calculation of the large deviation function of the spontaneous fluctuations of macroscopic observables (such as energy, exchanged heat etc...) in the equilibrium or non-equilibrium regime of classical systems described by solvable models of Statistical Mechanics. We show the existence of singularities in the distributions which in some cases may be attributed to a phenomenon of condensation of fluctuations resembling the Bose-Einstein condensation. We discuss the generality of such a behavior.

#145 - Coupled particle and heat transport: a dynamical system's perspective

Giuliano Benenti - Università degli Studi dell'Insubria, Como

The understanding of coupled particle and heat transport in complex systems is a fundamental problem, also of practical interest in connection with the challenging task of developing high-performance thermoelectric materials. We will discuss thermoelectric transport phenomena from the perspective of dynamical nonlinear systems, focusing on stylized classical and quantum models, including the disordered hard-point gas and asymmetric quantum-dot ring structures pierced by an Aharonov-Bohm flux. We will show that neither energy filtering nor strong coupling between particle and energy fluxes are necessary conditions for achieving the Carnot efficiency. In particular, we will discuss a mechanism for increasing the thermoelectric figure of merit in interacting systems with a single relevant constant of motion, typically in momentum-conserving systems. We will then focus on systems with broken time-reversal symmetry, for which the maximum efficiency and the efficiency at maximum power are both determined by two parameters: a "figure of merit" and an asymmetry parameter. In contrast to the time-symmetric case, the figure of merit is bounded from above; nevertheless the Carnot efficiency can be reached at lower and lower values of the figure of merit and far from the strong coupling condition as the asymmetry parameter increases.

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#146 - Amyloid-beta peptides from oligomers to fibrils: laser light, x-ray and neutron pictures

Laura Cantù (I) – Dipartimento di Biotecnologie Mediche e Medicina Traslazionale, Università di Milano

Elena Del Favero, Paola Brocca, Simana Motta, Valeria Rondelli (Università di Milano)

A hallmark pathological feature of Alzheimer's disease (AD) is aggregation and deposition of β-amyloid peptides (Aβ) in the brain. Recently we found an Aβ mutation at position two (A2V), associated with a very aggressive form of disease in homozygous carriers and resulting in enhanced fibril formation in vitro. Co-incubation of wild type Aβ with A2V mutant or even with 6-mer Aβ 1-6(A2V) inhibits amyloid formation. Understanding the structural organization of amyloid assemblies, formed by different forms of Aβ peptides alone and mixed is necessary for revealing the molecular mechanisms underlying the pathology and for providing insights towards developing possible therapeutics for AD. We performed laser light scattering measurements on different Aβ peptides to follow short time aggregation process in oligomers and SANS and SAXS experiments on aligned fibers. Aβ WT and Aβ A2V assemblies on all time scales differed in shape and stability, suggesting distinct packing of lateral units for these two peptides. Mixing of the two species showed a decoupling between aggregate elongation and aggregate stability.

#147 - Ultrafast force-clamp laser trapping of single molecular motors and DNA binding proteins

Marco Capitanio (I) - Università degli Studi di Firenze

Carina Monico (LENS-European Laboratory for Non-linear Spectroscopy, Sesto Fiorentino), Francesco Vanzi (LENS, Sesto Fiorentino e Dipartimento di Biologia, Università di Firenze), Francesco Saverio Pavone (LENS, Sesto Fiorentino e Dipartimento di Fisica ed Astronomia, Università di Firenze)

Force plays a fundamental role in a wide array of biological processes. For example, it modulates enzymatic activity, induces structural changes in proteins and nucleic acids, alters molecular bond kinetics, regulates motion of molecular motors, and plays a role in mechanical transduction and sensory functions. At the molecular level, these processes are ultimately related to the capability of force to modulate lifetimes of molecular interactions and transition rates in biochemical reaction cycles that involve motion. Single-molecule force spectroscopy techniques such as atomic force microscopy, optical and magnetic tweezers have opened up the possibility to study such fundamental processes at the molecular level. Protocols for single-molecule force spectroscopy have been devised for the study of stable and long-lived bonds between two molecules. When a molecular bond is weak, however, the unbinding kinetics becomes rapid and application of such protocols during the short lifetime of the molecular complex becomes challenging.

We developed an ultrafast force-clamp spectroscopy technique that uses a dual trap configuration to apply constant loads between a single intermittently interacting biological polymer and a binding protein. Our system displays a delay of only ~10 μs between formation of the molecular bond and application of the force and is capable of detecting interactions as short as 100 μs. The force-clamp configuration in which our assay operates allows direct measurements of the load-dependence of single molecular bond lifetimes. Moreover, conformational changes of single proteins and molecular motors can be recorded with sub-nanometer accuracy and a temporal resolution in the tens of microseconds.

#148 - Molecular dynamics and docking of fatty acids interacting with beta-lactoglobulin

Rita Guzzi – Dipartimento di Fisica, Università della Calabria, Unità CNISM

Stefania Evoli (Dipartimento di Fisica, Università della Calabria e CNR-IPCF, UOS di Cosenza, LICRYL e CEMIF.CAL, 87036 Rende (CS)), Rita Guzzi (Dipartimento di Fisica, Università della Calabria, Università della Calabria, Unità CNISM di Cosenza), Bruno Rizzuti (CNR-IPCF, UOS di Cosenza, LICRYL e CEMIF.CAL, 87036 Rende (CS))

Beta-lactoglobulin is the most abundant protein in cow milk, widely studied for its application in food technology. It binds and transports fatty acids of different length and several other ligands. The protein barrel has an open end with a conical shape forming a calyx, which constitutes the primary binding site for hydrophobic molecules. Other binding sites on the external surface have been hypothesized for fatty acids, but their location is debated.

In this work, molecular dynamics simulations have been used to investigate the dynamics of saturated fatty acids of different length (8-18 carbon atoms) in the protein calyx. The results indicate that atomic fluctuations in the protein are enhanced when ligands are bound, compared to the apo form. The anchoring of each fatty acid at the entrance of the binding site is provided by electrostatic interactions of the lipid head-group with Lys69 and Lys60 side chains. Interestingly, only the two fatty acids with the longest chain (i.e., palmitic and stearic acid), which experimentally have the highest affinity, are found in a fully extended conformation in simulation.

By combining molecular docking and dynamics simulations, two additional secondary binding sites have been identified for palmitic acid when the main site is already saturated. One is located in between a helical turn and a β-strand and consists in a small hydrophobic cavity in which the fatty acid molecule partially penetrates, either head-first or tail-first. The other one is located in between the α-helix and another β-strand and consists in a superficial crevice in which the fatty acid lies in an almost extended conformation. The location and properties of these two additional binding sites are discussed in connection with positions proposed in the literature.

#149 - Potassium channel Kcv interaction with model membranes

Paola Brocca – Università degli Studi di Milano

Monica Romanò, Elena Del Favero, Simona Motta, Valeria Rondelli, Anna Moroni , Laura Cantù (Università degli Studi di Milano)

K+- channels are transmembrane proteins abundant in virtually all biological systems [1]. Although these have been subject to intense experimental and theoretical investigation, basic relationships between their structure and their function are not understood sufficiently.

We are currently work on a viral K+- channel, Kcv [2], which is the smallest potassium channel known to be expressed naturally in a eukaryotic cell. A single Kcv subunit is composed of 94 amino acids that encode a short N-terminal helix and two transmembrane segments that are bridged by a pore forming region that contains the hallmark potassium channel selectivity filter. As with many other potassium channels, Kcv forms tetramers.

A particularly important feature of a membrane protein is the thickness of its hydrophobic, membrane-spanning region. The cost of exposing hydrophobic fatty acyl chains or peptide residues to water is such that the thickness of the hydrophobic region of the peptide should match the hydrophobic thickness of the bilayer. Hydrophobic mismatch between a protein and a lipid bilayer could be compensated for in a number of ways: the lipid bilayer around a protein could either thicken or thin to match the hydrophobic thickness of the protein, in a mixed bilayer the presence of the transmembrane protein can induce lateral segregation. Biochemical and functional evidence indicate that K+- channels, in addition to other ion channels, localize to lipid raft microdomains on the cell surface and that changes in membrane cholesterol can directly modulate ion channel function.

We present spectroscopic data revealing the structural changes induced by the presence of the transmembrane protein, on model biomimetic membranes as a function of membrane composition. Particular focus is given to mimic specialized membrane microdomains, lipid raft, composition and their typical asymmetry in the two leaflets.

WAXS measurements confirm that the protein insertion affects the average local order of the hydrophobic chains, so altering the membrane lipid chain arrangement over a wide surface area, likewise shifting the thermotropic behavior of the bilayer. This was expected and is confirmed by DSC. Moreover, at the bilayer scale (SAXS) it is seen that the channel arrangement 'match' the gel $P_{\beta'}$ geometry. Significant results from neutron reflectivity on single floating bilayer will be presented.

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#150 - Connection between covalent and physical interactions in cyclodextrin-based hydrogel as studied by vibrational spectroscopy

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Over the past years, great effort has been devoted in the physical-chemical research to the development of novel functional systems for effective molecular encapsulation and delivery of active compounds. These materials find important uses for advanced therapeutic methodologies in fast-growing technological fields, like drug delivery, tissue engineering and regenerative medicine. In this framework, cyclodextrin nanosponges (CDNS) are a very promising class of nanoporous soft materials which can swell in aqueous solution giving rise to an interesting gel-like behaviour, similarly to hydrogel. These polymeric networks are capable of encapsulating, carrying and releasing a variety of both lipophilic and hydrophilic compounds by forming with them non-covalent complexes.

In spite of these promising applications, several factors like the random nature of the growing process of the polymer, the presence of a large number of reaction sites on each monomeric unit, and the nature of the polymerization process yielding a large variety of amorphous systems, hampered a systematic structural and dynamic characterization of CDNS.

Here we present a detailed inspection of the vibrational dynamics of CDNS, in dry and hydrated state, performed by combining Raman and infrared spectroscopy and numerical simulations, with the aim to give a deep structural and dynamic characterization at molecular level of these innovative cyclodextrin-based materials. In particular, the analysis of the spectral features of some vibrational bands assigned to the vibration modes of specific chemical groups of the polymeric network is performed by using band deconvolution and fitting procedure. These data handling allows to in deep explore the state of the water molecules confined in the nano-pores of CDNS, the water-polymer interactions and the intra- and intermolecular hydrogen-bond network established in hydrogel. Starting from these experimental data, we propose a comprehensive model of the connection between covalent and physical interactions which determine the swelling behaviour and the mechanical properties of CDNS-hydrogel, i.e. the capacity of retaining water and the rigidity of the hydrogel network.

#151 - Dynamical stability of ovalbumin can provide insights into the molecular basis of serpinopathies

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Serpins are a class of proteins with large structural similarity playing a key role in proteolytic cascades by inhibiting the enzymatic action of serin proteases. The mechanism by which the inhibition occurs relies on the capture of the enzyme upon cleavage by a reactive loop, followed by a huge translocation of the molecule that definitely inactivates the enzyme and directs the complex for further degradation. Mutations or modifications in relevant serpins, such as neuroserpin or α1-antitrypsin, can induce the onset of severe, life threatening pathologies.

To address the molecular basis of serpinopathies, a reference protein belonging to that class, chicken egg albumin (ovalbumin), was studied by a synergistic approach integrating molecular dynamics and coarse grain simulations with single molecule force spectroscopy experiments. A central disulfide bond that blocks the main fold of ovalbumin was addressed, showing that its reduction, while not altering the three-dimensional structure, induces a relevant chenge in the dynamical stability. This effect, putatively associated to the presence of long range interactions inside the protein, seems to be peculiar of serpins and it could provide relevant insights into the molecular basis of serpinopathies.

#152 - Monitoring the structural order of peptides and proteins in supramolecular assemblies by FTIR spectroscopy

Antonino Natalello – Università Milano - Bicocca

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Ordered supramolecular structures of peptides and proteins are receiving great interest not only for their role in amyloid diseases but also for their possible use in the building of new scaffolds for tissue engineering applications. Here, we will present the formation of these assemblies starting from several model peptides differing for single amino acid substitutions that are responsible for their aggregation propensity and structural properties of the final aggregates[1, 2]. The assembling and disassembling processes has been studied by Fourier transform infrared (FTIR) spectroscopy thanks to the specific infrared response due to the formation of intermolecular β-sheet structures (1630-1620 cm^{-1})[3, 4]. Interestingly, this approach enables also to detect the overall structural order involving the peptide backbone NH groups in the 3300-3100 cm^{-1} spectral range, where the presence of an intense and narrow band can be taken as a marker of a high structural order in the assembled scaffold. This FTIR study allowed to characterize the aggregation propensity and kinetics and the stability of the final supramolecular structures, offering useful information to understand the role of specific amino acid substitutions on the peptide self-assembling process. In particular, highly efficient assembling was found for amino acid substitutions involving aromatic interactions, increased hydrophobicity, and polar residues substituted by Ala. The FTIR results were in agreement with the atomic force microscopy, X-ray diffraction, and rheological characterizations of the self-assembling peptides [1]. Moreover, the scaffold were found cytocompatible and, therefore, potentially useful in tissue engineering [1].
Interestingly, during amyloid protein aggregation the appearance of narrow bands due to the absorption of amino acid side chains can be also exploit to monitor the structure reorganization and stability of the fibrils, as reported in the case of the Ataxin-3 polyglutamine tract [4].

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#153 - Nanoparticles systems for gene delivery interacting with model cell membranes: a structural study

Simona Motta - Università degli Studi di Milano

Paola Brocca, Valeria Rondelli, Laura Cantù , Elena del Favero (Università degli Studi di Milano)

Gene therapy, the delivery of exogenous genes to the nucleus of target cells, is a very interesting approach for the treatment of genetic diseases and cancer [1]. For this purpose, reliable and efficient vectors are needed.
In the last years an increasing interest has been addressed to non-viral Nanoparticle Systems (NS) in which a plasmid DNA core is condensed with protamine sulphate [2], a cell penetrating polypeptide that protects DNA from degradation. In our study, such a core is complexed with highly-fusogenic multicomponent (DOTAP, DOPC, Dc-Cholesterol and DOPE) liposomes that have intrinsic endosomal rupture properties. By different spectroscopic technique we have characterized those systems. We have studied the structure of the protamine/DNA core depending on the length of the used DNA sequence. When DNA shorter that 2000 bp is complexed by protamine, a compact core of hundred nanometer size with surface fractal properties is obtained, while, for longer DNA, a mass fractal aggregate of larger size is seen [3]. This features affect the coverage by the lipid components. The NS systems are shown to consists in core-shell particles frequently bearing a single layer lipid coverage lying on the protamine/DNA core. Interestingly, SAXS and neutron reflectivity experiments have shown that NS are not prone to exchange their lipid component with some admixed membranes. We have obtained the opposite result using lipolexes nanovectors, nanosystems composed by the same lipid component of NS directly complexed with DNA without previous condensation with protamine. In particular, SAXS measurements have shown a progressive depletion in the lipoplexes multilayer structure during the interaction with anionic model membranes. Structural features of the NS and of lipoplexes, as they are and interacting with model cell membranes, is an aspect not yet deeply studied but of major importance. In fact the lipid component of the complexes and their structure are the key parameters in the interaction with cell membranes and for the improvement of transfection efficiency.

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#154 - Spin dynamics in molecular nanomagnets

Stefano Carretta (I) - Università degli Studi di Parma

Molecular nanomagnets (MNMs) are molecules containing a core of magnetic ions whose spins are strongly coupled by superexchange interactions. They form crystals which behave like ensembles of identical and almost non-interacting magnetic units. Being among the first examples of finite-size spin systems, MNMs have been test beds for addressing several quantum phenomena. In particular, one of the major current objectives is to exploit their coherent spin dynamics for quantum information processing. Indeed, for short-enough timescales the spin wavefunctions of MNMs evolve coherently according to an appropriate spin Hamiltonian, which can be engineered to meet specific requirements. Unfortunately, so far it has been impossible to determine these spin dynamics directly.

In this talk we show that recently developed instrumentation yields the four-dimensional inelastic-neutron scattering function in vast portions of reciprocal space and enables the spin dynamics to be determined directly [1]. We use the Cr8 antiferromagnetic ring as a benchmark to demonstrate the potential of this approach which allows us, for example, to examine how quantum fluctuations propagate along the ring or to test the degree of validity of the Néel-vector-tunnelling framework.

From a purely theoretical point of view we show that parameters of the spin Hamiltonian can be reliably calculated ab-initio. In particular, we present a flexible and effective ab-initio scheme to build many-body models for MNMs, and to calculate magnetic exchange couplings and zero-field splittings. It is based on the use of localized Foster-Boys orbitals as one-electron basis [2]. We have applied this scheme to three paradigmatic systems, the antiferromagnetic rings Cr_8 and Cr_7Ni and the single molecule magnet Fe4. In all cases we have identified the essential magnetic interactions and have found excellent agreement with experimental results.

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#155 - Spin coupling and charge transfer at molecule/metal interfaces

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Metal-organic complexes provide a variety of charge and spin states that can be used to tailor the conductance of single-molecule as well as multilayer electronic devices. Key to achieving this control is understanding how the molecular spin couples to electrons inside and outside a molecule. Here, we will discuss the competition between electron correlation, hybridization, and extrinsic doping effects for metal-organic complexes adsorbed on metals [1,2]. By combining scanning tunnelling spectroscopy and x-ray magnetic circular dichroism measurements, we argue that metal-organic adsorbates should be generally considered as strongly-correlated electron systems with either pure valence [3] or mixed-valence [4] behavior. Examples of phthalocyanine molecules with strong, weak, and zero mixed-valence character will be presented, leading to a consistent description of the magnetic moment and Kondo behavior of metal-organic adsorbates. We will further reveal the nature and efficacy of different charge transfer channels by individual manipulation of electron donor atoms, showing how the interplay of charge, spin, and vibrational degrees of freedom determines the site-specific magnetic moment and electrical conductance of molecular systems [5]. Finally, we will show that ligand-mediated superexchange between single molecule magnets (SMM) and a magnetic substrate can be used to stabilize the SMM magnetic moment at high temperature [6] and induce exchange bias [7].

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#156 - Very high-quality entanglement transfer through long uninform spin chains

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The ability to transmit quantum states and entanglement through quantum channels is one of the key tools for processing quantum information. Different solutions have been proposed to accomplish such a challenging task, which, however, require either an ad hoc engineering of the internal interactions of the physical system acting as the channel or specific initialization procedures.

We show that high-quality quantum-state and entanglement transfer can still be achieved in an unmodulated spin bus by letting it operate in the ballistic regime, occurring when only the extremal bond, or the two extremal bonds, at each end of the chain are allowed to be different from the intrachain exchange. We devise a general procedure to determine the optimal values of such extremal bonds interaction constants, which result smaller but comparable to the intrachain exchange. The quality of quantum transmission is only weakly affected by the chain length and it maintains very high even in the limit of arbitrarily long channels, being also almost independent of the channel initialization. The spin-1/2 XY chain has been thoroughly investigated when only one extremal bond at each end is different from the bulk ones, getting explicit results for the time evolution of different quantities characterizing the quality of quantum-state and entanglement transfer: for instance, the average quantum-state transmission fidelity

exceeds 90 % for any chain length. When two different bonds at each end are allowed to be adjusted, the fidelity of state transfer for the XX spin chain, and related fermion or boson hopping models, reaches values higher than 99 % for arbitrary chain lenghts. The high quality of transmission extends to quantities, e.g. magnetization, which may encode classical information, so that spin chains operating in ballistic regime can also be considered as possible alternatives to conventional transmission channels when power dissipation, and consequential heating of devices, represents a relevant issue.

#157 - Graphene-mediated exchange coupling between cobaltocene and magnetic substrates

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Using first-principles calculations we demonstrate sizable exchange coupling between a magnetic molecule and a magnetic substrate via a graphene layer. As a model system we consider cobal- tocene ($CoCp_2$) adsorbed on graphene deposited on Ni(111). We find that the magnetic coupling between the molecule and the substrate is antiferromagnetic and varies considerably depending on the molecule structure, the adsorption geometry, and the stacking of graphene on Ni(111). We show how this coupling can be tuned by intercalating a magnetic monolayer, e.g. Fe or Co, between graphene and Ni(111). We identify the leading mechanism responsible for the coupling to be the spatial and energy matching of the frontier orbitals of $CoCp_2$ and graphene close to the Fermi level, and we demonstrate the role of graphene as an electronic decoupling layer, yet allowing spin communication between molecule and substrate.

#158 - Micromagnetic analysis of demagnetization processes in exchange-coupled hard/soft bilayers with surface anisotropy

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A previously developed micromagnetic continuum model [1-3] for the study of demagnetization processes in exchange-coupled bi- and multi-layers of hard/soft type, with planar and perpendicular anisotropy, has been extended to take into account the effects of surface anisotropy in the soft layer, for fields applied along the easy direction.
In particular, we have studied in details the case of positive surface anisotropy and strong interface ferromagnetic coupling. Due to high anisotropy of the hard layer and strong coupling of the soft layer with the hard one, the interface anisotropies and the hard layer surface anisotropy can be neglected. The theoretical results have been applied to a bi-layer with perpendicular anisotropy in the hard layer, while the soft layer has been assumed to be ideal, that is, with shape anisotropy but zero volume anisotropy ($K_1= 0$), in order to clearly evidence the contribution of its surface anisotropy.
Moreover, we have only considered soft layer thickness t_1 and/or surface anisotropy K_{s1} values for which the nucleation field (the field at which the magnetization starts to deviate from saturated state) lies between the effective anisotropy fields of the two hard and soft materials. We have deduced the nucleation field equation and obtained plots of the nucleation field as a function of the soft layer thickness and of the soft surface anisotropy.
Demagnetization curves have been calculated both for K_{s1}/t_1=0 and $K_{s1}/t_1 \neq 0$, also considering the case in which the surface anisotropy is replaced by a corresponding soft volume anisotropy $K_1=K_{s1}/t_1$.
The nucleation process can be reversible (exchange-spring, ES regime) or irreversible (Rigid magnet, RM regime) depending on magnetic and geometrical parameters. The critical equation, which allows determining the boundary between RM and ES regions, has been deduced. Corresponding phase diagrams in the plane of soft (t_1) and hard (t_2) layer thickness have been obtained as a function of soft surface anisotropy K_{s1}.
The main conclusion of the above analysis is that concerning the comparison between the soft surface anisotropy K_{s1} and the corresponding soft volume anisotropy K_{s1}/t_1 in a typical exchange-coupled hard/soft system with perpendicular anisotropy, the results are almost equivalent.

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#159 - Local magnetic properties in Cr$_8$, Cr$_7$Cd and Cr$_7$Ni molecular rings from ^{19}F-NMR

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A detailed experimental investigation of the ^{19}F nuclear magnetic resonance (NMR) is made in the homometallic Cr_8 antiferromagnetic (AFM) molecular ring and in the heterometallic Cr_7Cd and Cr_7Ni rings at low temperature and as a function of the magnetic field. Since the F- ion is located midway between two magnetic metal ions in the ring, the ^{19}F-NMR spectra have a complicated field dependent structure, due to both isotropic transferred hyperfine contact interactions and anisotropic dipolar and

pseudo-dipolar interactions. In Cr_8 where the ground state is a singlet with total spin S=0 the ^{19}F -NMR spectra at T=1.6 K and low external magnetic field show a single narrow line, proving that the local spin density in the ground state is zero as expected for a molecular singlet state. By increasing the magnetic field towards the first level crossing field (Hc about 7 Tesla) a structure appears in the ^{19}F-NMR spectrum whose evolution as a function of temperature and external magnetic field proves that the thermal excitation to the first magnetic excited state generates a statistical distribution of molecules in the ground state and first excited state each with fixed values for the local moments at the Cr sites. This is a novel and unexpected result. On the other hand in Cr_7Cd and on Cr_7Ni the ground state is magnetic with a non uniform distribution of the local spin density [1]. This leads to a ^{19}F -NMR spectrum with a shifted line attributed to the ^{19}F nuclei that are located midway between a Cr_{3+} ion and a Cd_{2+} or Ni^{2+} ion, thus allowing the determination of the transferred hyperfine constant F^--Cr^{3+} and F^--Ni^{2+} for the specific site. The values of the hyperfine constants are compared to the ones known for F^--Mn^{2+} in $KMnF_3$and MnF2, for F--Ni$_{2+}$ in $KNiF_3$ and NiF_2 and for F^--Cr^{3+} in K_2NaCrF_6.

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#160 - Design of rare earth-free molecular clusters as cryogenic magnetic refrigerants

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Molecular nanomagnets (MNMs) represent an ideal playground to study interesting quantum phenomena and they're involved in many potential technological applications [1]. MNMs are now considered promising materials for ultra-low-T magnetic refrigeration, since they exhibit an enhanced magnetocaloric effect (MCE). Recent works on the MCE in MNMs involve clusters containing 4f ions or 3d–4f heterometallic complexes [2.] Since 4f elements are increasingly rare and expensive, the aim of our work is to provide a "recipe" to have an efficient molecular refrigerant containing 3d ions only. 3d ions in molecular clusters are often coupled by strong exchange interactions. Thus, the topology of these interactions plays a key role in optimizing the characteristics of the system associated with enhanced MCE. Our starting point is the Fe_{14}cluster [3], where the competition between many AF interactions and a negligible anisotropy provide an unusually large MCE. We first study the ideal cluster Ni_{14}, which has the same structure of Fe_{14} but a smaller Hilbert space. As a further step to understand the role of topology, we study different toy models representing the building blocks of the Fe_{14} magnetic core. We describe these systems by a Hamiltonian with only two exchange constants Js and no magnetic anisotropy, to understand the correlations between the energy spectrum and the MCE. Here we focus on a 5-sites cluster with a pattern of exchange interactions (a squared base pyramid) that can yield energy spectra optimal for MCE. To evaluate the performance of the system as a refrigerant we consider the Relative Cooling Power (RCP) [4] and the temperature T_{max} of the MCE peak. In fact, a cluster with high RCP and low T_{max} provides an efficient Carnot cycle at ultra-low-T. A large RCP guarantees that we can exploit all the available - ΔS for a wide temperature range. Hence, not only - ΔS but also the FWHM of the - $\Delta S(T)$ curve is crucial to have an efficient magnetic refrigerant.

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#161 - Complete magnetocaloric characterization of magnetic first order martensitic transformations

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The world's increasing energy need pushes the research to look for innovative energy conversion devices showing high efficiency and low environmental concerns. For this purpose the magnetocaloric effect (MCE) constitutes one of the most promising ways to follow.[1] The MCE is the consequence of the action of en external magnetic field on the state of a material. Changes of its entropy (Δs_T), temperature (ΔT_{ad}) as well as specific heat (cp) describe this effect, which is maximum across the magnetic phase transitions [2]. The relation between Δs_T, ΔT_{ad} and cp is not trivial, thus a reliable characterization of the thermomagnetic properties of the materials requires the measurement of at least two of the previous quantities [2]. The standard magnetocaloric characterization is generally performed making isothermal or isofield magnetization curves across the process to be investigated in order to calculate the Δs_T.

However the importance to compare the previous data with ΔT_{ad} measurements has been often remarked [2, 3]. The observation of large mismatches between calculated ΔT_{ad} values and the directly measured ones is among the main issues concerning this area of research [2]. We believe that this contributed to slow down the development of new materials during the last years.

Here we discuss a complete magnetocaloric characterization of a first order martensitic transformation made separately measuring Δs_T, ΔT_{ad} and cp as well [4]. For this purpose two ad hoc experimental set ups were realized together with a geometrical construction which allows to calculate ΔT_{ad} values from Δs_T deduced from magnetometry [4,5]. A detailed analysis of the errors of every technique was essential to show how the irreversibility and the kinetics of first order transformations are not the origin of the commonly reported mismatches between predicted and measured ΔT_{ad} values. On the other hand the material inhomogeneities together with demagnetizing effects if ignored could be deleterious.

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#162 - Information carrier bandwidth and speed tunability in magnonic crystals in the vortex state

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Magnonic crystals are artificial materials with periodic modulation of the magnetic properties that have recently received special attention due to the fact that slight changes of the external field can have dramatic consequences on the information carrier ("magnon") propagation, which can be boosted or delayed even to steadiness: in this way the same device can operate either as a memory or a waveguide. Employing the dynamical matrix method [1], we performed calculations on a squared 2D lattice of dots in the vortex state, varying the in-plane wavevector components to investigate the first Brillouin zone. We computed the dispersion relations for gyrotropic, azimuthal and radial modes. We discuss the dynamical coupling of modes with different cell wavefunctions, which is not purely dipolar as for the saturated states. We discuss how the circular polarization on the modes depends on the Bloch wavevector. We considered also the effects of application of a magnetic field, which moves the vortex core off the center of the disk: for a class of modes, propagation perpendicular to the direction of the applied field is speeded up, while parallel to the applied field is slowed down. These results can be important for designing versatile magnetic filters, in which variation of the applied field direction and intensity can turn the device from a waveguide into a memory, but also for spin logic devices, in which propagation or steadiness of the information carrier along a desired direction can be associated to different binary digits.

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#163 - Ultrathin oxide films on Fe(100)

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The growth of thin epitaxial oxide films on metal supports is attracting considerable scientific interest both on a fundamental level and for potential technological applications. In particular, the structural characterization of oxide structures is of crucial importance in order to get insight into the chemical and physical processes occurring in a variety of modern technological devices based on ultrathin oxide films, such as solid-state electronic devices, high-storage-density media, and metal oxide catalysts.
Among ultrathin oxide films, particular effort has been devoted to the investigation of single-layer oxides. The interest in one-layer-thick oxides is manifold, in particular (i) two-dimensional oxides can be seen as model systems for the oxide/metal interface, allowing investigation by means of high-resolution scanning probe techniques; (ii) the vertical confinement and the elastic and electronic coupling with the metallic substrate allows stabilizing stoichiometries and atomic structures that can differ with respect to the corresponding bulk terminations, with important implications in chemical reactivity, adsorption properties, and magnetic ordering of the resulting structures; and (iii) the wetting layer can represent the precursor phase for the growth of thicker films.
Single layers of transition metal oxides have been stabilized on noble and quasinoble metals. In these cases, growth techniques such as reactive deposition and/or postoxidation are typically applied, leading to ordered phases and well-defined oxide-metal interfaces. On the contrary, when a more reactive metal, such as Fe, is used as a substrate for the nano-oxide growth, these procedures fail to produce sharp metal/oxide interfaces. An alternative route to obtain a sharp interface between a single layer of transition metal oxide and a reactive substrate may be to exploit the oxygen adsorbed on the surface before metal deposition since, in this case, the amount of oxygen available is well defined.
I will present a systematic survey of structural and electronic properties of ultrathin oxide films of $3d$ transition metals grown on the Fe(001)-p(1x1)O surface characterized by one oxygen atom per surface unit cell, which can be used as a reservoir for the stabilization of two-dimensional oxides. The analysis will be performed mainly by applying scanning tunnelling microscopy and spectroscopy with theoretical modelling through density functional theory calculations, a combination that proved to be a powerful tool to understand the growth dynamics of oxide systems supported by metals. In particular, I will discuss the surfactant or antisurfactant role of the native oxygen and its importance to determine the growth of atomically flat and defect-free ultrathin oxide films.

#164 - Accretion disk origin of earth's water

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Earth's water is conventionally believed to be delivered by comets or wet asteroids after Earth formed. However, their elemental and isotopic properties are inconsistent with those of Earth. It was thus proposed that water was introduced by adsorption onto grains in the accretion disk prior to planetary growth, with bonding energies so high as to be stable under high temperature conditions [1]. This hypothesis is supported by the presence of water in the disks around young stars [2] and by numerical simulations [3] of water adsorption on silicate grains under conditions corresponding to those in the accretion disk.
We tested this hypothesis by laboratory experiments employing a supersonic molecular beam. The present experiments clearly indicate that when dosing at 138 K multilayer of water can be obtained and that subsequent water dosing at the same temperature but performed after annealing the surface above the molecular water desorption temperature lead to a lower uptake. This clearly indicates that while annealing part of the water layer desorbs and part of it must dissociate forming OH and H.
We found moreover that dosing water at high T causes the formation of a passivating layer of hydroxyls which is passive with respect to low T water adsorption and stable up to at least 900 K .We can thus conclude that water adsorbs dissociatively on the olivine {100} surface at the temperature ($\approx$ 500 - 1500 K) and water pressure ($\approx$ 10 - 8 bar) expected for the accretion disk, leaving an OH adlayer that is stable at least up to 900 K. This may result in the formation of many Earth oceans, provided that a viable mechanism to produce water from hydroxyl exists. This adsorption process must occur in all disk environments around young stars. The inevitable conclusion is that water should be prevalent on terrestrial planets in the habitable zone around other stars.

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#165 - Thermal effects on MoS$_2$ liquid exfoliated flakes: sulfur vacancies and doping

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We report a study of thermal effects on the electronic structure of liquid exfoliated molybdenite (MoS_2) by core levels and valence band X-ray photoemission spectroscopy (XPS).

Molybdenite has been exfoliated from its bulk phase using a liquid solvent, N-methyl-pyrrolidone (NMP), using a method similar to the one developed by Coleman and his co-workers: a solution of MoS_2 powder in NMP (concentration=7.5 mg/ml) has been sonicated for one hour. 10 μl of the solution have been deposited by drop casting technique on gold substrate, previously cleaned by "piranha" solution. The exfoliated flakes deposited have been analysed by XPS before and after thermal annealing in ultra high vacuum at 100, 200, 300 and 400°C. Two Gaussian-Lorentzian curves were used to fit each doublet, related to Mo 3d (5/2 and 3/2) and S 2p (3/2 and 1/2), one related to fully coordinated atoms, the other to defects and vacancies.

The quantitative analysis of the core level spectra demonstrates that, upon thermal annealing above 300°C, defect formation occurs in the form of single and double sulfur vacancies, similar to the ones observed after electron and ion bombardment. In particular, after thermal annealing at 400°C, we estimated that the relative double vacancies concentration among defects is equal to 35%. The presence of defects and vacancies induces states in the gap, which pin the Fermi level to lower binding energies. This pinning determines a rigid shift to lower binding energies of the Mo 3d and S 2p core levels, leading to n-type doping of the flakes. The energy difference between the core levels before and after thermal annealing at 400°C is 0.25 eV.

Accordingly, the occurrence of defect related surface states is determined from the analysis of the valence band XPS spectrum of the MoS_2 flakes. After thermal annealing at 300°C states in the gap are present: they are mostly due to the molybdenum atoms adjacent to the vacancy, with a contribution of the neighbouring sulfur atoms in the same sulfur plane of the vacancy.

#166 - Self assembling of titanyl-phthalocyanine on Ag(100) studied by scanning tunneling microscopy and low energy electron diffraction

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The interface structure is of paramount importance in tailoring the optical and electronic properties of the hybrid organic/inorganic interfaces.

Here we present a Scanning Tunneling Microscopy (STM) and Low Energy Electron Diffraction (LEED) investigation of titanyl-phthalocyanine (TiO-Pc) molecules deposited on Ag(100). The experimental results combined with Density Functional Theory (DFT) calculations allow a complete characterization of the TiO-Pc/Ag(100) interface.

The TiO-Pc molecule presents a non-planar structure with the O atom of the titanyl group pointing outward with respect to the macrocycle plane. Such a molecule is thus expected to interact with the substrate in two different ways: with the TiO group pointing toward the surface or away from it.

At very low coverage (isolated molecules) two different structures were detected by STM measurements at low temperature (5 K), attributed to molecules adsorbed with the TiO group pointing outward or inward with respect to Ag surface. The TiO-Pc molecules adsorbed with the TiO group toward the surface show two possible orientations (±30°) with respect to the Ag [011] direction, whereas the molecules pointing upwards tend to align along the [011] direction. Increasing the TiO-Pc amount deposited on the Ag(100) surface the molecules tend to organize to form an ordered film. Two distinct domains of the organic overlayer are detected by LEED and STM on the surface, presenting a square lattice rotated ±8° with respect to the Ag(100) surface lattice, in agreement with DFT modeling. STM measurements showed that the orientation of the single molecules in the overlayer changes from ±30° to ±27°, regardless the adsorption side of the interacting molecule. Two interesting features are observed in the organic layer: i) the domains are formed by both kinds of molecules with an apparent random arrangement; ii) in the two differently oriented domains the TiO-Pc molecules present opposite chiral structures. At coverage close to the complete monolayer (≈80%) the regions between the ordered domains present high molecular mobility even at 80K, the molecules pointing upwards showing higher mobility. When the organic layer reaches a complete monolayer the surface presents extensive domains limited by the substrate terraces.

#167 - Plasmon resonant (e,2e) spectroscopy

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The (e,2e) process has been largely used to investigate ionization mechanisms and electronic structure in atoms, molecules and solids. In solids, one of the most efficient channels of electron impact energy transfer is excitation of volume or surface plasmons (collective excitations of the electron gas). Two main plasmon decay mechanisms have been foreseen: the excitation of nearly free secondary electrons and the excitation of pair of correlated free electrons [1]. In competition with these two channels, the ejection of a secondary electron due to direct scattering within a medium described by its inverse dielectric function has been proposed [2]. To establish the relative relevance of these secondary electron generation channels is of importance in many branches of fundamental and applied science.

In this paper will be reviewed (e,2e) plasmon assisted experiments performed on Al and Be clean surfaces. The early experiment on Al [3] , performed at 100 eV incident energy, proposes that observed secondary electrons are emitted via a mechanism similar to photoemission with plasmon decay playing the role of photon absorption. The experiment performed always on Al at 500 eV [4] proves that surface plasmon decay accounts for roughly a quarter of the secondary electron spectrum. More recent experiment on Be

[5] point to plasmon resonant (e,2e) processes as a relevant channel for secondary electron generation and for building a resonant momentum spectroscopy.

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#168 - Angle-resolved energy loss spectroscopy experiments on epitaxial graphene on Pt(111) and Ru(0001)

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Angle-resolved electron energy loss spectroscopy has been used to study phonon and plasmon dispersion in monolayer graphene (MLG) on Pt(111) and in periodically rippled graphene on Ru(0001). We found that the dispersion relation of the low-energy plasmon mode (0-3 eV) confined in the graphene sheet is acousticlike. The linear dispersion relation of its frequency is caused by the non-local screening of the electrons in MLG due to the presence of the underlying metal substrate. Moreover, a quadratic dispersion of the ? plasmon of graphene/Pt(111) (6-8 eV) has been observed, in contrast to the linear dispersion reported for monolayer graphene grown on the semiconductor SiC(0001) substrate. The π plasmon is instead confined within graphene nanodomes on Ru(0001).
The elastic properties of a macroscopic graphene sample grown on Pt(111) and Ru(0001), extrapolated from experiments on phonon dispersion, showed values similar to the theoretical strength for free-standing graphene. Our results indicate that the excellent crystalline quality of graphene grown on metal substrates leads to macroscopic samples of high tensile strength. We also report on the differences in the phonon spectrum between graphene grown on Pt(111) and on Ru(0001).

#169 - Depth profiling of melting and metalization in Si(111) and Si(001) surfaces

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Surface melting has been studied for a long time in view of the importance of this phenomenon in understanding basic questions related to first-order phase transitions in solids (see [1, 2] and references therein). An original approach for measuring the depth profile of melting and metallization of the Si(111) and Si(001) surfaces is proposed and applied [3]. The different probing depths of the Auger electron and electron energy loss (EELS) spectroscopies are exploited to study the number of molten and metallic layers within 5–30 Angs from the surface up to about 1650 K. Melting is limited to 3 atomic layers in Si(001) in the range 1400–1650 K while the number of molten layers grows much faster (5 layers at about 1500 K) in Si(111) as also indicated by the L_3 -edge shift observed by EELS. The relationship between melting and metallization is briefly discussed and put in relation to low density and high density liquid transitions in tetrahedral bonding systems [4].

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#170 - Control of metal-oxide interface and tuning of exchange bias in Ni@NiO nanoparticles

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Magnetic metal-oxide core-shell nanoparticles (NP) have been the object of a vast amount of material research studies in the last years, because of their technological applications, like diagnostics, nanomedicine and magnetic recording. Smaller nanosized particles are required in order to realize advanced magnetic memory units, but this request is a major challenge, because of the superparamagnetic limit, resulting in instability of conventional recording media with three-dimensional particles. Particular efforts have been devoted to the application of the exchange bias effect as a possible way for stabilizing the magnetic state of NP, using an antiferromagnetic oxide coupled with a magnetic core [1]. To this purpose, the possibility to achieve an accurate control of the oxide shell thickness, crystallinity and of the oxide/metal interface quality is a fundamental step for the optimization of the desired NP magnetic properties. We performed a detailed study of pre-formed, mass-selected Ni@NiO NP with linear size values between 5 and 12 nm. Growth and characterization of the NP were carried out with an experimental system, equipped with three interconnected vacuum chambers for generation of a mass selected NP beam, deposition on substrate and in situ XPS analysis [2]. The Ni NP were

obtained with a gas aggregation source with a magnetron and a quadrupole mass filter, while NiO shells were produced by oxidising the NP with different procedures: deposition in oxygen atmosphere, post-annealing in air, co-deposition of NP with Ni vapour in oxygen. A study of Ni 2p XPS lineshape gave information about the chemical state of Ni in the core and in the oxide shell, while AFM and SEM have been used for investigation of the NP morphology. High quality HR-TEM and STEM-HAADF data allowed an in-deep analysis of the NP atomic structure, in both core and shell areas, and FC and ZFC magnetization curves and hysteresis cycles at T=5 K, recorded by a SQUID magnetometer, gave insight into the NP magnetic properties. In this way, the relation between magnetic properties and oxide shell structure has been assessed systematically, showing the role played by the control of the formation of oxide on the exchange bias and interparticle magnetic interaction.

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#171 - Terahertz mixers, fast detectors and single-photon counters based on superconducting ultrathin NbN films

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The recent advances in the superconducting NbN terahertz mixers, fast detectors and single-photon counters will be presented. The superconducting hot electron bolometer (HEB) mixers based on ultrathin films of NbN combine the best sensitivity at the frequencies well above 1 THz and a gain bandwidth of about 5-6 GHz which make them suitable for most sensitive instruments being developed in the far IR region for astronomical and atmospheric studies.

Direct detectors made from NbN and MoRe films are operated in 0.3-3 THz range exhibit response time as low as 50 ps and 1 ns respectively with noise equivalent power (NEP) of $3x10^{-13}$ W Hz$^{-1/2}$ (NbN) and $5x10^{-14}$ W Hz$^{-1/2}$ (MoRe). Another versions of these detectors have a broadband sensitivity in 0.1-30 THz range with the same response time and exhibit higher NEP but much higher dynamic range.

NbN superconducting single-photon detector (SSPD) is a planar nanostructure patterned from 4-nm-thick NbN film deposited on sapphire substrate. The sensitive element of the SSPD is 100-nm-wide NbN strip. The device is operated at liquid helium temperature. Absorption of a photon leads to a local suppression of superconductivity producing subnanosecond-long voltage pulses. In infrared (at 1550 nm and longer wavelengths) SSPD outperforms avalanche photodiodes in terms of detection efficiency (DE), dark counts rate, maximum counting rate and timing jitter. Recently several new improvements were introduced to the SSPD. The first one is the photon-number resolving SSPD (PNR-SSPD). This device realizes a spatial multiplexing of incident photons enabling resolving of up to 11 simultaneously absorbed photons. Another improvement is the increase of the photon absorption using a $\lambda/4$ microcavity integrated with the SSPD. High speed travelling wave single-photon detectors with near-unity quantum efficiency has been published very recently.

THz direct detectors and HEB mixers are used in a wide range of applications ranging from THz imaging for security (observation of hidden drugs, explosives and weapon) and medicine (THz probing of human tissues) to radioastronomy observation of stellar formation and dark matter (space observatories Herschel and Millimetron). SSPD due to their high quantum efficiency and picosecond timing resolution has already been successfully applied for non-destructive testing of CMOS integrated circuits, study of single-photon sources and quantum dot luminescence, and for quantum cryptography enabling quantum key distribution over 250 km distance.

#172 - Superconducting nanowire quantum detectors of molecules

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Superconducting nanowire detectors have been originally developed for single-photon detection in the visible and infrared regime where they are currently under intensive investigation. In literature this quantum detector is known as superconducting single photon detector (SSPD). It has been proved that SSPD is also sensitive to molecules and ions and produces fast signal pulses ranging from picoseconds to nanoseconds [1]. Indeed, when applied to the detection of heavy molecules this opens up a possibility of expanding the coverage mass region of time-of-flight mass-spectrometers (TOF MS) because traditional instruments use detectors which suffer a lack of efficiency for mass above 1 million AMU, which is the range of proteins complexes and DNA fragments. The interest in ion detection with SSPD extends also to fundamental experiments for the observation of de Broglie wave interference of molecules. Such experiments have been already performed with C60 molecules (720 AMU) [2]. The challenge is now to move to very massive neutral objects (mass of 105-106 AMU). For this purpose one needs a detector which is sensitive in this mass range and can be used in experiments of quantum matter wave interferometry of macroscopic objects. SSPD seems the detector of choice [3].

We present our recent achievements in the development of SSPD for molecular detection. We have invented a new configuration which allows to improve important key features like speed, collection efficiency, signal-to-noise ratio. With this technology we are able to increase the SSPD collection area without degradation of speed and improving the S/N ratio. We fabricate 2x2 mm^2 SSPD by electron beam nano-lithography. To our knowledge this device is the largest cryogenic detector for macromolecules with a nanosecond temporal response. We also present preliminary data that indicate sensitivity to the charge state of the molecules, which can be used to eliminate the charge/mass ambiguity in TOF MS which should represent a revolutionary improvement of this technique [4].

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#173 - Superconducting single photon detectors based on parallel NbN nanowires

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Superconducting single photon detectors (SSPD) based on ultrathin NbN nanowires are currently of interest for long distance quantum optics applications due to their good efficiency, dark count rate and timing jitter at 1550 nm wavelength. The focus of current SSPD research is the use of parallel nanowires for achieving pseudo photon number resolution, how to increase the efficiency at longer wavelengths and how to increase the area coverage. When increasing the SSPD area one must avoid the decrease in SSPD operation speed and maintain nanowire uniformity across large areas. Here we present how we solved these problems using parallel nanowires and show our results on SSPDs with area coverage up to 40 x 40 μm^2 based on 100 nm wide ultrathin NbN nanostrips with a 40% filling factor. Using a standard SSPD operation we achieved a maximum count rate of 33 MHz which is faster than the standard meandered serial SSPDs. Furthermore, we could achieve 80 MHz operation using an innovative operation procedure, that exploits the large signal amplitude of our parallel nanowire SSPDs. Due to the large area coverage we also identified a new operation region with two-photon sensitivity which we argue could be used to make a sampling photon number resolution SSPD. The increase in SSPD area coverage should open the way towards applications using multimode fibers or irregular photon emitters.

#174 - Developement of superconducting microwave microresonators for broad band high energy resolution particle detection

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We are running a project to develop new particle detectors based on the superconducting microwave microresonator technique. So far microwave microresonator were developed mostly for bolometric measurements in millimiter astronomy or in cosmic microwave mapping. These low temperature detectors are very sensitive devices compatible with large-scale multiplexed frequency domain read-out.

Our project aims to adapt and further advance the technology of microresonator detectors to develop new devices for single particle detection and high resolution spectroscopy. These devices   can find application in many fields. Our first aim is to develop detectors for neutrino physics. In particular we plan to realize detector arrays for calorimetric measurement of the energy spectra of 163Ho EC decay for a direct measurement of the neutrino mass.

We are also exploring the possibility of designing new devices for high energy resolution broad band (1-100 keV) photon spectroscopy. Kilo-pixel arrays of such devices may have a large impact in many frontier fields like astrophysics, material analysis, nuclear safety and diagnostic, archeometry, etc. In order to achieve these goals, we are optimizing the design and developing new materials for the detectors. A recent advance in microwave microresonator technology was the discovery that some metal nitrides, such as TiN, possess properties consistent with very high detector sensitivity.

We have developed a technique for producing sub-stoichiometric TiN device which allows a precise and reliable control of the transition temperature. We plan to investigate also nitrides of higher-Z materials, for example TaN and HfN, that are appropriate for achieving a high quantum efficiency in broad band photon spectroscopy.

We report about our first results obtained with several TiN and Al devices. In particular we discuss the film properties relevant to our detectors, such as quality factor, penetration depth and recombination time and we present the results obtained exposing the devices to low energy X-rays.

#175 - Single-photon detectors with superconducting nanowires integrated with passive optical elements for quantum information science

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The integration of single-photon sources and single-photon detectors with passive quantum photonic circuits would enable important functionalities in the field of quantum information processing. In this work we present our progress in the integration of superconducting nanowire single-photon detectors with waveguide optical circuits. The GaAs technology is the promising platform for the integration of quantum-dot single-photon sources and passive photonic circuitry. In the past we developed a superconducting single-photon detector on a GaAs/AlAs distributed Bragg reflector mirror [1], showing that a full integration of active and passive elements is possible using the GaAs technology. We have recently demonstrated the first waveguide single photon detectors (WSPDs), based on superconducting nanowires patterned on top of a GaAs/AlGaAs ridge waveguide, with a quantum efficiency of ~ 20 % and a jitter of ~ 60 ps [2]. Here we present the development of an integrated autocorrelator based on two separated detectors integrated on top of the same ridge waveguide. An efficiency >2 % at 1300 nm for both detectors and independent of the polarization of the incoming photons, is reported. The g(2)(τ) measurement of a laser source is experimentally demonstrated as a proof of principle. This ultracompact device enables the on-chip measurement of the second-order correlation function g(2)(τ) . We will further discuss ongoing work on the integration of detectors with single-photon sources and multimode interferometers. Photon number resolving functionality will be also discussed.

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#176 - Measurement of photon statistics with superconducting transition edge sensors

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The sharp transition between the superconducting and normal state of a thin film can be exploited to obtain very sensitive thermometers. Transition-Edge Sensors (TESs) are detectors based on small (≈ 100 µm^2) superconductive thin films biased on the transition. The very low heat capacity, in the range of fW/K, allows to make the detector sensible to single photons from the UV to the typical telecommunication wavelengths (1550 nm). Moreover the sensitivity is so high that the detector is intrinsically energy resolving, i.e. its response is proportional to the single photon energy. Working at fixed wavelength this property allows to discriminate the photon number in a light pulse. This capability is extremely important in the new quantum technologies and is fundamental for photon metrology.

Results here presented are obtained at INRIM with TESs based on a titanium/gold multilayer. Detectors with transition temperatures from 100 mK to 300 mK have been fabricated and characterized. Single photon counting has been demonstrated from visible down to NIR photons with response time constants from 10 µs to 200 ns, respectively. TESs with 10 µm x 10 µm active area provide an energy resolution lower than 0.2 eV, while detectors with 20 µm x 20 µm active area allow to discriminate up to 29 incident photons simultaneously. Quantum efficiencies on the order of 50 % has been obtained with the bare metal films, while better efficiencies are obtainable with antireflection coatings or optical cavities applied on top of the detector.

#177 - Photoresponse studies of proximitized superconductor/ferromagnet nanostructures for optical-photon detection

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We present our research on both superconducting and optical properties of ultrathin superconductor/ferromagnet (S/F) bilayers and patterned nanostripes. Recent advances in nano-patterning techniques opened the way for studying both fundamental aspects of superconductivity on the nanoscale, and advanced applications as Superconducting Single Photon Detectors (SSPDs). SSPDs are currently object of an extensive research, because of the high counting rate, low dark counting rate and high sensitivity for single infrared photons. The best realizations on these devices, at the moment, are based on ultrathin layers of low critical temperature superconductors.

Our S/F structures consisted of both metallic (e.g., NbN/Ni0.6Cu0.4 (NbN/NiCu)) and oxide-based materials (e.g., YBa$_2$Cu$_3$O$_7$/La0.7Sr0.3MnO$_3$ (YBCO/LSMO)). In the case of NbN/NiCu bilayers, an 8-nm-thick NbN film was sputtered first and, afterward, the sample was moved into another vacuum chamber to deposit NiCu overlayers with thicknesses ranging from 1 nm to 10-nm. All-oxide YBCO/LSMO bilayers were grown by Pulsed Laser Deposition (PLD) on MgO (110) substrates. A 50-nm-thick YBCO base layer was deposited first and capped with a 15-nm-thick LSMO film. The S/F bilayers are firstly optically characterized by using a pump-probe femtosecond optical spectroscopy technique to investigate nonequilibrium dynamics and estimate the electron-phonon relaxations times. Then, the films are patterned by using electron beam lithography and a very gentle ion milling, achieving widths in the range 100-300 nm and lengths up to 10 µm. The structures are configured in a serial connection of N blocks each consisting of 2 or 3 nanowires in parallel: in this way, large detection areas are achieved, while retaining a small total inductance per detector area, which is needed for high maximum count rates. All the devices have a detection area comparable with the laser spot in photoresponse experiments: in the longest ones, an area coverage of 10x15 µm^2 and a filling factor of 50 % have been achieved.

Photoresponse measurements have been performed by optical laser pulses at 1550 nm wavelength. In the case of YBCO/LSMO nanowires signals have been observed in a very broad temperature range, from 4 K up to the critical temperature of the nanowires, making these devices appealing for many applications. The operation working range is also very wide, since signals can be revealed by biasing the devices not only slightly below the critical current as in S/F structures based on NbN, but also on the whole resistive branch.

This last evidence shows a deep difference between devices based on YBCO and NbN whose working point is at the critical current due to basic mechanisms of the photoresponse related to the formation of an hot spot and cascade avalanche.

#178 - Silicon nanostructures for advanced photovoltaic: carrier multiplication effects

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The conversion of solar radiation into electric current with high efficiency is one of the most important topics of modern scientific research, as it holds great potential as a source of clean and renewable energy. Currently the exploitation of interaction between nanocrystals seems to be a promising route to foster the establishment of third generation photovoltaics. Here we adopt a fully ab-initio scheme to estimate the role of nanoparticle interplay on the carrier multiplication dynamics of interacting silicon nanocrystals [1]. Energy and charge transfer-based carrier multiplication events are studied as a function of nanocrystal's separation showing benefits induced by the wave function sharing regime. We prove the relevance of these recombinative mechanisms for photovoltaic applications in the case of silicon nanocrystals arranged in dense arrays, quantifying at an atomistic scale which conditions maximize the outcome.

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#179 - Anisotropic effective g-factor in IV-VI semiconductor quantum wells

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We consider the modifications of the electron g-factor due to the confining potential in multivalley IV - VI semiconductor nanostructures, extending recent work for III-V heterostructures [1]. Quantum confinement and magnetic field effects are considered within the Dimmock kp model of the IV-VI semiconductor band edge states describing the ellipsoidal shape of the multiple electron and hole pockets at the <111> Brillouin zone boundary. A new effective Hamiltonian for the quantum well (QW) electron and hole states in the presence of an external magnetic field is derived. The mesoscopic spin-orbit (Rashba type) and Zeeman interactions are taken into account on an equal footing, and the anisotropic electron and hole effective g-factors in IV-VI QWs are calculated. Some cases of interest are studied in detail as PbTe QWs grown along <111>, <110> and <001> crystallographic directions. The break of valley degeneracy is considered and the effective g-factor of electrons and holes in these IV-VI semiconductor QWs is shown to be highly anisotropic and affected (in different ways depending on the various orientations) by both the bulk anisotropy and the quantum confinement contribution akin to the Rashba spin-orbit coupling.

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#180 - Selective growth of InAs quantum dots on GaAs driven by As kinetics

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Advances in new generation devices for Nanophotonics and Quantum Information based on III-V Quantum Dots (QDs) rely on the capability to accurately control their size and lateral position on the substrate surface. In recent years, much experimental effort has been devoted to the search of methods to achieve position control of QDs. Until now, advances in this regard have been obtained by combining bottom-up and top-down methods, such as introducing ex situ processing-steps (e.g. standard lithography) before and/or after the epitaxial growth. Alternatively, a significant and appealing challenge would be to control the islands' position by a careful tailoring of the growth process.

In this work, we present a new Molecular Beam Epitaxy approach to obtain self-organization of InAs QDs on GaAs(001) that is based on an unexpected key role played by the element V. We show that, at relatively high growth temperatures, QDs alignment along oriented step bunching of mounds generated on the substrate can be controlled as a function of the As flux direction, so as to obtain an almost completely anisotropic surface distribution of QDs on the mounds. Generally, the role of As is neglected and the growth of GaAs and similar compounds is modeled as a simple one-component case. To the contrary, we show experimentally, by means of a suitable choice of the kinetic growth parameters, and theoretically, by developing a two-species rate equation model that the As role is crucial in the islands' stabilization and positioning [1]. We find that the very small As flux gradient between the two mound slopes ($\Delta F/F\sim$1-5%) originates a cations current flow from one mound slope to the other, so that the dots can develop only on one side of the mounds. The current is generated by the inhomogeneity of the cations adatom distribution between the two sides of the mound and activated by the relatively high temperatures.

A comparable behavior is expected for other compound semiconductors for which the adsorption kinetics of one of the elements involves the existence of a highly mobile precursor state.

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#181 - Conductivity and photoconductivity properties of single GaAs/AlGaAs core-shell nanowires

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A fundamental issue for the development of nanowire (NW) based devices is the investigation of the carrier transport properties in the single NW. To this aim, it is essential to produce high quality NWs, to deposit local electrical contacts in a controlled manner, and to adopt suitable characterization techniques. Photocurrent is a valuable tool to directly probe the striking properties related to the light absorption as well as the transport and collection of the photogenerated charges. Specifically, mapping techniques to probe local photocurrent properties results to have a great potential.

In this work, we present the conduction and photoconduction properties of individual GaAs/AlGaAs core–shell NWs under uniform and local optical excitation. The NWs were grown by Au-assisted vapor phase epitaxy and metalorganic vapor phase epitaxy (MOVPE), and electrical contacts were deposited on them by the electron beam induced deposition (EBID). The conduction properties of the single core-shell NW under dark conditions were investigated by I–V curves as a function of the temperature, pointing out that the nanocontacts have a blocking nature that is affected by an interface oxide layer. The photocurrent of the GaAs/AlGaAs core–shell NW is found to be much higher than the bare GaAs NW. In particular, the spectral photocurrent of the single core-shell NW was measured and the dependence of the polarization anisotropy ρ is found to vary from ~ 0.1 to ~ 0.55, depending on the absorption wavelength. High quantum efficiency values (10% at 600 nm) are obtained which are attractive for a wide range of optoelectronic devices. Finally, mapping photocurrent measurements show that the charge collection localizes near the contacts, consistently with the blocking contacts. Moreover, photocurrent-voltage characteristics and photocurrent spectra were measured with the optical excitation focused near the contacts, providing a better understanding of the charge collection mechanisms as well as a discrimination between the contribution due to the carriers photogenerated in the GaAs core and AlGaAs shell.

#182 - Multi-stacked ordering of quantum dots driven by As kinetics

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The growth of InAs on GaAs is characterized by a large lattice mismatch. The system evolves in the Stranski-Krastanov (SK) mode, next to the growth of a two-dimensional pseudomorphic InAs wetting layer, after a certain critical thickness, the development of 3D InAs islands, usually called Quantum Dots (QDs), becomes favoured as it partially relieves the accumulated strain.

Generally the InAs QDs are randomly distributed on the surface due to the stochastic nature of the self-assembly process. In principle more control over uniformity and spatial organization of the InAs QDs is necessary for many applications. For vertical ordering, the SK growth mode already produces excellent results exploiting the effect of strain field propagation when a GaAs spacer layer is grown between two QDs layers. In fact usually multilayer structures are grown starting by a single layer of QDs randomly positioned [1], a tendency of QDs self-ordering is observed and this effect is more evident the more the layers stacked. This method is indicated in literature as multilayer stacking and consists of a subsequent growth of alternating QDs layers and spacer layers (covering layers). We have shown that, at relatively high growth temperatures, QDs alignment along oriented step bunching of mounds generated on the substrate can be controlled as a function of the As flux direction [2], so as to obtain an almost completely anisotropic surface distribution of QDs on the mounds.

In this work, we employ the effect described above to achieve QDs lateral-ordering, by means of stacking of alternating InAs and GaAs layers. The achievement of well-defined rows of QDs, oriented along the [-110] direction, is demonstrated. Such lines are distributed over the surface with a high horizontal order. The lateral order has been highlighted with the help of the closest neighbour positions mapping and a codex has been developed to esteem the virtual line correlations. These analyses have demonstrated a remarkable tendency to lateral ordering, showing that while in the first layers the QDs ordering is well defined only locally, while it begins to be global after six multilayers.

Transmission Electron Microscopy of the samples contributed to understand the strain propagation in the spacer layers for the new QDs line formation.

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#183 - Optical determination of the strain field in GaAsN/GaAsN:H planar heterostructures

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It was recently found that marked polarization anisotropy of light emission can be obtained in GaAsN/GaAsN:H planar heterostructures. This is related to anisotropic strain in the sample growth plane. The strain field is due to the formation of N-H complexes along the hydrogen diffusion profile. In the present paper, we present Raman and photoreflectance results from GaAsN/GaAsN:H micro-sized wires made by an in-plane selective hydrogen incorporation controlled by H-opaque metallic masks. The strain field was mapped by measuring the variations in GaAs-like LO phonon frequency. The experiments also allow to monitor the hydrogen diffusion profile via the Ga-N local vibrational mode line, whose quenching is related to the formation of N-H complexes. On a macroscopic scale, photoreflectance experiments provide additional evidence of the in-plane strain re-distribution.

#184 - Embedded Ga nanoparticles on patterned Si substrate

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Metal nanoparticles (NPs) present unique optical properties, which are very different from those of bulk material. The localized surface plasmon resonance of these particles results in strong optical scattering and a strongly enhanced optical near-field around the particle. Recently, metal nanoparticles have been investigated as a possible way to improve the performance of thin-film solar cells. Metal NPs embedded in a semiconductor material act as antennas for the incident light and store energy in the localized surface plasmon resonance. The strong near-field absorption enhancement can be used to reduce the thickness of a thin film solar cell without a reduction of optical absorption.

Here we show that, by the combination of substrate patterning and droplet epitaxy, it is possible to obtain the fabrication of and ordered and controlled array of embedded Ga nanoparticles in a semiconductor matrix.

A Si(001) wafer patterned with regular arrays of half micron inverted pyramid pits was used as substrate for the subsequent fabrication of Ga nanoparticles embedded in GaAs islands using Droplet epitaxy (DE) technique. DE separates Ga deposition, used for the formation of an ensemble of localized Ga reservoirs on the surface, from the As supply, necessary to crystallize the droplets into GaAs nanostructures. The capture of the Ga droplet by the inverted pits is caused by capillarity forces. The occupancy ratio of the pits by Ga droplets, obtained from several similar images, is 80 %.

The chemical and structural quality of the GaAs nanoislands at the bottom of pits was studied by means of set of complementary characterization techniques. In particular cross-sectional TEM was employed in order to extract the exact shapes and composition of the islands. Strongly different concentration profiles of Ga and As are easily observable from EDS maps of the characteristic x-ray Kα emissions. Ga fills uniformly the pit, while As is detected only in limited crust close at the island surface. Extracting the EDS spectrum from narrower areas along the vertical axis of the pit shows that the As:Ga ratio nearly approaches 1 at the very top of the As map whereas it strongly decreases on going deeper in the island. The inner part of the island is constituted by a pure Ga NP. This NP is then fully embedded within a semiconductor matrix, constituted by the pit Si sidewalls and the GaAs crust which is formed during the crystallization process with As. Kinetic Monte Carlo simulations examining nanostructural evolution in the Ga droplet nucleated in the pit during the crystallization process support the observed phenomenology.

#185 - Strain-controlled generation of silicon nanopillars

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Silicon metal-assisted chemical etching (MACE) is a nanostructuring technique exploiting the enhancement of the silicon etch rate at some metal-silicon interfaces. Compared to more traditional approaches, MACE is a high-throughput technique, and it is one of the few that enables the growth of vertical 1D structures of virtually unlimited length. As such, it has already found relevant technological applications in fields ranging from energy conversion to biosensing. Yet, its implementation has always required metal patterning to obtain nanopillars. Here we report how MACE may lead to the formation of porous silicon nanopillars even in the absence of gold patterning. We show how the use of inhomogeneous yet continuous gold layers leads to the generation of a stress field causing the spontaneous local delamination of the metal - and to the formation of silicon nanopillars where the metal disruption occurs. We observed the spontaneous formation of nanopillars with diameters ranging from 40 to 65 nm and heights up to 1 μm. Strain-controlled generation of nanopillars is consistent with a mechanism of silicon oxidation by hole injection through the metal layer. Spontaneous nanopillar formation could enable applications of this method to contexts where ordered distributions of nanopillars are not required, while patterning by high-resolution techniques is either unpractical or unaffordable.

#186 - Laser emission from core or shell transitions in self-assembled microcavities of CdSe/CdS colloidal nanorods

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Chemically synthesized colloidal semiconductor nanocrystals have well established light-emitting properties. They have been proposed for lasing applications, [1,2] even if in this contest the gain competes with the non-radiative Auger recombination[3]. Interesting solutions are core/shell dots with thick shell or elongated nanorods (NRs).

Here we consider NRs made by wet-chemical synthesis in which a CdSe dot (~ 3 nm diameter) is embedded in a CdS rod (with lengths between 20 and 60 nm). We study the photo-physics by fs pump-probe technique and we observe long living gain [4] (> 300 ps) with Auger recombination suppressed in the biexciton regime [5]. Data are fitted assuming electrons delocalized over the rod and holes localized in the core [5]. We obtain amplified spontaneous emission (ASE) from films of these NRs under excitation by 100 fs laser pulses at 400 nm. The novelty lies in the fact that ASE arises not only from CdSe core states, but also from CdS shell states, in the red or in the blue-green spectral region respectively, depending on the NR length (short or long respectively)[6].

A further very interesting property of these NRs is their capability to self-assemble, which we exploit to fabricate micro-resonators by capillary jet deposition of NR solution, in a scalable and reproducible way [7]. These assemblies combine gain and feedback constituting efficient micro-lasers.4 We study the optical resonator and model the optical feedback. We show laser emission either from core states either from shell states, depending on the NR length. Laser action is characterized by a very low pump threshold (down to ~ 0.2 mJ/cm^2) and a FWHM of ~ 0.6 nm. Integrations of these microlaser into devices such as lab-on-a-chip systems are envisaged.

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#187 - Silicon-Germanium Nanowires: chemistry and physics in play, from basic principles to advanced applications

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The end of the last century has seen a progressive interest in materials and devices with reduced size and dimensionality and semiconducting nanowires (NWs) have emerged as the strongest candidate to provide the change of paradigm needed by the new generation of electron devices [1]. While Si and Ge NWs have been widely studied, only recently SiGe NWs are attracting an increasing interest for their multiple potentialities in many different fields [2].

One-dimensional SiGe nanostructures have acquired a prominent role in several cutting-edge research topics in nanoscience, thanks to the latest relevant advances in synthesis, processing and characterization. These materials present unique structural, electronic, optical and transport properties, which are intrinsically associated with their low dimensionality. What is particularly fascinating in these nanosystems is that by bringing together two similar elements –Si and Ge, neighbors in the periodic table–, a rich variety of new chemical and physical properties emerge, stimulating both fundamental and application-driven research in nanoscience.

The physical properties of SiGe NWs are strictly related not only to the size of the system, but also to the relative composition of Si and Ge atoms, and to the geometry of Si/Ge interface. Substituting some of the atoms of a pure Si NW with Ge in random as well as ordered configurations of different compositions, can strongly affect some fundamental properties such as band gap, effective mass, phonon and electron scattering processes and excitonic properties. As a consequence, SiGe NWs are the target of the most intriguing and exciting technological applications in the field of high performance nanoelectronics, thermoelectrics, photovoltaics, biomedicine, superconductivity and spintronics. From another point of view, since in these materials the size is at or below the characteristic length scale of some fundamental solid-state phenomena, their investigation aids in clearer and deeper insights into basic research in material science.

In this presentation I will review both the achieved milestones and outline the current research efforts, focusing on theoretical modeling. The investigation of the matter at nanoscale with experimental techniques is often complicated by several factors not always well controlled (such as impurities, surface reconstructions, dislocations, etc.), which can hide the right comprehension of the basic properties. In this context the role of theoretical modeling and simulations is extraordinarily important and must be joined with the experimental observations, in particular to understand the basic concepts involved in device operation, typical failure modes, and their relative advantages and limitations.

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#188 - I-AMICA: a high technology infrastructure for south Italian Mediterrean environmental and climate monitoring

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I-AMICA (Infrastruttura di Alta tecnologia per il Monitoraggio Climatico Ambientale - Infrastructure of High Technology for Environmental and Climate Monitoring) is a three years challenging project, co-funded by Italian National Operative Program (PON) and European Regional Development Fund. A lot of effort distinguish the project to strengthen the environmental monitoring in Italian South Mediterranean with the aim to support the integration among research, high training, and innovation. A special issue is also to be proactive in synergies among public and private research organizations. The activities are focused on actions addressed to strengthen the observational infrastructures for atmosphere, forest and coastal areas in the regions of Southern Italy, whose economic growth and social well-being are strongly related to the environment quality. In such Convergence Regions (Campania, Apulia, Calabria and Sicily), instrumental networks (e.g. advanced sensors, software tools, integrated platforms and mobile laboratory and stations) dedicated to the environmental and climatic monitoring in the Mediterranean area, in terms of air quality, forest and agriculture, coastal marine ecosystems will be promoted and developed.

In order to raise the national and international competitive capacity, four "pillar" activities are aimed to (1) strengthen observing infrastructures for climate and environment and data processing systems, (2) promote innovation, technological development and industrial transfer, (3) integrate these observational activities into international programs (i.e. GAW-WMO, ACTRIS, EARLINET, GMOS, ICOS, FLUXNET, SHARE, NEXT DATA) that will allow I-AMICA to effectively be integrated with important networks. Finally, (4) through the implementation of observations, networking, technological applications and territorial services in the Convergence Regions, I-AMICA provides an important support to the local and regional communities.

#189 - ERMES-WORLD: Environmental Radioactivity Monitoring for Earth Sciences-WOrld Reference Laboratory and new Developments

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On behalf of the ERMES-WORLD Collaboration

The Environmental Sciences are approaching an important crossroad for understanding complex processes such as Climate Change, Earth's interior and its heat budget, global geodynamic processes. The phenomenological study needs a comprehensive characterization for connecting past-present processes, which can be performed only through time-space markers such as radionuclides. The numerical modeling of complex systems such as those mentioned need, a growing number of experimental data with the highest possible accuracy for the scientific validation. This fundamental synergy requires an ultra-low level background environment as only found underground and ERMES-WORLD has been designed to achieve it. ERMES-WORLD will also promote and support other synergies providing to the scientific community the best reference facility. ERMES-WORLD delivers a high quality and innovative research program and will, as well, open new research opportunities for Environmental and Nuclear Sciences increasing the synergy between these fields and contributing to the development and monitoring of peaceful nuclear applications in other fields of interest for Science and the International Community: Astroparticle Phyiscs, Non-proliferation, Nuclear Safety, Safeguards, Reference Materials, Biomedical Applications, Nanoelectronics. The synergy proposed by ERMES-WORLD also combines the study of environmental radioactivity, using the most powerful technology in the best ultra-low level background environment around the world (INFN-Gran Sasso National Laboratory, Italy).

#190 - Hydrogen storage in solid state, recent developments

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Storage of hydrogen, the possible energy vector of the future, in light-weight solids has some advantages (especially in volumetric terms) compared to current technologies, such as compressed gas or liquefied hydrogen. Fundamental knowledge of the atomistic processes is required to design optimized novel materials with new physical properties. Physisorption of hydrogen molecules on very high specific surface materials is an option, effective specially at cryogenic temperatures. On the other hand, chemisorption in nanostructured conventional hydrides or in light-weight complex hydrides is being very intensively studied. Nanoparticles confined by scaffold materials exhibit improved properties in the hydrogen absorption/desorption process. Some recent results achieved at the Padova University are presented.

#191 - Magnesium nanostructures for hydrogen storage

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The continued interest in novel light element solid-state hydrogen (H) storage media has triggered the investigation of an impressively rich diversity of candidate materials. However, a lightweight hydride capable of reversible H-storage close to ambient temperature at pressure has not yet been synthesized. Nanoscale materials engineering aims at this ambitious goal by exploiting several interacting effects: microstructure refinement down to the nanometer range, reduced dimensionality, addition of nanocatalysts, synergy and physical coupling among complementary phases.

In this work, we present a comprehensive approach to the study of Mg-based nanostructures for H-storage, including: i) synthesis with advanced physical deposition techniques [1-2]; ii) high-resolution structural analysis using state of the art electron microscopy [1-2] and in situ diffraction with synchrotron radiation [3]; iii) experimental characterization of H-sorption kinetics and thermodynamics [1-7]; iv) modelling by means of classical molecular dynamics.

Several physical phenomena will be highlighted, such as the size-dependence of H-sorption kinetics [1]; the occurrence of nanoscale reactions between matrix and catalyst [2-4]; the possibility to modify the formation enthalpy by elastic confinement [7]; the synthesis of nanocomposites between immiscible hydride forming phases, and the morphological stability of nanostructures [5]. This study benefits from the collaboration with several European Universities and Research Centres, partly in the framework of the running COST Action MP1103 "Nanostructured Materials for Solid State Hydrogen Storage" [8].

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#192 - Ionic conductivity in light metal fullerides

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Fast-ion conductors are materials displaying a very large ion conductivity in the solid state, which could be comparable to that of liquid organic electrolytes, commonly used in Li-ion batteries. It is known that fullerenes are able to intercalate small alkali (Li, Na) and alkali-earth ions (Mg) and this often leads to the formation of polymers, in which C_{60} units are interconnected by covalent bonds. In particular, either in Li or Mg intercalated C_{60}, the charge transfer of four electrons from the metal to the fullerene stabilizes a peculiar two-dimensional polymer structure [1, 2], where Li^+ and Mg^{2+} ions can easily diffuse also at low temperature with a low activation energy [2, 3]. The polymer arrangement is of paramount importance for the onset of fast ion diffusion in such compounds; it is supported by the presence of intrinsic unoccupied Mn^+ interstitial sites in the crystalline structure, connected by three-dimensional pathways. In particular, we recently found that in Mg_2C_{60} polymer the onset of Mg^{2+} diffusion is observed already at T=120 K. Above this temperature, ion conductivity increases following an Arrhenius law and reaches the noticeable value for the of $0.5 \cdot 10^{-4}$ S/cm at room temperature, with an unusual low activation energy of only ΔE_a=100 meV [3]. Impedence measurements also evidenced that Mg^{2+} diffusion follows the ideal Debye model in this system. This material appears very promising for the production of the future and still unexplored Mg ion batteries.

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#193 - Ge-rich SiGe multilayers for thermoelectric applications

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Thermoelectric materials are presently used in a number of applications for both turning heat into electricity and also for using electricity to produce cooling (Peltier cooling). Despite the significant scientific progresses reported in the recent years, one of the crucial issues to be overcome is the relatively low efficiency which characterizes the actual technology. While Bi_2Te_3 alloys have demonstrated the best performances at room temperature, $Si_{1-x}Ge_x$ is the best performing bulk thermoelectric material for high temperature applications. We have deposited and characterized Ge-rich SiGe multilayers on Si substrates with the aim of demonstrating micro- and nano-fabricated room temperature thermoelectric generators monolithically integrated on silicon. SiGe heteroepitaxy is a mature growth technology, scalable, cheap and integrable with nowadays CMOS micro-power circuits (i.e. used in autonomous systems) which would allow improved figure of merit (*ZT*) materials based on low dimensional structures to be engineered. Two kinds of multilayer structures have been designed and realized: lateral and vertical structures, where heat and current flow along the in-plane or out-of-plane direction respectively. In the first case quantum confinement effects are used to enhance the electrical properties, while in the second phonon scattering is expected to reduce thermal conductivity. In order to obtain

useful thermoelectric effects the heterostructure must be several microns thick. Therefore, a growth technique which is capable of producing, in a reasonable time, high quality material with nanometer-scale control over a range of several microns is required. Low-energy plasma-enhanced chemical vapor deposition (LEPECVD) has been used in our case. Crystal quality and strain control have been investigated by means of high resolution X-ray diffraction and transmission electron microscopy. The thermoelectric characterization performed on both lateral and vertical multilayers indicates the viability of this material for the realization of thermoelectric devices. Values of ZT exceeding 0.1 at 293 K have been recently demonstrated.

#194 – QCL - optical feedback cavity enhanced spectrometer for trace gas analysis in the mid infrared: validation of non thermal plasma

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A highly sensitive spectrometer has been developed for pollutant trace gas detection in the mid infrared. The analyzer based on a Quantum Cascade Laser (QCL) and the Optical Feedback- Cavity Enhanced Absorption Spectroscopy (OF-CEAS) technique [1,2], is capable to measure concentration values in the pptv range of Formaldehyde (CH_2O) and Formic Acid (HCOOH).

In particular CH_2O has been classified, by the International Agency for Research on Cancer, as a carcinogenic substance. It also represents a good indicator of indoor pollution level since it is an oxidation product of many Volatile Organic Compounds (VOC). Furthermore there is a growing interest for Non Thermal Plasma (NTP) in environmental applications due to their high chemical reactivity at a low energetic cost. The most advanced application of NTP for the environment is the abatement of diluted pollutants, especially for indoor air treatment [3]. Therefore, the new spectrometer has been employed in a preliminary study of depollution processes by means of a Dielectric Barrier Discharge (DBD) plasma reactor.

The implemented OF-CEAS system is based on a thermoelectrically cooled, continuous wave Distributed-Feedback Quantum Cascade Laser, realized at Thales-III-V labs, emitting at a wavelength of 5.65 μm [4]. The laser radiation, which can be tuned over about 7 cm^{-1}, by changing the temperature, is directly coupled to a high finesse V-shaped cavity. The high reflectivity of the mirrors provides an optical interaction path of about 10 km. Working at a cavity pressure of about 50 mbar, with a sample gas flow in the range of tens standard cubic centimeter (sccm), a minimum detectable absorption coefficient of 1.6 x 10-9 cm^{-1} was demonstrated in 100 ms of integration time (single laser scan), which for CH2O corresponds to a detection limit of 60 pptv. The Allan Variance analysis displays an optimum integration time of 12 s leading to a detection limit down to 4.9 pptv for formaldehyde molecules [5].

The compact and robust QCL-OF-CEAS instrument has been successfully exploited as a diagnostic tool to validate Non Thermal Plasma indoor air treatment. A packed bed like DBD reactor was evaluated in terms of formaldehyde destruction. The destruction efficiency has been studied with varying input energy into the plasma at different values of formaldehyde concentration in the ppbv range. Moreover the QCL-OF-CEAS device allows a real time monitoring of other byproducts generated by the plasma treatment, such as HCOOH and O_3, with a detection limit at pptv and ppmv levels, respectively.

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#195

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#196 - Thermal transport in nanostructured semiconductors

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Thermoelectrics represent an important class of energy materials due to their ability of converting heat into electricity. Nevertheless, thermoelectric devices are mainly used only in niche markets (where reliability and durability are more important than the overall performance) because of their low efficiency. The key issue is to maximize the heat-to-current conversion efficiency for which purpose a material with high electrical conductivity, high Seebeck coefficient, and low thermal conductivity is actually needed. Such a material is unfortunately not provided by Nature. A way to increase the thermoelectric efficiency involves reducing the thermal conductivity (still preserving a good electrical one), which requires to design new materials where phonon transport is more largely affected by some addition structural feature than in pristine systems. It has been proposed that a primary approach to obtain this reduction is to generate suitable nano-structured (ns) semiconductors, where the typical grain size is smaller than the phonon mean-free-path, but it is still larger than the electron (or hole) one [1].
In this work I will discuss proof-of-concept computer experiments based on non-equilibrium molecular dynamics simulations aimed at understanding the role of crystallinity, granularity, and stoichiometry on lattice thermal conductivity in ns-Si and ns-SiGe systrems.

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#197 - Simulation of charge transport in ovonic materials

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Ovonic materials feature an electrical switching behavior, i.e., a sudden change in resistivity by several orders of magnitude when a threshold field is reached. Such behavior became recently of great technological interest and it can be studied by means of computational models based on new experimental data.
Carrier transport in ovonic materials is here investigated assuming thermally-assisted trap-limited conduction [1,2] and following different approaches. The hydrodynamic-like approach [2] is a 1D analytical model based on the use of the carrier energy distribution to calculate the local carrier concentration and the average electron energy, as well as the charge and energy fluxes. The results reproduce and interpret the available experimental findings in phase-change memory cells and provide a reasonable interpretation of the physical mechanisms governing the SNDR of this class of materials, but the extension to 3D geometries is not trivial. Thus a Monte Carlo simulation (MCS) of the transport problem has been set up. MCS can account for the microscopic dynamics of charge carriers in a nanometer amorphous system, provided that the transition rates describing the trap-limited conduction are given together with some coupling parameters and an appropriate description of the interaction between the ovonic nano device and the external contacts [3]. Coupling MCS with the solution of the Poisson equation in 3D is a necessary step in order to obtain a transport picture consistent with the electrostatic potential produced by the fixed charges in the localised states inside the amorphous material. However, due to the computational burden required by the Monte Carlo-Poisson computational framework, it is useful to design an effective and fast simulative tool, still catching the relevant microscopic aspects for the transport process at hand. This model is the most recent development of our group: it includes a 3D network of randomly-placed nodes, each of them coarse-graining a region of the device. Two sets of equations can be derived by imposing the charge-flux and charge energy-flux balances at each node. The model is current driven, following the experimental set up, and is coupled to the Poisson equation. Results can be obtained for the nanostructures used in the experiments and can be employed to explore innovative device and contact geometries. The above model is being extended to include lattice heat transport by adding the lattice heat balance equation to the set of the equations describing electric and carrier-energy transport, thus providing a simulation tool that can account for the amorphous-crystalline phase transformation taking place at high external currents in this class of devices.

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#198 - The glassy state, magnetically viewed from the frozen end

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It is by now an established fact that the glass transition is accompanied by the formation of so-called dynamical heterogeneities (DHs) or coherently re-arranging regions (CRRs) in the supercooled liquid below the melting temperature T_m. These DHs continue to exist well below T_m till the Kauzmann temperature T_K and their mutual hindering is responsible for the rigidity of the amorphous solid1. However, below T_K the DHs become static inhomogeneities which can take the form of crystal embryos (CEs), regions of enhanced regularity (RERs) (in the purest glass) or even nano- and micro-crystals (in the multi-component glasses). These entities are the frozen remnants of the DHs or CRRs and are ubiquitous in the amorphous solid state. Their manifestation has been discovered [1] at the lowest temperatures ($T < 1$ K) when the remaining degrees of freedom are acoustic phonons and the so-called tunneling systems (TSs). The TSs become quantum-mechanical probes of the existence of the CEs and specialize into two types: ordinary two-level systems (2LSs) and anomalous TSs (ATSs) which turn out to be extremely sensitive to weak magnetic fields (a few Oe). A simple model made up of a dilute gas of 2LSs and ATSs will be shown to be able to explain all of the magnetic effects reported for the cold multi-silicate and organic glasses in the last 15 years or so: thermal, dielectric constant, dielectric loss, and polarization echo response to weak magnetic fields. In particular, the model stemming from the existence of the CEs probed by the ATSs explains the dependence of the polarization echo amplitude on the magnetic field, on the electric field, on the isotopic composition (novel isotope effect) and on the pulses waiting time (oscillations in the amplitude disappearing at the higher fields) [2]. The agreement between theory and experiment is excellent and there is no need to resort to nuclear electric quadrupoles in the glasses to explain the experimental data. At the lowest temperatures (ca. 5 mK) the interactions between ATSs lead to the freezing of the dynamics of the ATS electric dipoles which manifests itself in the form of a spin-glass like transition and a cusp in the dielectric constant (as observed [2]).

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#199 - Phonon softening and structural instabilities in TiSe2

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Titanium diselenide is a transition-metal dichalcogenide showing an intriguing phase transition at a critical temperature T=200 K. Several mechanisms have been proposed to clarify its origin, but the matter is still under debate. Recent theoretical works support the idea of excitonic insulator mechanism [1] but a Jahn-Teller effect has also been proposed, and it is clear that the electron-lattice interaction plays and important role in this structural instability [2].
In this work we investigate the lattice distortion calculating phonon frequencies and eigenvectors for the undistorted structure within DFT-LDA. We also perform total energy calculations for distorted structures in a 2x2x2 supercell.
We underline the key role of pressure and lattice constants optimization in such phonon calculations, showing that neglection of the zero stress condition may affects strongly the theoretical predictions [3].

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#200 - Intrinsic nature of the excess electrons distribution at the TiO₂(110) surface

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Among the many fascinating and interesting properties of the TiO₂, the Ti-3d gap state that appears when the surface is reduced plays a crucial role. Even if TiO₂ is a subject of many studies, the origin of this gap state and its spatial localization are still unclear. In order to get more insight into its spatial localization, we have reduced the TiO₂(110) surface in a chemically controlled way by depositing Na alkali atoms and exploited the resonant photoelectron diffraction (RESPED) technique. This synchrotron radiation technique is based on the measurement of the angular distribution of the intensity of photoemission peaks as a function of the angle of analysis, recorded in the Na doped TiO(110) case for photoelectrons from the Ti-3d gap state excited at the Ti 2p-3d resonance. By comparing the experimental patterns with multiple scattering calculated ones we have found that the excess electrons are shared by several surface and subsurface Ti sites, with the dominant contribution on a specific subsurface site (in agreement with density functional theory calculations), with negligible contribution from interstitial Ti ions, strikingly similar to the defective TiO₂(110). These findings are clear evidence that the distribution of the charge found in the band gap is an intrinsic property of TiO₂(110) and it is independent from the way excess electrons are created.

#201 - Azimuthal dichroism in near-edge X - ray absorption fine structure spectra of planar molecules

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The dependence of the near-edge x-ray absorption fine structure (NEXAFS) spectrum of molecules on the photon electric field direction is investigated by means of first principles simulations based on density-functional theory with the transition-potential approach. In addition to the well-known dependence of the NEXAFS resonances on the orientation of the electric field with respect to the molecular plane, we demonstrate that for planar molecules with sufficient in-plane anisotropy such as pentacene, a dichroic effect is computed with a splitting of the σ^* resonance as a function of the azimuthal orientation of the photon electric field in the molecular plane. The σ^* splitting is investigated as a function of the length of acenes and closely related molecules. A proper assignment of such spectral features guided by theory together with variable polarization experiments, may allow one to completely determine the orientation of molecules at interfaces.

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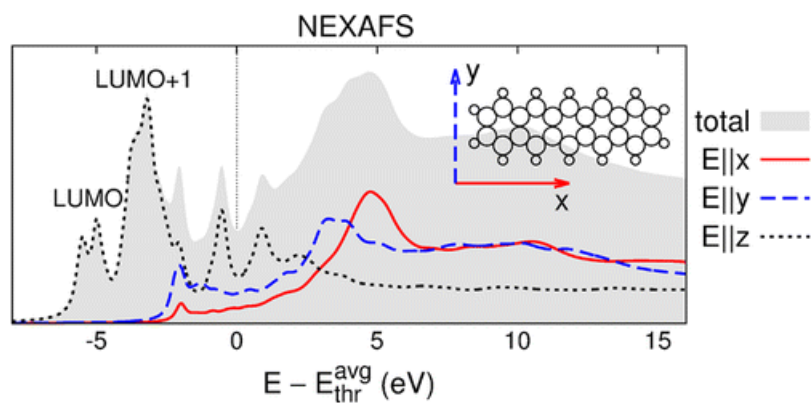
#202 - Competing phenomena at n-type interface between polar insulating-oxides and SrTiO₃ band insulator

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The discovery of a two dimensional electron gas (2DEG) at the interface between $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) heterostructures raised a huge interest since its discovery [1], because of the intriguing functionalities related to this phenomenon, including high electron mobility [2], large magnetoresistance [3], and superconductivity [4]. The mechanism behind this phenomenon have not yet fully understood and several issues, like the real ground state of the system, are still hotly debated.

In this contribution, I will present an overview of the most interesting experimental results appeared in the last few years on this topic, together with new insights on the phenomena obtained from x-ray [5] and STS spectroscopy measurements [6-7] of LAO/STO and of other novel artificial titanate heterostructures.

We find that a structural and electronic reconstruction of the interface precede the appearance of the 2DEG. In particular, it is shown that the intrinsic instability of the weakly polar (001) $SrTiO_3$ surface is the main driving force for the inversion of the 3d-band hierarchy at the interface. This reconstruction can be or not accompanied by the appearance of a metallic state, depending on the extent of localisation of doped electrons in in-gap interface-states [8]. These results challenge some of the most accredited theoretical models describing this system.

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#203 - Inverse magnetoelectric effects at ferromagnet-ferroelectric interfaces

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Interfacial magnetoelectric coupling for electrically altering the magnetization of ferromagnetic electrodes is a viable path to achieve the electrical writing of the magnetic information in spintronic devices. Exploiting the piezoelectric behavior of a ferroelectric material (FE) in contact with a ferromagnetic (FM) thin film, the electric control of the magnetic anisotropies can be achieved [1]. However strain-mediated methods seems hardly suitable for integration in spintronic devices, where the piezoelectric activity of a FE layer would be inhibited by the growth on a substrate. This is the reason why there is a growing interest towards "purely electric" magnetoelectric effects. For the paradigmatic $Fe/BaTiO_3$ (BTO) system, sizable changes of the interfacial Fe magnetic moment upon reversal of the dielectric polarization of BTO have been predicted [2]. Furthermore in Fe/BTO/Co tunneling junctions, huge variations of the magnetoresistance have been obtained by reversing the BTO polarization [3]. Nevertheless, so far a clear understanding of the basic physical mechanisms leading to such a macroscopic effect is still lacking.

In this paper we demonstrate that the effect of reversing the BTO polarization is not a modest change of the interfacial Fe magnetic moment but the full switching of the interface magnetic ordering, eventually leading to the cancellation of the average Fe interface magnetization. By XMCD measurements on patterned Co(6ML)/Fe(2ML)/BTO/LSMO micro-capacitors, we found that, at RT, the average magnetization of the FeOx interface layer disappears for the dielectric polarization vector of BTO pointing outwards from the FeOx layer. LSDA+U calculations show, indeed, that the switching from the ferromagnetic to the antiferromagnetic ordering within the interface FeOx layer can be driven by the BTO polarization reversal. A "giant" interface inverse magnetoelectric effect results, which can be fruitfully exploited in devices such as tunneling junctions, where just the interface magnetization determines the magnetoresistance. In view of the exploitation of magnetoelectric effects in a wider class of devices, where the entire magnetization of a magnetic layer should be switched, some recent results on the purely electric control of the magnetic anisotropy in FeCoB thin films on BTO will be finally presented.

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#204 - Inhomogeneous superconductivity in oxide interfaces

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The two-dimensional electron gas at the the $LaAlO_3/SrTiO_3$ or $LaTiO_3/SrTiO_3$ oxide interfaces becomes superconducting when the carrier density is tuned by gating. The measured resistance and superfluid density reveal an inhomogeneous superconductivity resulting from percolation of filamentary structures of superconducting "puddles" with randomly distributed critical temperatures, embedded in a non-superconducting matrix [1]. Following the evidence that superconductivity is related to the appearance of high-mobility carriers, we model intra-puddle superconductivity by a multi-band system within a weak coupling BCS scheme. The microscopic parameters, extracted by fitting the transport data with a percolative model, yield a consistent description of the dependence of the average intra-puddle critical temperature and superfluid density on the carrier density [2].

Assuming that the sizable Rashba spin-orbit coupling in these systems is responsible for the occurrence of the inhomogenous state [3], we investigate the interplay between electronic phase separation and superconductivity [4].

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#205 - Competing Magnèli-like phases driven by substrate-induced strain in TiO_2 anatase thin films

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We used high-resolution transmission electron microscopy (HRTEM), high angle annular dark field scanning TEM (HAADF/STEM) and simulation together with density functional theory (DFT) calculations to characterize the structure and defects in $LaAlO_3$(LAO)-supported TiO_2 anatase thin films. The analyses provided evidence of a peculiar growth mode of anatase on LAO characterized by the formation of an epitaxial layer at the film/substrate interface. The film is split into two adjacent slabs of about 20 nm each characterized by a different family of crystallographic shear (CS) superstructures, namely (103)- and (101)-oriented CS plane structures, in the outer film region and in proximity of the film/substrate interface, respectively [1]. HAADF/STEM and Energy Dispersive X-ray Spectroscopy (EDXS) revealed the presence of Al interdiffusion from the substrate into the first slab of the film. By combining HRTEM results and relevant image simulations with DFT calculations we determined the atomic structure of the CS planes and showed that they are based on the cubic TiO structure resembling the classical rutile-derived $TinO_{2n-1}$ Magnéli phases [2]. DFT-derived thermodynamic predictions provided information on the stability of the observed structures as well as on the relations to the growth dynamics and to the matching with the bare substrate. Interestingly, we found that the crossover in the film between the two regions hosting the two different Magnéli-like phases corresponds to the transition from a three-dimensional to a two-dimensional growth mode in the film structure, as observed by in-situ reflection high energy electron diffraction (RHEED) during film growth [3].

Based on the experimental and theoretical evidences, we proposed a model for the peculiar growth mode of the overlayer and drew conclusions on the role of cation interdiffusion on film nucleation, providing an explanation for the relative predominance of (103) and (101) CS planes in the body of the film and close to the interface with the substrate, respectively.

Our findings open intriguing perspectives toward the possibility of engineering new heterostructures with targeted properties based on anatase by the control of oxygen vacancies and to the technological application of Magnéli phases in anatase.

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#206 - Ordering and multiple phase transitions in ultrathin nickelate superlattices

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We interpret via advanced ab initio calculations the multiple phase transitions observed recently in ultrathin $LaNiO_3/LaAlO_3$ superlattices. The ground state is insulating, weakly charge ordered, and antiferromagnetic due to concurrent structural distortion and weak valency disproportionation. We infer distinct transitions around 50 K and 110 K, respectively, from antiferromagnetic order to moment disorder, and from a structurally dimerized insulator to an undistorted metallic Pauli paramagnet (exhibiting a cupratelike Fermi surface). The results are in satisfactory agreement with experimental results.

#207 - MuSR spectroscopy in the skyrmion candidate single crystal $Ba_2CuGe_2O_7$

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A muon spin rotation/relaxation (muSR) investigation of the magnetic phase diagram of the two-dimensional spiral antiferromagnet $Ba_2CuGe_2O_7$ is presented. Neutron scattering measurements [2,3] identified three different magnetic phases in $Ba_2CuGe_2O_7$ as a function of magnetic field: an almost AF cycloidal spin structure, an incommensurate (IC) double-k AF-cone phase and an AF commensurate Neel phase along z-axis [3].

The complex spin structure is a consequence of the crystal symmetry that makes this material very attracting for at least two reasons: firstly the multiferroic properties are theoretically predicted for this class of helimagnets to produce a strong coupling between ferroelectric and ferromagnetic order parameters, a feature of potential applicative interest. Secondly, a skyrmion lattice is expected from theoretical studies [1].

Skyrmions, a spin textures analogous to hair licks, have both a fundamental interest, as localised excitations, and a potential as self assembling nanoscopic magnetic dots. They are similar to vortices, hence they modify the the internal field distribution.

Here we address the analysis of muon spectroscopy, which provides clear zero field signatures of the magnetic transitions, by means of the spectrum of precession frequencies, determined by the internal field distribution. The modifications induced by applied fields will be discussed in terms of a parallel DFT investigation, aimed at the ab-initio determination of the muon stopping site.

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#208 - Gaps and hidden orders in correlated fermionic systems

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The one dimensional (1D) Hubbard Hamiltonian exhibits hidden long-range orders in its two gapped phases, namely the Mott insulating and the Luther-Emery liquid phases [1]. The discovery opened the way to a general result obtained in [2], stating that long-range order is present in every gapped phase of 1D fermionic systems. It is captured by two-point correlators of charge and/or spin operators of nonlocal type, known as string and parity operators. At least one of them remains asymptotically finite in each gapped phase, vanishing at the transition. Their identification allows for a classification of the different microscopic orders underlying the phases, among which one can recognize also the Haldane charge order. These type of orders are directly accessible to experimental detection via single-site/single atom imaging in optical lattices. We discuss the above findings and give some preliminary result about their generalization to the two-dimensional case.

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#209 - Defect states and excitations in a Mott insulator with orbital degrees of freedom: Mott-Hubbard gap versus optical and transport properties

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We address the role played by charged defects in doped Mott insulators with active orbital degrees of freedom. It is observed that defects feature a rather complex and rich physics, which is well captured by a degenerate Hubbard model extended by terms that describe crystal-field splittings and orbital-lattice coupling, as well as by terms generated by defects such as the Coulomb potential terms that act both on doped holes and on electrons within occupied orbitals at undoped sites. We show that the multiplet structure of the excited states generated in such systems by strong electron interactions is well described within the unrestricted Hartree-Fock approximation, once the symmetry breaking caused by the onset of magnetic and orbital order is taken into account. Furthermore, we uncover new spectral features that arise within the Mott-Hubbard gap and in the multiplet spectrum at high energies due to the presence of defect states and strong correlations. These features reflect the action on electrons/holes of the generalized defect potential that affects charge and orbital degrees of freedom, and indirectly also spin ones. The present study elucidates the mechanism behind the Coulomb gap appearing in the band of defect states and investigates the dependence on the electron-electron interactions and the screening by the orbital polarization field. As an illustrative example of our general approach, we present explicit calculations for the model describing three t_{2g} orbital flavors in the perovskite vanadates doped by divalent Sr or Ca ions, such as in $La_{1-x}Sr_xVO_3$ and $Y_{1-x}Ca_x VO_3$ systems. We analyze the orbital densities at vanadium ions in the vicinity of defects, and the excited defect states which determine the optical and transport gaps in doped systems. (published in PRB 87, 045132 (2013)).

#210 - New results in quantum simulation with cold atoms

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Cold atomic ensembles and Bose Einstein condensate have proved to be very versatile system to implement Feynman's idea of "quantum simulators". This is largely due to the possibility to control their coherent dynamics as well s to control the mutual interaction between the atoms. Most of the attention sofar has been focussed on the tailored implementation of many body hamiltonians. Here we will show how cold atoms can simulate engineered environments . In particular we will discuss the case of pure dephasing, showing a rich non markovian dynamics. Further example of systems we will discuss are polarons in two components BEC and the simulation of many body hamiltonians in BEC trapped in field cavities.

#211 - Design of a Lambda system for population transfer in superconducting nanocircuits

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The implementation of a Lambda scheme in superconducting artificial atoms could allow detection of stimulated Raman adiabatic passage (STIRAP) and other quantum manipulations in the microwave regime. However symmetries which on one hand protect the system against decoherence, yield selection rules which may cancel coupling to the pump external drive. The tradeoff between efficient coupling and decoherence due to broad-band colored Noise (BBCN), which is often the main source of decoherence is addressed, in the class of nanodevices based on the Cooper pair box (CPB) design. We study transfer efficiency by STIRAP, showing that substantial efficiency is achieved for off-symmetric bias only in the charge-phase regime. We find a number of results uniquely due to non-Markovianity of BBCN, namely: (a) the efficiency for STIRAP depends essentially on noise channels in the trapped subspace; (b) low-frequency fluctuations can be analyzed and represented as fictitious correlated fluctuations of the detunings of the external drives; (c) a simple figure of merit for design and operating prescriptions allowing the observation of STIRAP is proposed. The emerging physical picture also applies to other classes of coherent nanodevices subject to BBCN.

#212 - Weak measurement of the Goos-Hänchen shift

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It is well known from quantum physics that weak measurements offers a platform of amplifying and detecting very small signals. In this letter, we present the first experimental observation of the Goos-Hänchen shift. A bounded beam of light, reflected at a planar interface does not obey the ray optics predictions, it suffers diffractive correction to the law of reflection or Snell's law. The most prominent of these are the Goos-Hänchen shift (GH) [1] and the Imbert-Fedorov (IF) [2] shift. Angular analogous to the GH and the IF effect have recently been observed, as well as the spin Hall effect of light (SHEL) [3].The last one is connected with the IF shift, being a separation orthogonal to the plane of the incidence of the two spin components of the reflected or transmitted beam. These effects are not only common for simple planar interfaces but were also observed or predicted in photonic crystals, waveguides or resonators.

Generally the measurements of these optical shifts are challenging tasks because they are tiny phenomena. A weak measurement approach is considered to be a successful method for the observations of these effects. A weak measurement is one in which the coupling between the measuring device and the observable to be measured is so weak that the uncertainty in a single measurement is large compared with the separation between the eigenvalues of the observable. In a remarkable experiment, Hosten and Kwiat [3] where the firsts that applied this experimental scheme to the measurement of optical beam shifts. They reported the first experimental observation of the SHEL.

In this article we present the first experimental observation of the GH effect by a weak measurement scheme. The "weak measurement device" [4] is a prism which introduces a small lateral displacement Dp (Ds) for the p(s) polarization of a Gaussian beam in total internal reflection (TIR).

A polarizer and an analyzer select the initial and the final linear polarizations to be at angles α and β with respect to the horizontal in the xy plane. The weak measurement scheme works as follow [4,5], if the polarizer and the analyzer are set to $\alpha=\pi/4$ and $\beta=\alpha+\pi/2+\varepsilon$ ($\varepsilon \ll 1$) respectively, the emerging beam is laterally shifted of a quantity $\frac{1}{2}\Delta GH\cot(\varepsilon)$ where $\Delta GH=Dp–Ds$. We measure the separation $\Delta GH\cot(\varepsilon)$ in between the two beams corresponding to the two polarizations settings $\alpha= \pi/ 4$ and $\beta= \alpha+\pi/ 2\pm \varepsilon$. The small beam displacement ΔGH introduced by the GH effect is thus amplified by a factor of $\cot(\varepsilon)$.

In summary, we have demonstrated that the weak measurement is a valuable approach for observing the GH shift in TIR. Although our results are strictly valid only for TIR, furthermore we expect that they can be extended, experimentally and theoretically, to the case of metallic mirrors and multilayer dielectric mirrors. This technique, based on an amplification scheme, can be particularly interesting in applications where the GH shift is used as a sensitive meter, such as in bio-sensing or position detection. Beam shift can also be very important for photo-lithography where the partial spatial coherence plays a critical role.

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#213 - Theoretical modelling of strongly coupled anthracene microcavities

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Strongly coupled organics based microcavities are presently much investigated. Apart from the large oscillator strength of their Frenkel excitons, common to J-aggregate based microcavities, molecular crystal microcavities are often characterized by the presence of well developed vibronic replicas that take part into the polariton formation and affect their luminescence properties [1]. In particular, recent experiments reporting the observation of polariton lasing in anthracene microcavities [2,3] have attracted much interest. We discuss here a simple phenomenological model accounting for the onset of the non-linear threshold based on a master equation including the relevant relaxation processes and employing realistic material parameters. The mechanism governing the build-up of the polariton population is identified and the role of polariton-polariton bimolecular quenching discussed.

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#214 - Correlations, entanglement or nothing: recent results on bilinear interactions of light modes

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Entanglement is at the heart of quantum technology. During the last two decades much attention has been devoted to the generation and the characterization of entanglement in bipartite and multi-partite systems. In the realm of continuous variables, attention has been focused to Gaussian states and, among the the possible mechanisms to generate Gaussian entanglement, the one consisting in the mixing of squeezed states at a beam splitter is of special interest in view of its feasibility. A beam splitter is a simple, passive device whose action is described by a bilinear Hamiltonian and, in view of this simplicity, its fundamental quantum properties are often overlooked.
Correlations - We first review few simple paradigmatic examples of the generation of two correlated light beams by mixing single-mode continuous variable states with the vacuum at a beam splitter.
Entanglement - Then we address the interaction of two Gaussian states (i.e., states with Gaussian Wigner functions) interfering at a beam splitter and analyze the correlations exhibited by the resulting bipartite system. We show that nonlocal correlations (entanglement) arise if and only if the fidelity between the two input Gaussian states falls under a threshold value depending only on their purity and on the transmissivity of the beam splitter. Our result clarifies the role of squeezing as a prerequisite for entanglement and provides a tool to optimize the generation of entanglement by passive devices [1].
Nothing - We finally present the peculiar case of the interference of two modes exited in the same Gaussian state: now no correlations build-up at all and, furthermore, if the first moments are equal to zero, then the two-mode state is left unchanged, as the beam splitter is not present. Nevertheless, we show that it is possible to unveil "hidden correlations" between them, thus discovering the presence of the beam splitter [2].

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#215 - Ultrafast cavity-polariton relaxation dynamics in a strongly-coupled J-aggregate microcavity

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Cavity-polaritons have attracted interest [1] due to the possibilities of interesting applications like low-threshold polariton lasers [2] and also to study the fundamental properties like Bose-Einstein condensation [3]. Most of the advances made until now are in the case of strongly coupled inorganic-semiconductor quantum wells in a microcavity which work primarily at cryogenic temperatures due to the small vacuum-Rabi splitting. J-aggregates of cyanine dyes have an oscillator strength an order of magnitude higher leading to observation of vacuum-Rabi splitting of ~ 80 meV in strongly coupled microcavities at room-temperatures [4]. We have studied the ultrafast relaxation dynamics of cavity polaritons in a J-aggregate microcavity using pump-probe spectroscopy [5] and time-resolved up-conversion [6]. Using 15 fs broadband visible pulses centered at 590 nm, pump-probe spectroscopy was performed on the strongly coupled J-aggregate microcavity at resonance condition to observe the role of exciton-reservoir (ER) on the relaxation dynamics of the upper (UPB) and lower polariton branches (LPB). As calculated in theoretical models [7], ultrafast non-radiative relaxation from the UPB into the ER in 150fs and a slower relaxation from the ER to the LPB in a time of 3.2 ps were observed, along with ultrafast radiative decay of the polaritons in 60 fs. These dynamics were successfully modeled for the relaxation processes and found to be in agreement with expected values [8]. Vacuum-Rabi oscillations, periodic exchange of energy between the polariton states, are the consequence of strong-coupling between the exciton and cavity modes. For vacuum Rabi splitting of 133 meV, 30 fs period oscillations can be expected between the polariton states before they radiatively decay out of the microcavity. To

observe these oscillations, the transmission of 7 fs broadband visible pulses, was gated using a 13 fs nIR pulse centered at 915 nm, to generate the sum-frequency by overlapping temporally and spatially on a type-I phase-matched 20 µm BBO crystal. The transmission was resolved by changing the delay of the gate-pulse with respect to the cavity transmission. At resonance, the polariton modes showed 30 fs oscillations as expected. These experimental evidences are important steps towards realization of polariton based room-temperature applications.

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#216 - Formation and optical pumping of ultracold RbCs molecules

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Andrea Fioretti (CNR- INO, Pisa)

Ultracold RbCs molecules have been produced starting from laser-cooled Rb and Cs atoms in a double MOT by short-range photoassociation on both sides of the $Rb(5S_{1/2})+Cs(6P_{3/2})$ dissociation limit. The photoassociated levels, assigned to the low vibrational levels of the 5th 0^+ excited electronic state correlated to the $Rb(5P_{3/2})+Cs(6S_{1/2})$ dissociation limit, mainly decay into deeply bound levels of the ground triplet electronic state. The molecules radiatively stabilized in the a $^3\Sigma^+$ state are detected by resonant enhanced two-photon ionization. We are now trying to transfer the population either to the lowest vibrational level of the a $^3\Sigma^+$ state or to the ground singlet state by an optical pumping process using uncoupled or coupled excited states respectively. The process is firstly simulated considering the relevant potential curves and different possible laser sources.

#217 - Open quantum systems in the parametric representation and the spin-1/2 Heisenberg star with frustration

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A physical quantum system whose interaction with the surrounding environment can not be neglected is usually denoted as an Open Quantum System (OQS). In quantum information theory, OQS are usually treated in terms of reduced density matrices, an approach which in principle allows one to take into account the full quantum behaviour of the environment and to describe in a natural way the entanglement between it and the system, but at the same time suffering of serious loss of phase information in its actual implementations. A rather different situation, where the presence of a "classical" environment is implicitly acknowledged, is considered when one supposes that the Hamiltonian of a quantum system has a parametric dependence on external variables, which may lead to the appearance of peculiar quantum features as, e.g., the Berry phase.
We propose a parametric representation of OQS, based on the use of generalized coherent states for the environment, which is exact, and at the same time gives the possibility to follow the crossover from a quantum to classical environment.
As a prototypical example, we have considered the antiferromagnetic Heisenberg star with frustration, i.e. a qubit (or spin-1/2, the principal system) surrounded by a set of interacting spins, which represent the environment and which can finally be described as a single spin S, whose magnitude depends on the ratio between the intra-environment and qubit-environment couplings. The description of the spin star by the parametric representation shows that the emergence of a geometric (Berry) phase for a spin in an external magnetic field does follow from the fact that the true physical set up, of which the "spin in a field" is just a semiclassical-like parametric representation, is that of a quantum composite system in an entangled state. In fact, the Von Neumann entropy of the spin-1/2, which is finite due to the existence of the environment (the spin-S), turns out to be the binary entropy of the normalized Berry's phase.

#218 - Some recent developments in non equilibrium statistical mechanics

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We shall discuss some results in non equilibrium statistical mechanics obtained in the study of macroscopic fluctuations of thermodynamic variables and currents. In particular the study of macroscopic fluctuations shows that phase transitions not permitted in equilibrium are possible and actually take place in simple models of lattice gases. Furthermore the work in a transformation from a stationary state to another one, suitably renormalized, satisfies a Clausius type inequality which implies that also out of equilibrium quasistatic transformations are optimal. The talk is based on work carried out during the last decade in collaboration with L. Bertini, A. De Sole, D. Gabrielli, C. Landim.

#219 - On the Riemann problem of gas dynamics

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Luigi Quartapelle (Primo autore, Dipartimento di Scienze e Tecnologie Aerospaziali , Politecnico di Milano)

The talk provides a tutorial introduction to the subject of the Riemann problem of gasdynamics. This is a particular initial value problem for the Euler equations governing compressible flows in one dimension. The initial data consist of two uniform distributions of the flow variables - mass, momentum and total energy density - separated by a discontinuity. A prototypical example is the so-called shock tube experiment, where a fluid at rest inside a straight tube is in two different thermodynamic states separated by a diaphragm that is removed instanteneously. In the last fifty years, the general Riemann problem with non-zero initial velocities has also played a pivotal role in the field of numerical simulations of compressible flows, particularly transonic and supersonic ones around aircrafts, and of gasdynamical phenomena of astrophysical interest, possibly coupled with magnetic effects. Indeed, the representation of the flow variables provided by the solution to local Riemann problems has replaced the discretization paradigm based on the Taylor series approximation, since it embodies the basic conservation principles governing fluid dynamic systems, by construction.

The self-similar solution emerging from the initial condition of the Riemann problem consists of two nonlinear waves, with a contact discontinuity propagating in between. Within the nonlinear waves, the fluid properties vary due to irreversible and reversible processes, associated respectively to shock waves and continuous isentropic transitions. Across the intermediate jump, the pressure and the velocity are instead continuous. A system of two algebraic equations is thus obtained for the two unknown values of any thermodynamic variable - excluding pressure - on the two sides of the contact discontinuity. For the ideal gas with constant specific heats, only compression shocks and rarefaction fans are entropically admissible and an analytic representation of the fluid state within the nonlinear waves allows for an explicit closed-form expression of the Riemann problem. The ideal gas model is however only a very special case, while thermodynamic principles allow for nonlinear waves of different kinds, endowed with a richer structure. When the gas model exhibits a region of non-convex isentropes, as, e.g., the van der Waals gas with sufficiently complex molecular arrangement (more than 7 atoms), nonlinear waves with opposite behavior with respect to that of the ideal gas may occur, such as rarefaction shocks and compressive fans. Moreover, also composite waves may arise, consisting in a discontinuity attached to a fan, both cooperating to gas compression or to its rarefaction. Furthermore, triple composite waves may occur, consisting of shock-fan-shock or fan-shock-fan combinations, with the three wave parts all contributing to either compression or rarefaction, respectively.

#220 - Normal fluid profiles in Helium II counterflow channels

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Superfluid ^{4}Helium turbulent flows in counterflow channels are investigated via two-dimensional self-consistent numerical simulations. The range of the heat fluxes employed in the simulations implies that the superfluid phase is characterized by the presence of quantized vortex lines (vortex points in 2D) which are responsible for the mutual interaction between the two components, normal and superfluid, constituting the low-temperature liquid phase of ^{4}He (also referred to as He II). The temporal evolution of the vortex distribution in the channel is determined integrating the Langrangian equation of motion deduced by Schwarz [1], while the calculation of the time dependent normal fluid velocity at a lengthscale δ smaller than the average inter-vortex spacing λ is performed applying the Ψ - ω formulation to the two-fluid Landau-Khalatnikov [2] equations extended in order to take into account the mutual friction interaction arising from the quantized vortex motion. This mutual friction term is first calculated at a macroscopic lengthscale $\Delta > \lambda$ employing the theoretical framework elaborated by Hall and Vinen [3] and then interpolated on the mesoscopic computational grid on which the normal fluid equation of motion is solved. The results obtained are investigated at the macroscopic lengthscale Δ determining the coarse-grained superfluid and normal fluid velocity profiles and the coarse grained superfluid vortex density profiles, for different values of the average vortex-line density. The vortex density profiles confirm the vortex polarization predicted by Barenghi et al. [4] while the velocity profiles of the two He II components show a clear vorticity locking, as illustrated in [5]. The results are compared to the achievements obtained in past numerical studies [6], where no interaction of the vortices on the normal fluid was taken into account, and to the analytical laminar steady solutions determined applying Geurst's approach [7] to cartesian geometry. In addition, statistical analysis of the superfluid velocity field are performed showing a non-classical behaviour, coeherently with the numerical simulations realized by White et al. [8].

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#221 - Dynamical imaginary-time correlations from auxiliary fields Quantum Monte Carlo

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Quantum Monte Carlo (QMC) simulations of many body fermionic systems are considerably complicated by the well known sign problem [1]. Although very accurate approximation schemes have been developed for the calculation of static properties, like structure functions and energy, the possibility of extending such methodologies to the investigation of dynamical properties is still largely unexplored [2]. Recently, a number of innovative QMC methods have been conceived which map the imaginary time evolution into a random walk in the abstract manifold of Slater determinants. In such approaches the sign problem is not circumvented and still requires approximations, but emerges in a different - and hopefully easier to handle - way.
We have focused on the phaseless auxiliary Fields QMC method (AFQMC), developed by Shiwei Zhang [3]. Generalizing the formal manipulations suggested by Assaad et al. [4], we propose a practical scheme to evaluate dynamic correlation functions in imaginary time, giving access to the study of excitations and response functions of interacting fermionic systems.
We have explored systematically the effects of the phaseless approximation, underlying the AFQMC technique and its dynamical generalization, via the study of exactly solvable simple models, comparing AFQMC predictions with exact solutions. We will present also results about a two-dimensional electron liquid, providing comparisons with other QMC techniques.

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#222 - Quantum Gibbs ensemble Monte Carlo

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We present a new path integral Monte Carlo method to study the gas-liquid coexistence line of a quantum fluid of Bosons which is a natural extension of the classical Gibbs ensemble Monte Carlo method of Panagiotopoulos. As an illustrative application of our method we apply it to the $\mbox{}^4$He and to the square well Bosons in their large mass regime, close to the classical result, and at an intermediate mass.

#223 - Static and dynamic friction in sliding colloidal monolayer

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In a recent experimental breakthrough, the controlled sliding of two dimensional colloidal crystals over perfectly regular, laser generated periodic or quasi-periodic "corrugation" potentials has been realized in Bechinger's group [1].
Based on realistic molecular dynamics simulations which reproduce the main experimentally observed features, we explore the potential impact of colloid monolayer sliding in nanotribology [2]. The free motion of edge-spawned kinks and antikinks in smooth incommensurate sliding is contrasted with the kink-antikink pair nucleation at the large static friction threshold in the commensurate case. The Aubry pinning/depinning transition is also demonstrated as a function of parameters including the corrugation amplitude. Colloid simulated sliding data allow the extraction of frictional work directly from particles coordinates and velocities as a function of classic friction parameters, primarily speed, and corrugation strength (representing "load"). Analogies with sliding charge-density waves, driven Josephson systems and the sliding of rare gas islands, and other novel features suggest further experiments and insights, which promote colloid sliding to a novel friction study instrument [3].

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#224 - Zero - sound mode in a neutral Fermi liquid: dynamic fermionic correlations applied to two - dimensional 3He

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Recent neutron scattering experiments on 3He films have observed a zero-sound mode, its dispersion relation and its merging with – and possibly emerging from– the particle-hole continuum [1].
We develop a practical quantum Monte Carlo scheme to calculate imaginary time correlation functions for moderate-size fermionic systems. Combined with an efficient method for analytic continuation [2], this scheme affords an extremely convincing description of the experimental findings.

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#225 - New metrics for economic complexity: measuring the intangible growth potential of countries

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Economic Complexity is a new line of research which portrays economic growth as an evolutive process of ecosystems of technologies and industrial capabilities. Complex systems analysis, simulation, systems science methods, and big data capabilities offer new opportunities to empirically map technology and capability ecosystems of countries and industrial sectors, analyse their structure, understand their dynamics and measure economic complexity. This approach provides a new perspective for data-driven fundamental economics in a strongly connected, globalised world.

In particular here we discuss how it is possible to assess the competitiveness of country and complexity of products starting from the archival data on export flows which provides the matrix of countries and their exported products. According to the standard economic theory the specialization of countries towards certain specific products should be optimal. The observed data show that this is not the case and that diversification is actually more important. Specialization may be the leading effect in a static situation but the strongly dynamic and globalized world market suggests instead that flexibility and adaptability are essential elements of competitiveness as in bio-systems.

The crucial challenge is therefore how these qualitative observations can be turned into quantitative variables. We have introduced a new metrics for the Fitness of countries and the Complexity of products which corresponds to the fixed point of the iteration of two nonlinear coupled equations. The information provided by the new metrics can be used in several ways. As an example, the direct comparison of the Fitness with the country GDP per capita (Fitness-Income Plane) gives an assessment of the non-expressed potential of growth of a country. This can be used as a predictor of GDP evolution or stock index and sectors performances.

The global dynamic in the Fitness-Income Plane reveals, however, a large degree of heterogeneity which implies that countries can evolve with different level of predictability according to the specific zone of the Fitness-Income plane they belong to. This heterogeneous dynamics is often disregarded in usual economic analysis. When dealing with heterogeneous systems, in fact, the usual tools of linear regressions become inappropriate. Making reliable predictions of growth in the context of economic complexity will then require a paradigm shift in order to catch the information contained in the complex dynamic patterns observed.

These methods and concepts can give concrete contributions, as other possible applications, to risk analysis, investment opportunities analysis, policy-modelling of country growth and industrial planning.

#226 - Fast two dimensional "bubble" analysis of biopolymer filamentous networks pore size from confocal microscopy thin data stacks

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The average pore size ξ_0 of filamentous networks assembled from biological macromolecules is one of the most important physical parameters affecting their biological functions. Modern optical methods, such as confocal microscopy, can non-invasively image such networks, but extracting a quantitative estimate of ξ_0 is a non-trivial task. We present here [1] a fast and simple method based on a two-dimensional "bubble" approach, which works by analyzing one-by-one the (thresholded) images of a series of three-dimensional thin data stacks. No skeletonization or reconstruction of the full geometry of the entire network is required. The method was validated by using many isotropic in silico generated networks of different structures, morphologies and concentrations. For each type of network, the method provides accurate estimates (a few percent) of the average and the standard deviation of the three-dimensional distribution of the pore sizes, defined as the diameters of the largest spheres that can be fitted in the pore zones of the entire gel volume. When applied to the analysis of real confocal microscopy images taken on fibrin gels [2], the method provides an estimate of ξ_0 consistent with results from elastic light scattering data.

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#227 - Modelling DNA organisation and ejection in viral capsids: hints from topology

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The packing of DNA inside bacteriophages certainly yields the simplest example of genome organisation in living organisms.
Recent experiments, based on single-molecule manipulation and imaging techniques, showed that the linear double-stranded DNA packed in bacteriophage capsids is both highy knotted and neatly structured. Some of the main questions that arise in this context are the following: What is the physical basis of the geometrical and topological DNA organization in the capsids? What controls and sets the timescales of DNA ejection into the cytosol of their bacterial hosts? Here we show evidence from stochastic simulation techniques that suggests that a key element is the tendency of contacting DNA strands to order, as in cholesteric liquid crystals. Accounting for this local potential allows us to reproduce the main experimental data on the geometrical and topological DNA organization in phages. In addition, an analysis of DNA trajectories during ejection shows that the predominance of torus over twist knots, found in equilibrium and experimentally, persists at all stages in the ejection.

#228 - Modelling genome organisation in 3D: applications to bacterial DNA and chromosomes

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While we now know in details the sequence of most eukaryotic genomes, we still have only a rudimentary idea of how these genomes fold in space, or how structure affects function. In both eukaryotes and bacteria, DNA is invariably associated with a number of proteins, such as histones, polymerases, promoters etc. Rather than merely using DNA as a track on which to diffuse around or track along, these proteins often profoundly change the 3-dimensional structure of the genome.
I will present a coarse grained Brownian dynamics simulation study of an ensemble of DNA and DNA-binding proteins, and show that under a variety of conditions proteins cluster and lead to genome organisation. I will discuss these results with respect to known facts on the 3D organisation of bacterial DNA and of human chromosomes. I will also present a finer grained molecular dynamics study of chromosome 14, comparing the structure we obtain in simulations with the contacts found by our experimental collaborators via fluorescence in situ hybridization (FISH) and chromosome conformation capture (3C) experiments.

#229 - Protein translocation in narrow pores: inferring bottlenecks from native-structure topology

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In voltage driven translocation experiments, an applied voltage across two electrolytic cells connected through a nanopore induces the migration of proteins and other macromolecules across the nanopore. The macromolecule engaging the pore produces detectable ion current variations very informative on its physical chemical properties.
An increasing accumulation of data [1,2,3] supports the view that protein translocation across narrow pores is a multistep process characterized by a sequence of dynamical "stall events" (bottlenecks) representing to some extent the fingerprint of the passing molecule.

Our simulations on a coarse-grained model of the protein-pore system support the multistep scenario which results from the tight coupling between translocation and unfolding. Moreover simulations strongly indicate the relationship between: i) stall events, ii) ascending ramps in the free-energy profile G(Q) of a translocation reaction coordinate Q, and iii) regions of the protein richer in "backward native-contacts" (i.e. native non-bonded interactions among those aminoacids that have not yet entered the pore).
We thus can argue that the sequence and nature of such bottlenecks might have a clear interpretation in terms of the structural properties of the protein native-state. Therefore, inference on the presence of a multistep translocation dynamics of proteins can be done from the knowledge of the native-state topology.

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#230 - Time resolved experiments on amyloid-beta peptide fibrillization

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We present a combination of time-resolved Small Angle X-ray Scattering and Dynamic Light Scattering experiments on amyloid-β (Aβ) peptide fibrillization. The pathology of Alzheimer's Disease is featured by the presence of extracellular deposits of misfolded and aggregated Aβ in the form of amyloid fibrils. Amyloid fibrils usually consist of 2–6 unbranched protofilaments, each about 2–5 nm in diameter, characterized by a cross-β spine, with β-strands perpendicular to the fibril axis and β-sheets along the length of the fibril [1]. According to literature, the amyloid aggregation process should follow a typical nucleation-polimerization kinetics, characterized, in each phase, by structural intermediates presenting specific dimensions, morphologies and citotoxic activity [2,3]. Mature fibril formation is always preceded by the peptide assembly in several metastable non fibrillar forms, known as prefibrillar forms. Substantial evidence suggests that small, prefibrillar oligomers, that form at the beginning of the aggregation process, are the crucial species in the onset of the disease and in neuronal cell degeneration. The study of Aβ fibrillization pattern in solution and at a protein concentration quite resembling that in vivo [4], provides noticeable information to develop basic knowledge about the molecular mechanisms at the basis of this aggregation, hence for the development of a new therapeutic approach for Alzheimer's Disease treatment and prevention. In particular, the combined use of Small Angle X-ray Scattering, with Synchrotron Light, and Dynamic Light Scattering experimental techniques enables the characterization of the prefibrillar species and of the mature fibrils, due to the different range resolution.

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#231 - Interaction between amyloid oligomers and phospholipid membranes: a neutron diffraction study

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Proteins undergoing amyloid aggregation convert from their native state to ordered fibrillar aggregates. The deposition of amyloid fibrils is associated to severe pathological conditions, such as Alzheimer's and Parkinson's diseases and systemic amyloidoses. Oligomeric prefibrillar aggregates have been indicated as the major responsible for cytotoxic activity which results in cell membrane destabilization and impairment of calcium homeostasis, ultimately leading to cell death. Therefore, it is crucial to obtain information about the interaction of oligomeric aggregates with the membrane.
In this work we have used neutron diffraction to study the interaction of oligomers of the protein HypF-N and biomimetic phospholipid membranes. HypF-N is the N-terminal domain of the hydrogenase maturation factor from *E. coli*. This disease-unrelated protein under appropriate solution conditions is able to undergo amyloid aggregation forming prefibrillar oligomeric aggregates endowed of cytotoxic activity. Therefore, it represents a useful model system to get insight into the aggregation process and aggregate-membrane interaction.
We performed lamellar neutron diffraction measurements on oriented lipid bilayers obtained by the deposition of POPC/POPS (92:8 mol/mol) liposomes on solid support, with or without incubation in the presence of monomeric or oligomeric HypF-N. We found that the bilayer spacing decreases from pure lipid membranes to membranes containing the oligomeric protein. This decrease is caused by the disorder of the alkyl chains. The increasing alkyl chain disorder is also reflected in the membrane density profiles, where secondary maxima caused by the unsaturated bonds in the hydrocarbon chains, clearly visible in the pure lipid, decrease in the presence of the protein. This indicates that Hypf-N penetrates into the membrane hydrophobic core.
Interestingly, the deuterium distribution indicates that HypF-N oligomers increase water penetration inside the membranes. This result agrees with the hypothesis that amyloid oligomers create defects in the lipid membranes.

#232 - Charge transport in nano-structures: a percolative approach correlating electrical and topological properties

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Recent measurements performed on biological matter revealed unexpected current responses under the application of an external bias. In particular, these features are shared by samples of different proteins, investigated with different techniques i.e. they constitute an intrinsic property of this kind of matter [1-5]. The common traits of these features are mainly two:

a. The current response is definitely linked to the protein structureand its modifications;

b. The current response assumes a typical non-linear shape, at increasing the applied bias.

These behaviours can be attributed to a sequential tunneling mechanism of charge transport, in particular, Direct Tunneling (DT) at low bias, and Fowler-Nordheim Tunneling (FN) at high bias. Usually to achieve the FN regime is a quite difficult task, due to the high fields involved, anyway it has been done, by using the c-AFM technique [4] onto a nanolayer of the protein bacteriorhodopin (bR) [6]. These measurements have explored a wide bias range and revealed the cross-over between the DT and FN regime. To describe these results, a microscopic model, hereafter called INPA (impedance network protein analogue) has been set up. This model describes the protein as an impedance network [7] andis able to determine its electrical properties as a functionof the the 3D structure.Furthermore, by using INPA, it has been possible to investigate the conductance associated to the experimental data and to estimate its variance: the analysis of these global quantities traces the cross-over as a second order phase transition [8]. Moreover, since the DT-FN transition is an appealing phenomenon also in inorganic solids [9], the model is here used with regular structures,in order to evidence similarities and differences on respectnon-regular structures (proteins), both on the electrical response and also on the main emerging statistical properties. In present communication we compare the bR with some regular structures (cubic structures) of increasing size. In such a way, it is possible to investigate, for example, the size effects on the phase transition.

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#233 - Smart systems for societal challenging applications

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In the coming years the whole societies in teh world will be faced with serious demographic changes. In several industrialized countries the population's average age will drastically increase. The "ageing society" is becoming not only an evident challenge for the social security systems but also for the societies as a whole. These trends have several implications:
• there will be more aged people in absolute as well as relative terms, with fewer family carers (i.e. informal carers), and a smaller productive workforce to contribute to the financing of social and health services, posing significant challenges to the organisation of these services;
• there will be - also due to rapid progress in medicine - more frail and disabled older people in need of social, home and long-term care services at the same time as there are fewer informal family carers and increased cost-containment pressures on the formal services.
Despite the tremendous socio-economic impact of the ageing problem on the modern society, and the substantial research efforts being carried out on this topic from the physiological, psychological, and sociological point of view, an integrated effort in bringing technology at the service of the elderly people is still in its infancy.
Smart Systems solutions can be identified as technological innovations that will assist the elderly individual to maintain autonomy, independence and dignity by:
• extending the time people can live in a decent way in their preferred environment by increasing their autonomy, self-confidence and mobility
• promoting the eventual risk profile of individuals to better and healthier lifestyle
• enhancing the security, to prevent social isolation and to support maintaining the multifunctional network around the individual
• supporting careers, families and care organizations
• supporting maintaining health and functional capability of the individuals, especially the elderly and/or persons with chronic illnesses or disabilities
• increasing the efficiency and productivity of used resources in the ageing societies
• improving equal access to services.

#234 - Nanofacility Piemonte: three years of activity in the field of nanofabrication by ion and electron beams

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Nanofacility Piemonte is the most recent nanofabrication laboratory of Istituto Nazionale di Ricerca Metrologica, realized with the contribution of Compagnia di San Paolo Foundation in 2009. The laboratory completed the already existing facilities dedicated to microfabrication of quantum devices and nanostructures, the QR Laboratories. Nanofacility Piemonte is composed of a FEI SEM FEG Inspect F™ for online characterization and microanalisys (EDAX) and a FEI DualBeam ESEM FEG Quanta 3D™, equipped with Focus Ion Beam, Scanning Transmission Detector, four nanomanipiulators by Kleindiek Nanoteckink, NanoPattern Generator System from J. C. Nabity and Gas Injector System (Platinum). Nanofacility is available with skilled personnel, to any academic and industrial body through simple rules (http://www.nanofacility.it).
Since its starting, the two electron microscopes of Nanofacility Piemonte worked uninterruptedly, day and night, for thousands of hours, characterizing, fabricating and manipulating nanostructures, innovative materials and new families of solid state devices. In these last three years, a number of young researchers and technicians have been trained on advanced microscopy techniques, developing new cooperations and strenghtening the existing ones.
More than fifteen research projects ran or are still active at the moment in different fields of physics of matter, chemistry and nanotechnology, ranging from quantum devices for the Voltage standard and Single Electron Transistors to silicon nanowires, graphene devices, magnetic materials and devices, high Tc superconductors, Directed Self-Assembly of single objects and diblock copolymers, nanophotonics, bio-sensors, detectors and TEM lamella preparation. This work is a review of the main achievements and processing methods in the fabrication of new families of nanostructures and nanodevices by electron and ion beams.

#235 - From MEMS dream to today reality

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Starting from International "Technology Road Map for Semiconductor" (ITRS) the presentation enter in detail on "More Than Moore" field with some stories on MEMS starting from Ink Jet to different sensors like accelerometer, gyroscope, microphones and pressure transducers, to new scenario that include new products on actuation using piezoelectric materials.

#236 - High sensitivity nano-SQUIDs for nanomagnetism investigations

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In the recent years, it has been shown that the magnetic response of nano-objects (nanoparticles, nanobead, small cluster of molecules) can be effectively measured by using a Superconducting Quantum Interference Device (SQUID) with a small sensitive area. In fact the sensor noise expressed in term of the elementary magnetic moment (Bohr magneton, μB) is linearly dependent on the SQUID loop side length. For this reason, LTc SQUIDs have been progressively miniaturized in order to improve the sensitivity up to few tens of μB per unit of bandwidth .

In the present work, high sensitive niobium nanoSQUIDs and their employment to the magnetic properties measurements of iron oxide nanoparticles will be presented. Two different type of nanoSQUIDs have been developed. The first one is based on Dayem nanobridges and is fabricated by using Electron Beam Litography (EBL) and the other one is based on three dimensional sub-micron Josephson tunnel junctions (JTJ) fabricated by Focused Ion Beam (FIB) sculpting.

The main advantage of nanobridges is the large critical magnetic field of thin niobium films; allowing to the use the nanoSQUIDs in magnetic field up to few Tesla necessary to reach the saturation magnetic field of interesting magnetic material. On the other hand, they have a limitation in the critical current reproducibility and exhibit low critical current modulation depth (20-30%). The nanoSQUIDs based on sub-micron Josephson tunnel junctions (JTJ) starts from a Nb/Al-AlOx/Nb trilayer which represents the best approach to the fabrication of reliable and reproducible Josephson tunnel junctions. They have a planar configuration with a loop area down to 0.2 μm^2, and two square JJs having a 0.2-0.4 μm side. The main advantage of JTJ nanoSQUIDs is a better control of the critical current, high modulation depths and ultra low noise. The drawback is the smaller critical magnetic field respect to the nanobridge, allowing the applicability to magnetic field smaller than about 200G. However, such fields are large enough to study relaxometry of nanoparticles and for many other applications. These nanosensors have been successfully employed to measure the field dependence and the time relaxation of the magnetization of iron oxide nanoparticles having a mean diameter of 4.2 nm and 7.8 nm. Field dependence of magnetization measured at 4.2 K by will be showed for different particle size. Relaxation measurements have been also recorded by cooling the sample in a magnetic field B=100 G from 300K t o 4.2K, then inverting the magnetic field. The time resolution for the beginning of the measurement was few tenths of se cond which is well below the limit of commercial magnetometers. These measurements prove that nanoSQUIDs reported here allow to successfully perform nanomagnetism investigations.

#237 - A multisensor platform for thin film polymeric-based transducers

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A method and system for the sensing of thin polymeric layers is presented. This method is based on a differential measurement of the complex impedance of two polymeric layers, which constitute active and reference layers. To enhance the sensitivity of the method to structural changes in the polymer a thermal analysis is performed as well. In this way a complete thermal-dielectric spectroscopy is achieved.

Polymers are well known to be very sensitive to a wide range of mechanical, chemical and physical inputs. They are also of high interest for their functionalization capabilities. When doped with the right component the selectivity on the input quantity of these polymers can be highly increased, leading to very versatile and general purpose sensor platforms. A single sensor board can be tuned to detect different gases just by controlling the doping species. In polymer based sensors the secondary transducer rely on different types of interaction: electrical, thermal, optical, mechanical. Common transducing methods measures electric impedance, refractive index, viscosity, elasticity, mass or thermal capacity.

The combination of thermal and dielectric spectroscopy was chosen to enhance the sensitivity of these methods. With this combination of interactions a multi-dimensional response map of the polymer under test can be achieved. Moreover, the differential approach allow the comparison of the functionalised polymer with a reference, reducing the effect of interfering quantities.

The system here presented is comprised of a pair of interdigit structures, electric heaters and thermocouples. The three elements of the sensor are stacked to form a multilayer device which is able to sense electric impedance and temperature of the substrate at the same time. The multilayer device has been implemented onto a substrate of polyimide Kapton® 0.1mm thick film. Metal structures were obtained via thermal vapour deposition. A third electrode positioned in the middle point of the heater resistor is used to compensate small variations in temperature and power between the two sensing areas. The differential interdigit structure was made with the same process. Two thermocouple sensing elements are positioned above the two halves of the heater structure.

#238 - Multilayer structures, pi-conjugated polymers and optical detection of nitroaromatic compounds

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In the last years, the detection of explosive traces and nitroaromatic compounds has become a major analytical problem which requires highly sensitive, fast and handy sensors for its solution. Several techniques have been adopted to solve this difficulty, among which mass and Raman spectroscopy, X-ray imaging and canines. However, cost, complexity and robust portability are tricky issues for several of these methods. Canines, for example, are at present the most reliable tool for explosive detection, but their employment is expensive and unsuitable for continuous monitoring since dogs can get easily tired. An hopeful technology uses conjugated fluorescent polymers as sensible element in optical sensors to rapidly detect the presence of explosive vapours [1,2]. Optically excited conjugated systems exhibit a quenched fluorescence upon exposure to vapours of nitroaromatic compounds. The quenching

is related to the photoinduced electron transfer from the conjugated system to the electron-poor analyte. This process strongly depends on the relative position of the LUMO states of the conjugated material with respect to those of the analyte.

In this communication, we report on the development of a photonic device able to enhance the fluorescence signal of an organic layer used as a sensitive material. The first part of the work was aimed to identify, synthesize and test the most sensitive and stable materials for the detection of nitroaromatics. Synthesis, absorption, fluorescence, and ellipsometric characterization of Poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(1,4-benzo-{2,1'-3}-thiadiazole)] (F8BT) and other new conjugated systems, designed and synthesized ad hoc, is reported. Moreover, we tested the ability of these polymers to detect dinitrotoluene and benzoquinone by fluorescence quenching both in solutions and as thin films. Results are then compared to those obtained by commercial F8BT.

The second parallel activity has been focused to identify the most suitable and efficient photonic structures and configurations for the amplification of the fluorescence signal used for detection.

Bragg organic multilayers have been prepared by spin coating deposition [3] and characterized by reflectance, transmittance and ellipsometry and the results compared with computational simulations. Looking for the best coupling conditions for pumping and emission of a thin layer of the active material, we successfully measured in the final structure a fluorescence enhancement.

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#239 - 2D-detectors for photoionization studies of atoms, molecules and clusters at ELETTRA and FERMI@ELETTRA

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In the study of the electronic structure of atoms, molecules, and clusters, Velocity Map Imaging (VMI) of charged particles produced by photon impact is a valuable research tool that continuously profits from advances in both 2D detectors and light sources.

At Elettra, the ongoing collaboration between the atomic and molecular physics group, and the Instrumentation and Detector Laboratory, has resulted in a prototype set-up [1,2] which successfully tackles the challenges posed by such diverse applications as Synchrotron Radiation (SR) and Free Electron Laser (FEL) experiments (notably differing in the rate of events produced and detected). The VMI spectrometer is suitable for the detection of electrons and ions; in the first case, then a Time-of-Flight (TOF) mass spectrometer allows to acquire simultaneously photoion spectra, too.

In SR experiments, a crossed delay line detector is used, coupled to a 4-channel time-to-digital converter that reconstructs the position of the electrons. PhotoElectron-PhotoIon-Coincidence detection (PEPICo) allows correlating the kinetic energy and angle of photoemitted electrons with the mass of photo-ions, i.e. to the specific ionic state produced by photon absorption.

The same system cannot be use with a FEL source, because of the huge event rate; instead, a Micro Channel Plate (MCP) a phosphor screen and a CCD camera allow shot-to-shot (albeit not time-resolved) collection of practically all events.

Recent experiments on metallic clusters and rare-gas atoms performed at the GasPhase beamline of Elettra and at the LDM beamline (Low Density Matter) of the FEL Fermi@ELETTRA will be presented.

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#240 - Organometallics architectures on surfaces

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Supramolecolar assemblies of organometallic complexes containing transition metals can create networks of active centers for electronic and magnetic functions. Metal Phthalocyanines (MPcs) are π-conjugated complexes with planar structure that easily arrange on atomically periodic surfaces. Very different behaviour is expected for different MPc on surfaces depending on the interaction process.

MPcs assembled along the Au(110) reconstructed channels form 1D chains and 2D ordered structures [1]. The orbital and spin configuration of FePc, CoPc and CuPc chains are strongly modified upon adsorption on the Au(110) surface, if the orbitals responsible of the magnetic moments are involved in the interaction process. The magnetic moment for a single layer of molecular chains is completely quenched for the CoPc single layer, fully preserved for the CuPc molecules and reduced for the FePc ones, as deduced from X-Ray magnetic circular dichroism (XMCD) [2]. The FePc chains assembled in the 5x5 phase switch from a non-magnetic to a magnetic state, when at increasing molecular coverage the FePc forms a 2D 7x5 reconstructed phase. The evolution from single molecule to quasi-unidimensional Kondo lattice to a magnetic state is a model system to unravel the interrelationship between the Kondo state and the molecular orbitals localized on the central metal atom involved in the process [3].

Electronic state coupling between the molecule and the metal substrate may be avoided by using an appropriate buffer layer, like graphene. Graphene grown on Ir acts as a buffer layer decoupling FePc from the underlying metal surface, without affecting the electronic states of the molecular layer. Despite this weak effect on the electronic properties, the FePc layer presents a high adsorption energy on graphene. The decoupling of FePc from the metal substrate due to graphene allow to maintain a significant magnetic state of the arrays of Fe ions. Furthermore XMCD reveals that FePc atoms present an in-plane magnetic easy axis resulting from an enhanced magnetic anisotropy, which is on the strategic trend to prepare regular two-dimensional (2D) architectures tailoring the electronic and magnetic properties of organic nanostructures on graphene.

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#241 - Transparent plasmonic nanowire electrodes via self-organised ion beam nanopatterning

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A self-organised approach for the synthesis of transparent metal nanowire arrays is based on defocused ion beam sputtering of polycistalline metal films [1,2]. The nanowire arrays, supported on low-costdielectric substrates (glass slides), feature a dual functionality: they exhibit anisotropic conductivity, with sheet resistances which are reduced in comparison to those of transparent conductive oxides, and additionally they support localised plasmon resonances. The latter represents an attractive feature in view of plasmon enhanced photon harvesting applications, in which the nanostructured metal electrodes are employed as an alternative to conventional transparent conductive oxides. In an alternative approach Noble metal nanoclusters with tunable plasmonic properties are grown by guided agglomeration on nanostructured templates fabricated by defocused ion beam sputtering (IBS) on low cost glass substrates. The self-organized IBS process induces the formation of a ripple pattern with selected periodicity in the 200 nm range, vertical dynamic up to 70 nm and asymmetric steep facets exceeding 30°. Glancing Angle Deposition (GLAD) of Au on these nanostructured templates allows to confine anisotropic metallic nanoclusters on the tilted facets illuminated by the atom beam. At low metal doses, isolated anisotropic nanoclusters are formed, which confer to the substrate a strong dichroic optical behaviour due to the excitation of localised plasmon resonances. At higher metal doses connected tilted Nanowires are formed on the illuminated ridge of the glass ripples. The tilted nanowire arrays exhibit macroscopic electrical conductance with sheet resistances in the 10 Ohm/square range, coupled to high optical transparency and plasmonic properties.

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#242 - Unveiling the electronic and optical contribution of rebonded-step surface reconstruction in Ge/Si heteroepitaxy

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The continuous scaling of semiconductor technology has driven increased interest in the spontaneous formation of coherent islands during Stranski-Krastanow (SK) growth of strained epitaxial layers.

In this context, Ge on Si(001) is considered a prototypical model system for studying the fundamental mechanisms of strain relaxation in lattice-mismatched semiconductors as well as for modeling the electronic and optical properties of three-dimensional (3D) heterostructures. The evolution of grown Ge islands is basically due to the stability of the {105} facets which lowers significantly the free energy of the system for compressively strained Ge.

Moreover in quantum-dots (QD), due to the high surface-to-volume ratio, the surface role becomes increasingly important and even

comparable to that of confinement; then it is crucial to identify the surface contribution to the QD electronic and optical properties. Despite its importance, the electronic structure and the optical properties of the RS-reconstructed facets of Ge quantum-dots grown on Si(001) remained, up to now, largely unknown. This is likely due to the narrow size of island facets (a few nm²) which hinders most of the experimental probes.

Recently, we have shown that Ge epitaxy on peculiar Si(001) vicinals leads to a surface which is completely RS-reconstructed and, thus, is an excellent model system for analyzing the electronic states associated to the RS-(105) surface.

We have combined Reflectance anisotropy spectroscopy (RAS) with scanning tunneling microscopy (STM) to unambiguously correlate the optical anisotropies with the atomic surface structure of the RS reconstruction. The close connection between the spectral fingerprints and the distinctive structural motifs of the RS-reconstructed surface is fully confirmed by first-principles calculations of the electronic bandstructure and optical RAS spectra. The existence of surface states related to the RS reconstruction, totally disentangled from that observed on the (2x1)-reconstructed Si and Ge on Si(001) surfaces, is a decisive indication that the structure of the Ge/Si(105) surface cannot be interpreted as that of a Si(001) vicinal composed by a staircase of (001) nanofacets, but is indeed consistent with that of a new singular face.

#243 - H2 molecules formation on W(110) surface

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Recombination of atomic hydrogen is of interest in several fields: industrial plasma reactor used for microelectronics, etching and among them the thermonuclear fusion. The realization of nuclear fusion reactor like ITER has revealed the need of new data on hydrogen recombination on tungsten at high temperature level. The calculations of hydrogen atoms recombination catalyzed by a tungsten surface have been the subject of few papers. Some works in the last years has been devoted to the study in the framework of Density Functional Theory to the determination of adsorption and diffusion properties of hydrogen atoms on the W(001) and W(110) [1-5]. Reaction dynamics studies using Molecular Dynamics (MD) simulations are reported for the interaction of low-energy atomic hydrogen on the W (001) [6] and for recombination of hydrogen atoms on W(001) [7].

In this contribution, according to the experimental evidence that the face (110) is the most prominent in polycrystalline tungsten, used in the experiments, we consider, the recombination of hydrogen atom on W(110).

We performed MD calculations to investigate the probability for the recombination and for other surface processes occurring when an H atom is adsorbed on the surface and an H atom impinges from the gas-phase (Eley-Rideal mechanism). The study was made in the framework of a semiclassical collitional method, largely described in different previous publications (see for example Rif. [8,9]), that takes into account the coupling of gas species dynamics with the lattice motion during the interaction.

Different dynamical aspects of this heterogeneous system are considered and discussed in details. In particular we focus on the reaction mechanism, the energetics of the recombination reaction, the vibrational energy distribution of the nascent H_2 molecules, the energy exchanges between the gas-phase particles and the W surface.

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#244 - Tunable wettability through independent tuning of micro and nano scale features of self - assembled hierarchical material

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The control of the wetting properties has been demonstrated to be crucial for a wide range of applications. Superhydrophobic surfaces have recently gained the attention of both the scientific and industry community for self-cleaning surfaces to anti-icing coating while superhydrophobic/hydrophilic are playing key role in the fabrication of microfluidic device. When a liquid is dropped on a superhydrophobic surface low interfacial surface area is present and thus high contact angles (CA, angle between the surface and the tangent to the drop profile) are observed. In the ideal situation, the liquid does not wet the surface and it is free to roll-off (CA close to 180°). In contrast a hydrophilic material allows a very high liquid adhesion and poor CA. Superhydrophobicity, which is usually caused by the surface energy of the solid being lower than the one of the liquid, can be achieved by either acting on the chemistry of the material, usually by addition of fluorinated ligands, or on its roughness (i.e. the ratio between effective and geometric surface area), increasing the nanostructuration to reduce the points of surface-liquid contact. In this work we present a quasi-1D self-assembled TiO_2 nanostructured with independently tuneable multiscale features allowing fine control over its surface wettability. The materials, with a hyperbranched shape, are fabricated by Pulsed Laser Deposition, present features that range from few nanometers (leaves) to few micrometers (branches) and are intrinsically superhydrophilic. Varying deposition parameters and

wet and thermal post treatments it is possible to tailor respectively the nano and micro features obtaining contact angles going from zero (superhydrophilic) to nearly 180 degrees upon sensitization of fluorinated polymer. UV/Vis spectroscopy showed that these surfaces have high light transmittance (nearly 100% in the visible). Beside the fact that wetting properties have been demonstrated to be stable to wetting/de-wetting cycles with water, the controllability and the possibility to locally switch between superhydrophobic/superhydrophilic makes this technology a potential breakthrough in any field where the wettability plays a role.

#245 - Non-adiabatic ab initio molecular dynamics of supersonic beam epitaxy of silicon carbide at room temperature

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In this work, we investigate the processes leading to the room-temperature growth of silicon carbide (SiC) nano-crystals by supersonic molecular beam epitaxy technique. We present both experimental data and computational modeling of the collision of fullerene on a silicon surface inducing strong chemical-physical perturbations and, for sufficient velocity, disruption of molecular bonds, and cage breaking with formation of nanostructures with different stoichiometric character. We show that in these out-of-equilibrium conditions, it is necessary to go beyond the standard implementations of density functional theory, as *ab initio* methods based on the Born-Oppenheimer approximation fail to capture the excited-state dynamics. In particular, we analyse the Si-C60 collision within the non-adiabatic nuclear dynamics framework, where stochastic hops occur between adiabatic surfaces calculated with time-dependent density functional theory. This theoretical description of the C60 impact on the Si surface is in good agreement with our experimental findings.

#246 - Frictional anisotropy of crystalline surfaces and its relationship with surface structure studied by atomic force microscopy

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Friction forces play a key role in mechanical phenomena occurring on all scales, from the operation of microelectromechanical systems to interplate earthquakes. The study of friction forces is also useful for understanding a large spectrum of physical properties of surfaces. Thanks to the development of nanoscale investigation tools such as scanning probe microscopy, the investigation of friction and wear phenomena down to the atomic scale is becoming a leading topic within the field of surface physics, and has given rise to the science called nanotribology. We focus here on the anisotropic aspects of nanotribology, related in particular to the surface of crystalline materials. Frictional anisotropy is characterized by a dependence of the friction force intensity on the sliding direction and friction force components orthogonal to the sliding direction. We show how an atomic force microscope can be used to map in two dimensions the frictional anisotropy at the nanoscale and how to carry out data interpretation to unravel the friction– surface structure relationship. As model systems, we analyzed the basal plane of organic molecular single crystals, often characterized by marked corrugations, and interpreted the data in terms of constitutive models of anisotropic friction.

#247 - Soft x-ray photoemission spectroscopy on buried complex oxide interfaces

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At the interface between complex oxides, unexpected electronic properties different from those of the constituent bulk materials can arise. A particularly interesting example is the appearance of 2-dimensional conductivity at the interface of the band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) [1–3] above a critical LAO thickness of 4 unit cells (u.c.) [4].

A very recent related heterostructure is the diluted system of $(LaAlO_3)_x(SrTiO_3)_{1-x}/SrTiO_3$ (LASTO:x/STO) which also shows interfacial conductivity above a certain critical LASTO thickness which scales inversely to the LAO content [5].

The interfaces of LAO/STO and LASTO:0.5/STO heterostructures have been investigated by soft x-ray photoelectron spectroscopy for different layer thicknesses across the insulator-to-metal interface transition. The valence band and Fermi edge were probed using resonant photoemission across the Ti $L_{2,3}$ absorption edge. We measured, for the first time to our knowledge, clear spectroscopic signatures of Ti^{3+} signal at the Fermi level in fully oxygenated samples of LAO/STO and the related system of mixed LASTO:0.5/STO. Our results show that Ti^{3+}-related charge carriers are present in both systems, but only for conducting samples. No Fermi-edge signal could be detected for insulating samples below the critical thickness. Furthermore, the angular dependence of the Fermi intensity allows the determination of the spatial extent perpendicular to the interface of the conducting electron density.

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#248 - Computer modeling of surface-confined intermixing phenomena at epitaxial interfaces

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The present study outlines an important area of application of computer modeling in nanoscale surface and interface phenomena. Being relevant to the fundamental physical problem of competing atomic interactions in systems with reduced dimensionality, these phenomena have found exacting academic interest. On the other hand the fine atomic structure of surfaces and interfaces correlates with a large number of technological problems in material science. Typical examples are: formation of nanoscale surface patterns and two-dimensional superlattices, atomic intermixing at epitaxial interface, atomic transport phenomena, structure and stability of quantum wires on crystal surfaces. On that physical background, we discuss a variety of diffusion mechanisms that control surface-confined atomic exchange, vacancy-mediated diffusion, formation of alloyed atomic stripes and islands, relaxation of pure and alloyed atomic terraces, island diffusion in external field. The computational model refines important details of surface diffusion behavior of adatoms accounting for the energy barriers at specific atomic sites (smooth domains, terraces, steps and kinks) located on the crystal surface and the subtle interplay between energy gained by mixing and elastic strain energy. Being in agreement with recent experimental findings, the presented ensemble of diffusion scenarios opens a way for nanoscale surface design and preparation of regular interface patterns with exotic physical characteristics.

#249 - Effective doping and chemical scaling law in Fe-based superconductors

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Transition-metal substitutions are of great interest in the superconductivity of Fe-based superconductors and have been intensively studied both theoretically and experimentally, as they induce two main different effects that are both relevant to the pairing mechanism: the first one is a direct effect on the number of carriers while the other is related to the possible pair breaking effect. While the superconducting transition temperature is generally seen to linearly depend on the number of carriers introduced by doping, so that the occurrence of a "chemical scaling" relation has been proposed, there have been several cases where this simple rule does not hold. This is the case of Pt –doped $CaFe_2As_2$ [1] and Ru-doped $BaFe_2 As_2$. In the first case, Pt addition resulted in a complete suppression of superconductivity, while Ru, although isovalent with Fe, was reported to decrease the carrier number without, unexpectedly, affecting superconductivity [2].

After several theoretical and experimental studies (mainly ARPES) the issue regarding the role played by transition metal substitutions in superconductivity is still not ascertained and greatly debated.

In the present study we perform an ab-initio calculations on the electronic properties of $CaFe_2As_2$ and $BaFe_2 As_2$ under several different transition metal substitutions (Co, Ni, Pt, Rh) considering supercells up to 40 atoms and applying a novel defolding procedure which allows us to to directly compare our results with photoemission experiments. The presence of atomic substitutions, in fact, causes disorder, i.e. loss of periodicity, thus leading to state folding into a smaller Brillouin zone and to an increased complexity of the band structure. However, ARPES experiments find that the effective periodicity seen by the out coming electrons can still be casted in the 1-Fe per cell framework taking into account the proper phase, despite the symmetry of the overall (disordered) cell. Our findings clearly show that the simple rigid band picture leading to the empirical "chemical scaling law" does not hold and that substitutions cause structural, bonding, electronic and magnetic changes that strongly depend on the substituting atom and the host compound and that have to be carefully evaluated in each single case.

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#250 - Quantum physics with superconducting electrical circuits

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Solid state electrical circuits that behave as artificial quantum atoms are now developed for processing quantum information. After a broad introduction to superconducting quantum bit circuits, I will describe quantum physics experiments based on the Cooper pair box quantum bit circuit, and in particular the operation of an elementary quantum processor that demonstrates the quantum speed-up of the Grover search algorithm. I will introduce hybrid structures in which superconducting qubits and microscopic spins are combined together for performing different quantum information processing tasks.

#251 - Effect of Ru substitution on atomic displacements in the layered SmFe$_{-x}$Ru$_x$AsO$_{0.85}$F$_{0.15}$ superconductor

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Since the discovery of high-Tc superconductivity in doped LaFeAsO, the iron-based superconductors continue to attract substantial interest of the condensed-matter community. Among these, the RFeAsO (R stands for rare earth), with highest Tc of 55 K for the $SmFeAsO_{1-x}F_x$, are highly studied materials. The fundamental electronic structure, characterized by Fe 3d interacting with the As 4p states, is generally manipulated by controlling the RO spacers, e.g., by substitution at the R site and/or by substitution at the O site. In this regard, the interlayer interaction between the active FeAs layers and the RO spacer layers is of particular interest, with atomic disorder and local strain being the key issues [1]   .

Recently, several efforts are made to manipulate the effect of disorder in the active FeAs layers by substitution. In particular, isovalent substitution [2] at the Fe site has been used to study the effect of disorder on the superconductivity. Apart from the effect on the superconductivity, these studies were also motivated by the possiblity to answer the question of the symmetry of order parameter in the iron-based superconductors, either in the spin-fluctuation approach with anion height as a parameter, or the orbital fluctuations mediated superconductivity with iron phonons. Aiming to address these issues we have studied the local structure of $SmFe_{1-x}Ru_xAsO_{0.85}F_{0.15}$ superconductors as a function of Ru substitution [3]. The EXAFS and XANES spectra obtained at the As K and Sm L_3 edges have permitted us to obtain information on the local structure of the active FeAs layers and the SmO spacer layers. The EXAFS data reveal distinct Fe-As and Ru-As bond lengths and the local disorder being confined in the FeAs layer, while the SmO spacer layer sustaining a local order. Therefore, the effect of Ru substitution in the FeAs layer appears similar to what has been found in the rare-earth substituted RFeAsO with different rare-earth size. It was found that the coupling between the two layers gets weaker for bigger size of rare earth while the FeAs layers get thinner, similar to the increasing Ru substitution at the Fe site. These results demonstrate the importance of interlayer atomic correlations for describing the electronic properties of the layered 1111-type superconductors

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#252 - Selective Mottness as a key to iron superconductors

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The phase diagram of the high-Tc cuprates is dominated by the Mott insulating phase of the parent compounds. As we approach it from large doping, a standard Fermi-liquid gradually turns into a bad non-Fermi liquid metal, a process which culminates in the pseudogap regime, in which the antinodal region in momentum space acquires a gap before reaching a fully gapped Mott state. Here we show that experiments for electron- and hole-doped $BaFe_2As_2$ support an analogous scenario. The doping evolution is dominated by the influence of a Mott insulator that would be realized for half-filled conduction bands, while the stochiometric compound does not play a special role. Weakly and strongly correlated conduction electrons coexist in much of the phase diagram, a differentiation which increases with hole doping.

We identify the reason for this selective Mottness in a strong Hund's coupling, which decouples the different orbitals. Each orbital then behaves as a single band Hubbard model, where the correlation degree only depends on how doped is each orbital from half-filling. Our scenario reconciles contrasting evidences on the electronic correlation strength and establishes a deep connection with the cuprates [1].

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#253 - Study of macroscopic quantum phenomena and phase dynamics in moderately damped Josephson junctions

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In the last few years, studies on phase dynamics and macroscopic quantum phenomena have been extended to Josephson junctions (JJs) composed of materials other than the traditional low critical temperature superconductors (LTS). Measurements of switching current distribution (SCD) have turned to be more and more standard tools to investigate phase dynamics in unconventional and hybrid systems and nano-structures. High critical temperature superconductors (HTS) are an example of unconventional systems, because of the d-wave order parameter symmetry and of the presence of low-energy quasiparticles, which are expected to induce high level of dissipation. Measurements of SCD constitute a direct way of discriminating the phase dynamics and the transport also in nontrivial cases of moderate damping, which are going to be more and more common with advances in nanopatterning superconductors and in materials science with novel possibilities of synthesizing also hybrid coplanar systems.

We have proved the existence of a transition between thermal activation and macroscopic quantum tunneling both in LTS NbN and in HTS YBCO grain boundary (GB) JJs, in the moderately damped regime (MDR). While MDR seems to be to a large extent intrinsic in HTS JJs, in LTS JJs is controllably induced by low critical current I_c, thus by low Josephson energy E_J. More importantly we have found distinctive signatures of phase diffusion, as the appearance of an anticorrelation between temperature and the width of the switching distributions. Measurements of SCD have been supported by Monte Carlo simulations of the phase dynamics, providing a solid and reliable method to estimate the damping factor Q in the MDR. We have performed numerical simulations in a wide range of dissipation conditions and junction parameters, and direct comparison between measurements and Monte Carlo simulations allow us to reconstruct a $(Q, k_BT/E_J)$ phase diagram summarizing the various activation regimes. Such a phase diagram constitutes a guideline for moderately damped systems over a large range of junction materials, geometry and dissipation level. We have explored a new region of the $(Q, k_BT/E_J)$ phase diagram and we have demonstrated a direct transition from quantum activation to diffusive motion in GB YBCO JJs. Such an experiment sets a relevant reference in the study of the influence of dissipation on the switching statistics of JJs and to understand interaction of a quantum system with the environment.

#254 - Materials and technologies of superconducting devices for quantum computation

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It is well known that a main source of decoherence in superconducting devices for quantum computation, such as Josephson phase qubits, is the microscopic two-level state (TLS) defects in the dielectric materials that are used to form the tunnel barrier and to organize a wiring insulation. In addition, also the superconductor's native oxides and the interface between superconductor and substrate have been suspected as regions with high density of unpaired surface spins (magnetic TLS) [1]. Hydrogenated amorphous silicon (a-Si:H), because of its lower loss tangent among conventional dielectrics (a-SiO, a-SiO$_2$,), is considered as the best amorphous dielectric for superconducting qubit application. We have developed a reliable method for the direct measurement of

dielectric losses in amorphous dielectric thin films using a novel design based on lumped superconducting LC resonators. The plasma enhanced chemical vapor deposition (PECVD) at T=250 °C was utilized for deposition of the a-Si:H as a dielectric of LC resonators with Nb electrodes. The devices were tested at the conditions of a qubit application (0.5 - 10 GHz frequency range and low temperatures). Our a-Si:H material have demonstrated the loss tangent of 2.5 x 10^{-5} at T=4.2 K, which is in a good agreement with data for best a-Si:H published in literature [2]. We have studied the influence of a-Si:H deposition by PECVD on the superconducting, normal-state and structural properties of Nb film [3]. A suppression of the Tc and an increase of the residual resistivity of Nb film were observed due to hydrogen diffusion and decomposition of the native oxide, with subsequent oxygen diffusion caused by heating up to T=250 °C. Our results have indicated that the integration of a-Si:H deposition by high temperature PECVD in Nb technology, toward the realization of a superconducting qubit with a low decoherence time, requires the employment of an amorphous Si layer as an effective method to protect Nb films against oxygen and hydrogen diffusion. Alternatively to the Nb technology, NbN as superconductor is considered as the materials for qubit realization because NbN films tend to form smaller amount of a native surface oxide in comparison with Nb films. We have fabricated and tested NbN/AlN/NbN Josephson phase qubits and we have carried out the experiment on phase diffusion process which can be relevant in development of qubit devices based on advanced materials [4].

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#255 - Analysis of soliton dynamics and noise induced effects on the superconductive lifetime in long Josephson junctions

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The influence of various noise sources on the transient dynamics of long Josephson junctions (LJJ) is investigated in the presence of an oscillating bias current signal and a noise source with Gaussian or non-Gaussian (i.e. Cauchy-Lorentz or Lévy-Smirnov) probability distributions.

These systems are computationally analyzed integrating the perturbed Sine-Gordon equation describing the phase evolution. We found evidence of noise induced effects on trends of the mean escape time (MET) from the superconductive metastable state, varying different system parameters, as the bias frequency, noise intensity and junction length. In particular, we find *resonant activation* (RA) and *noise enhanced stability* (NES), and we study the connections between these phenomena and the creation/evolution of *solitons* (i.e. kink and antikink solutions) in the LJJ phase string dynamics. Pronounced changes in RA and NES are observed by using Lévy noise sources with different statistics.

MET is also studied considering spatially homogeneous and inhomogeneous bias current distributions. In the latter case, in the presence of Gaussian noise, we observe an enhanced non-monotonic behavior, that, conversely, almost vanishes using noise sources with different statistics.

#256 - Coherent quantum manipulation of superconducting qubits by fast flux pulses: decoherence, adiabaticity and speed issues

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A double SQUID can be used as a solid state flux qubit. Its behavior is described by an effective potential the shape of which can be modified by two independent bias magnetic fluxes. In particular, it is possible to pass from a single-well to a double-well shape, and it is also possible to modify its symmetry/asymmetry. A rapid modification of the potential allows the manipulation of the quantum state in a very fast manner: we observed coherent oscillations with frequencies up to 70 GHz, to be compared with the typical oscillations obtained by microwave manipulations on similar systems, below 1 GHz. This is an interesting advantage from the point of view of quantum computing, since for similar decoherence times a greater speed means a large number of possible coherent operations. Moreover, the manipulation based on fast flux pulses allowed a deep insight in decoherence mechanism acting on the system. The drawback of this scheme concerns the fact that the manipulation must be in the same time non-adiabatic (for the two lower energy levels, the computational states), and adiabatic (for the upper ones). This is possible thanks to the energy level structure, but requires an accurate characterization of the system. We present principles and recent results, and discuss issues and perspectives about this scheme.

#257 - Kink instabilities and magnetic reconnection in plasmas from millimetric to parsec length scales

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Magnetic field-line reconnection is a very efficient mechanism for the conversion of magnetic energy to plasma energy and fast-particles acceleration. It is often invoked to explain phenomena in a variety of extremely different environments, from extragalactic gamma-ray emitters [1], to acceleration of electrons to peV energies in the CRAB nebula [2], to the generation of anomalous cosmic rays outside the heliospheric termination shock [3], to more familiar ones like solar flares, magnetospheric substorms, and rapid collapse events in laboratory plasmas. Despite the very different conditions, e.g. different sources of free energy, different ratios between Alfvén and light velocities, and different dissipation mechanisms (coulomb collisions, inverse Compton scattering etc.), most of the mentioned phenomena show the common feature of rapid releases of magnetic energy after long phases of quasi-steady accumulation. The rapidity of magnetic reconnection and the intensity of the associated electric field were subject to intense experimental and theoretical studies that will be reviewed in this work.
Kink perturbations of the magnetic configuration are investigated in tokamak research as their development sets an upper limit to the pressure that the plasma can reach [4]. Magnetic reconnection is fostered by such deformations, as they tend to produce intense current sheets that are the natural location of reconnection phenomena. Furthermore, kink instabilities are candidate explanations for morphological and dynamical features of astrophysical jets. Laboratory and space observations on kink instabilities will be summarized.

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#258 - Intense laser-plasma interaction as a tool for fundamental physics

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Classical electrodynamics (CED) and quantum electrodynamics (QED) are well established theories and have been tested experimentally in different regimes. However, there are still areas of CED and QED and fundamental problems in such theories that deserve theoretical and experimental investigation. In view of the increasingly stronger available laser fields, it is becoming feasible to employ them to test CED and QED under the extreme conditions supplied by ultra-intense fields [1].
After an overview on still open fundamental problems in the realm of strong-field CED and QED, we will indicate how the interaction of super-intense laser pulses (intensity exceeding 10^{20} W/cm^2) with solid targets can represent a unique tool to investigate such open problems experimentally for the first time. Among them we will discuss
1. the problem of radiation reaction in CED and QED, i.e., how the dynamics of charged particles is affected by the electromagnetic field emitted by the charge itself, when driven by a super-strong background electromagnetic field;
2. the theoretically predicted but still experimentally unobserved ability of intense electromagnetic fields to modify the dielectric properties of the vacuum (the so-called vacuum polarization effects);
3. the production of dense electron-positron plasmas in laser-solid collision.

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#259 - Efficient extreme ultraviolet and soft X-rays plasma sources at ENEA Frascati

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Extreme ultraviolet (EUV) sources based both on a laser produced plasma (LPP) and a discharge produced plasma (DPP) have been developed at the UTAPRAD-SOR Laboratory at the ENEA Frascati Research Centre.
In contrast with hard X-rays laser plasma sources, where typically ultra-short laser pulses are used, laser pumping pulses with temporal duration from tens up to hundreds of nanoseconds are preferable for an efficient emission of EUV radiation and soft (<2 keV) X-rays when using the LPP.
The ENEA LPP source can be driven by two different XeCl excimer lasers (λ=308 nm): a high-repetition-rate Lambda Physik LPX 305 PRO laser with 30 ns pulse duration and 0.5-J energy per pulse, and the high-output-energy Hercules laser, developed by ENEA, having 120 ns pulse duration and 5-J energy per pulse. A characterization of the LPP source in both pumping conditions will be presented and the problem of the plasma emitted debris and relevant mitigation will also be shortly discussed.
EUV pulses having time duration of about 100 ns have been obtained also with the ENEA DPP source. After a brief description of the experimental apparatus, a DPP source characterization and its performances, compared with a simplified theoretical simulation, will be presented.
Several examples of application of the sources concerning photonic materials and photoresists treatments will be shown. Both sources are operative and available for experiments.

#260 - Investigation of non-neutral complex plasmas

Massimiliano Romè - Università degli Studi di Milano

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Complex or dusty plasmas are ionized gases that also contain a distribution of micrometer-sized particles with a surface charge of the order of a few thousand electron charges. These plasmas are characterized by the interplay between a wide range of time and spatial scales. Laboratory complex plasmas generally satisfy a global (quasi-)neutrality condition. Recently the concept of magnetization of a dusty plasma has drawn a considerable interest [1]. A magnetic field may influence the dust charging process and hence the electrostatic interaction between grains, their diffusion and confinement time, affecting in turn the dynamics of the overall plasma. Penning-Malmberg traps [2] are an established tool for the study of magnetized non-neutral plasmas. These plasmas can be easily confined for long times under ultra-high vacuum conditions with a combination of static electric and magnetic fields, and their evolution can be monitored by means of electrostatic and optical systems. The DuEl (Dust-Electron) device is a modified Penning-Malmberg trap under development at the University of Milano, aimed at investigating a non-neutral complex plasma, i.e. a plasma of electrons contaminated with a fraction of dust grains [3,4]. The physical aims of the project and the design of the apparatus are presented. A physical process of fundamental interest is the diffusion of dust in the electron plasma and its influence on the fluid instabilities therein. In this respect, to support the experimental investigations a dedicated two-dimensional particle-in-cell code has been developed, that simulates the transverse dynamics of a magnetized electron plasma contaminated by a massive, charged species. A mass-less fluid (drift-Poisson) approximation for the electron component is exploited, while the motion of dust grains, including the effects of gravity, is integrated kinetically. The possibility of effective dust confinement and the effects of dust contamination on the equilibrium and stability properties of the electron plasma (with the formation of coherent structures) are studied as a function of relevant parameters, e.g. dust size, degree of contamination and magnetization.

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#261 - Barriers in the transition to global chaos in collisionless magnetic reconnection

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In this work we analyze the transitional phase from local to global chaos in the magnetic field produced during a collisionless threedimensional magnetic reconnection numerical experiment [1]. In the corresponding magnetic field topology, regions where the magnetic field lines are stochastic coexist with regions characterized by the presence of regular KAM surfaces. In the stochastic domains the field of the Lyapunov exponents, computed by following the magnetic field line trajectories for a finite amplitude interval, the so called Finite Time Lyapunov Exponents, shows a structure with ridges. These ridges, which are special gradient lines that are transverse to the direction of the minimum curvature of this field, are Lagrangian Coherent Structures (LCS) [2] that act as barriers for the transport of field lines [3]. A careful spectral analysis of the radial position of the magnetic field lines shows that their motion through the chaotic domain is characterized by different frequencies which strongly depend on the coherent structures that they are winding around [4]. Transport increases and the transition to global chaos occurs when the LCS's are destroyed during the advancing reconnection process.

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#262 - Experimental fast electron transport studies in a counterpropagating scheme

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A detailed knowledge of the physical phenomena underlying the generation and the transport of fast electrons generated in high-intensity laser-matter interactions is of a great interest both for fundamental research, e.g. laboratory astrophysics and for applications such as the development of ultra-fast X-ray and particle sources and the Fast Ignition approach to Inertial Confinement Fusion, where a laser-generated fast electron beam is envisaged to deposit its energy in a precompressed fuel capsule heating it to the point of ignition.

Typically a few tens of percent of the laser energy is converted into kinetic energy of the fast electrons, which are injected into the target material in a cone of about 60°-80°, generating huge currents (up to hundreds of MA). Therefore, the transport of the fast electrons in the dense target material is accompanied, in addition to collisions of the electrons with the target atoms, by self-generated electric and magnetic fields, the onset of a neutralizing return current and beam-plasma instabilities.

Here we report on an experiment carried out with the VULCAN Petawatt beam and aimed at investigating the role of collisional return currents in the dynamics of the fast electron beam. To that scope, in the experiment counterpropagating electron beams were generated by double-sided irradiation at relativistic laser intensitiy of a layered target foil containing a Ti layer. The experimental

results were obtained for different time delays between the two laser beams as well as for single-sided irradiation of the target foils. The main diagnostics consisted of two bent mica crystal spectrometers placed at either side of the target foil. High-resolution X-ray spectra of the Ti emission lines in the range from the Ly-α to the K-α line were recorded. In addition, 2D X-ray images with spectral resolution were obtained by means of a novel diagnostic technique, the energy-encoded pin-hole camera, based on the use of a pin-hole array equipped with a CCD detector working in single-photon regime.

The spectroscopic measurements suggest a higher target temperature for well-aligned laser beams and a precise timing between the two beams. The experimental results are presented and compared to simulation results.

#263-Stability criteria in compressible reduced magnetohydrodynamics and analogy with the magnetorotational instability

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A stability analysis for the Hamiltonian compressible reduced magnetohydrodynamics (CRMHD) model is carried out by means of the Energy-Casimir method. Two destabilizing effects are found and, by means of a comparison with the classical delta W criterion applied to ideal MHD, such effects are identified with the kink and interchange instabilities. Further analogies between the expression of the second variation of the free energy functional for CRMHD and the expression of delta W for ideal MHD are obtained, such as for instance, the stabilizing role of compressibility. With the help of the Energy-Casimir method, we obtain also stability conditions for CRMHD in the presence of toroidal flow. We establish then a formal analogy between CRMHD and a reduced incompressible model for magnetized rotating disks. The energy stability analysis, in the light of such analogy, shows that the condition for magnetorotational instability for the latter model, corresponds to the condition for interchange instability in CRMHD, with Coriolis term and shear velocity playing the role of the curvature term and of the pressure gradient, respectively. By means of the Energy-Casimir method, we obtain stability conditions for the rotating disk model, for a large class of equilibria, accounting also for non-uniform magnetic fields. In particular, this shows the possibility, for such system, to undergo, in addition to the magnetorotational instability, also an analogous of the kink instability. In the purely fluid limit, on the other hand, the Rayleigh hydrodynamical stability condition is recovered.

#264 - 21st SILS Conference

Federico Boscherini - Dipartimento di Fisica e Astronomia, Alma Mater Studiorum, Università di Bologna

An introduction of the 21st SILS Conference.

#265 - Exploiting X-ray phase contrast imaging in medical diagnostics: towards clinical applications

Paola Coan (I) - Ludwig Maximilians University, Münich

X-ray imaging has been the most important and widespread diagnostic tool in Medicine over the last century. X-ray radiography, which is based on recording the inhomogeneous transmission of radiation passing through a sample, still represents the gold-standard technique for a large number of biomedical applications.

Despite its huge success, for example in imaging bone structure, X-ray diagnostics ultimately reaches its limits in the examination of soft tissues, such as small tumours in healthy tissues, lungs or articular cartilage. Moreover, medical diagnostic imaging requires high contrast at low radiation dose: a condition that often limits the sensitivity of the method.

In this scenario, the application to biomedical imaging of coherent X-ray phase-contrast imaging (PCI) methods, which explicitly utilise the wave character of X-ray light, has attracted a vivid interest in medical imaging. The unprecedented contrast enhancement that this new radiographic modality may provide indicates the potential to overcome the intrinsic limitations of standard radiology in the examination of soft tissues with similar or even reduced radiation doses.

Over the last decade, different PCI modalities have been largely applied to biomedical applications. Comparative studies in which PCI images are correlated to results obtained with conventional diagnostic imaging tools have demonstrated the high sensitivity of PCI techniques for clinically relevant cases such as breast and cartilage tissues.

In this presentation, the principles of PCI are introduced and an overview of the main results produced in in-vitro and in-vivo experiments on clinically relevant medical cases is reported. The feasibility of low dose, high energy and high resolution PCI-CT and its sensitivity for imaging clinical-like human specimens will be discussed and demonstrated.

The scenario of PCI in the perspective of the clinical application of the method will be also discussed. Today, PCI techniques are mainly performed at synchrotron facilities since these X-ray sources possess key characteristics such as a small source size, high beam collimation and high fluencies that are important for PCI and medical applications. However, the availability of compact, intense monochromatic sources, which are under development worldwide, may fundamentally change the practice of X-ray imaging and can largely extend the application of imaging techniques that are presently confined into synchrotron radiation facilities.

#266 - New opportunities with coherent hard X-rays at the refurbished ESRF beamline ID10

Federico Zontone - European Synchrotron Radiation Facility, Grenoble

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In the frame of the upgrade of the European Synchrotron Radiation Facility the ID10 beamline went through a major reconfiguration in 2012. The previous multi station based on the beam multiplexing via semi-transparent diamond monochromators, known as Troika, has been replaced by a serial double-station setup operating in 50% time-sharing mode with independent fully optimized optics. The first station has a dedicated setup for liquid scattering experiments in various grazing incidence geometries while the downstream station has a longer hutch hosting experiments based on the scattering of coherent hard X-rays (7-10 keV), with techniques like X-ray Photon Correlation Spectroscopy (XPCS) for quantifying temporal fluctuations in slowly varying speckle patterns to look into the dynamics of the system and Coherent X-ray Diffraction Imaging (CXDI) for retrieving the exact spatial arrangement of static disordered samples from coherent far-field diffraction patterns.

Here we illustrate the new opportunities with coherent hard X-rays by showing an example of aging dynamics in metallic glasses studied by XPCS and the first successful 3D CXDI result at 60 nm resolution of a micrometric agglomerate obtained from the spontaneous self-assembly of Fe_2P nanoparticles.

#267 - Edge illumination phase-contrast imaging: nanoradian angular resolution at synchrotrons and translation to conventional sources

Paul Claude Diemoz - Dept. of Medical Physics and Bioengineering, University College London

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The edge illumination (EI) x-ray phase-contrast imaging (XPCi) technique has been under intensive development over the last years at UCL [1,2]. First developed and applied at the Elettra synchrotron radiation (SR) facility, it was later demonstrated to be efficiently applicable also to conventional, lab-based x-ray sources. The technique is insensitive to beam polychromaticity and provides high phase sensitivity even with source sizes of up to at least 100 μm. Besides, the required setup is simple, scalable and relatively insensitive to mechanical vibrations and thermal stress.

In this talk, we first present the results obtained at two SR facilities, ESRF (France) and Diamond (UK), by using very high (85 keV) and very low (12 keV) x-ray energies, respectively. A newly developed method for quantitative separation of the absorption and refraction object properties was applied to the experimental data. The very good agreement with the theoretically predicted values proves the high accuracy of the method. Furthermore, the uncertainty on the refraction values was calculated to be only a few

nanoradians, which is about one order of magnitude improvement compared to previously reported values for other XPCi techniques, proving that EI allows achieving extremely high angular resolution [3]. The high sensitivity and the very wide energy range over which it can applied make this technique very promising for the imaging of a variety of samples of different size and composition.

We then describe how this technique can be applied to conventional x-ray tubes. In particular we show, using experimental data and a new theoretical model, how the phase sensitivity is influenced by the size of the x-ray source. Two EI setups have been installed in the UCL laboratories and have been used for imaging a variety of samples. We present examples of some of the considered applications, which include mammography, the imaging of murine cartilage, detection of cracks and defects in composite materials. Great improvements over conventional methods are demonstrated, obtained with radiation doses that are acceptable for both biological and clinical applications.

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#268 - Photofragmentation of halogenated pyrimidine molecules in the VUV range

Mattea Carmen Castrovilli – CNR - Istituto di Metodologie Inorganiche e dei Plasmi, Monterotondo Scalo

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The harmful influence of electromagnetic radiation on biological systems has long been known, but the microscopic mechanisms, acting at the single molecule level, are just recently being unraveled [1]. Selective irradiation of the nucleus or the cytoplasm shows the DNA to be the most sensitive target in the cell, its damage leading to dramatic consequences such as cell death or mutagenesis. Experiments performed on isolated DNA bases have the invaluable property to disentangle the effects induced directly on the DNA building blocks from the indirect effects induced by secondary processes from the surrounding environment.

On the other hand, the harmful effects of radiation damage are proficiently used in medicine to selectively increase the effects of radiotherapy on tumor cells. Within this frame, the halogenated pyrimidines constitute an important class of prototype radiosensitising molecules. The study of their fragmentation dynamics is of potential interest to understand the fundamental mechanisms of the enhanced radiation damage when these molecules are selectively incorpo-rated in the DNA of tumor cells.

We have undertaken a joint experimental and computational study of the appearance energy (AE) potentials of the 2Br, 2Cl, and 5Br pyrimidine molecules. The targets are chosen with the purpose of investigating the effect on the fragmentation dynamics of the specific halogen atom and of the site of halogenation.

The experiments were performed at the 'Circular Polarization' (CIPO) beamline of the Elettra synchrotron radiation source, Trieste, Italy. We have measured the m/z spectrum of the molecule at 14eV photon energy and then a specific m/z cross section has been studied as function of the photon energy. In this way the AE of the fragment ion has been measured.

The ab initio calculations of the molecular structures involved in the investigated fragmen-tation paths have been performed using Gaussian 09 program. The relative energies for the reactants and products have been calculated using G3B3 [2] methods. The study of the mass spectra, the fragmentation channels and the theoretical calculations compared to the expe-rimental AE values suggest the positioning of the halogen atom in site C2 as the most favorable configuration for the releasing of the halogen radical, in particular for the Br case.

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#269 - Toward ambient pressure scanning photoemission imaging and spectromicroscopy - a feasibility test and first results

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Aleman Llorente, Luca Gregoratti (Elettra - Sincrotrone Trieste SCpA, SS14 Km163.5 in Area Science Park)

X-ray photoelectron spectroscopy (XPS) is a powerful experimental tool for surface science studies due to its high surface and chemical sensitivity. The standard approach to this technique suffers from two major limitations: 1) spatial resolution (material gap) and 2) the requirement for high-vacuum conditions (pressure gap). In the last decades important technical improvements have been addressed to overcome both limitations, the first being the development of synchrotron based photoelectron microscopy techniques such as the approach used for the Scanning PhotoEmission Microscope (SPEM) of the Elettra synchrotron light source, that uses a small focused photon probe to illuminate the surface. The focusing of the X-ray beam is performed by using a Zone Plate and the sample surface is mapped by scanning the sample with respect to the focused beam. The X-ray beam can be downsized to a diameter of 120 nm which allows an effective imaging resolution of less than 50 nm. The overall energy resolution is better than 200 meV. Some recent achievements in the chemical, physical and electronic characterization of nano- and micro-structured materials, such as carbon nanotubes and semiconducting nanowires, will be presented providing an overview of the capabilities of this powerful technique. Other examples will illustrate the characterization of the surfaces of Solid Oxide Fuel Cells under operating conditions showing how dynamic phenomena such as mass transport can be monitored by the SPEM [1]. Only recently the development of electron energy analyzer with differentially pumped lens systems allowed to address the "pressure gap" and to perform in situ XPS measurements up to few mbar (near ambient pressure). Due to their cost, technical complexity and intrinsically low efficiency it was not possible to export such solution to photoemission spectromicroscopy and conventional XPS stations so far. Feasibility test and

first results of innovative and cheap solutions developed at Elettra for photoemission microscopes, which can be potentially used to address the "pressure gap" in any XPS system, will be presented and discussed [2].

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#270 - Magnetic, orbital and charge fluctuations in layered cuprates studied by resonant soft x-ray scattering

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High resolution resonant soft x-ray scattering is a powerful tool for understanding the physics of high T_c cuprates (HTS), as we have recently demonstrated using the AXES and SAXES spectrometers at the European Synchrotron Radiation Facility (ESRF, Grenoble) and at the Swiss Light Source (SLS, Switzerland) respectively.
Here I will present some of the results obtained with these instruments on insulating and superconducting layered cuprates using Cu L_3 edge RIXS. This technique is shown to be the optimal probe to study magnetic, orbital and charge fluctuations in the CuO_2 planes of these compounds, allowing energy and momentum-resolved measurements and adding crucial pieces to the puzzle of high temperature superconducitivity.
In particular, I will show that a large family of high T_c cuprates exhibits high-energy damped spin excitations (paramagnons) over a wide range of doping, with dispersions and spectral weights closely similar to those of magnons in undoped compound, thus supporting the paramagnons as strong candidates to cover the role of glue for the Cooper's pairs [1]. We find similar results in artificial cuprate-based superlattices (SLs), both insulating and superconducting, that exhibit magnon and paramagnons dispersions down to very small cuprate layer thickness and despite the chemical and structural alterations at the interfaces [2]. Moreover the orbital excitations, visible in the spectra together with magnons and due to the ligand field felt by Cu^{2+} ions, reveal a pyramidal coordination of copper atoms at the interfaces. These findings open the way to the production of new, artificial HTS based on cuprate/noncuprate SLs where the charge reservoir layer is constituted by the interface itself. Finally I will show that two-dimensional incommensurate charge fluctuations are present in the CuO_2 planes of $(Y,Nd)Ba_2Cu_3O_{6+x}$ [3]. In combination with earlier observations, these data and their temperature dependence indicate an incipient charge density wave (CDW) instability that competes with superconductivity and, for the first time, we have the evidence that the anomalously low T_c found in underdoped cuprates is due to CDW, and not other phenomena.

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#271 - Discrete representation of local orientation in grains using diffraction contrast tomography

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Wolfgang Ludwig (European Synchrotron Radiation Facility, Grenoble and University INSA Lyon), Kees Joost Batenburg (CWI Amsterdam and University of Antwerp)

The reconstruction of the 3D grain microstructure in the bulk of polycrystalline materials is a problem that presents many challenges, both from an experimental and data analysis point of view. In non-destructive techniques based on monochromatic beam X-Ray diffraction, the local orientation of the crystal lattice, whose knowledge is the aim of the reconstruction, is also responsible for the deformation of the images recorded by the detector.
Different computational approaches have been proposed over the years, to deal with the different available experimental techniques. One of the common shortcomings has been the restriction to single voxel optimization. It has been shown that stochastic optimization techniques can be used to approach the solution, matching the diffracted intensities and data acquisition schemes (namely, line beam illumination or 3D volumes from stacking of 2D layers), requiring however long acquisition times. Ideally, reconstruction of the 3D orientation field would be achieved from extended beam diffraction data and the optimization should be performed over the volume of a grain or ultimately the sample volume.
X-Ray Diffraction Contrast Tomography is an extended beam tomographic imaging technique which demands shorter acquisition time compared to other techniques. If the reconstruction of the local crystal orientation is restricted to only a 2D slice of a volume, the problem will be intrinsically five-dimensional, because the 2D orientation field assumes a three-dimensional orientation space. However, it will always be possible to describe the reconstruction as the solution to a linear system A x = b, where x* is the true solution to the system. Unfortunately the availability of components in b will be less than required by the number of unknowns in the vector x. The developments in mathematical optimization, during the last 15 years, have shown that tools like l1-minimization, applied to the Haar transform in the solution domain, can recover specific solutions to heavily under-determined systems.
We propose a practical representation of the orientation space, which avoids higher degrees of under-determinacy, and we describe the application of the FISTA algorithm to DCT data. This approach overcomes the single voxel optimization restriction.
Finally we present promising results obtained on simulated data.

#272 - SR-FTIR imaging of carbon dioxide diffusion in cordierite-like structures

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Cordierites and beryls are isostructural microporous minerals that may contain significant amounts of H_2O and CO_2 in their structural channels [1]. The crystal chemical study of these minerals may thus be important for both petrological and technological applications. Experimental introduction of CO_2 in cordierite was studied by several authors [2, 3], who pointed out the extreme difficulty to reach sample saturation and homogenization. Hence, knowledge of the actual distribution of the volatile molecules is crucial to evaluate the diffusion within the minerals. In this work, we addressed this problem by using FTIR spectroscopy.

Experimental introduction of CO_2 was carried on both cordierite and beryl CO_2-free starting materials. Single-crystals were treated in CO_2-saturated environment at different pressure, temperature and time conditions using a non end-load piston-cylinder press at INGV (Rome). The run products were analyzed via micro-FTIR spectroscopy at INFN-LNF (Frascati) in order to quantify the CO_2 content and its distribution across the sample. Preliminary data show that pressure plays a major role in diffusing gaseous CO_2 across both in cordierite and beryl, whereas the effect of temperature is less pronounced. High-resolution FPA (focal-plane-array of detectors) SR-FTIR imaging was done at beamline B22, Diamond laboratory (Oxford, UK). The data show that the diffusion of CO_2 occurs exclusively along the structural channels, along the *c*-axis direction. The diffusion path of CO_2 does not exceed 200 µm even after 10 days treatment. Sample cracks formed during the experimental runs speed up diffusion; measured CO_2 contents along these cracks are even 4 times higher.

Several CO_2-rich samples were heat-treated up to 1200° C using a Linkam heating stage to investigate the rate of CO_2 evacuation as a function of T. In situ FTIR spectra showed that the decarbonation process starts around 800° C, but temperatures of at least 950° C are needed to remove up to 95% of CO_2 from the sample in the first 30 minutes.

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#273 - TDDFT-based nonadiabatic dynamics with classical and quantum trajectories

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Basile Curchod (EPFL, Lausanne)

In the mixed quantum-classical description of molecular systems, only the quantum character of the electronic degrees of freedom is considered while the nuclear motion is treated at a classical level. In the adiabatic case, this picture corresponds to the Born-Oppenheimer limit where the nuclei move as point charges on the potential energy surface (PES) associated with a given electronic state. Despite the success of this approximation, many physical and chemical processes do not fall into the regime where nuclei and electrons can be considered decoupled. In particular, most photoreactions pass through regions of the PES in which electron-nuclear quantum interference effects are sizeable and often crucial for a correct description of the phenomena.

Recently, we have developed a trajectory-based nonadiabatic molecular dynamics scheme that describes the nuclear wavepacket as an ensemble of particles following classical trajectories on PESs derived from time-dependent density functional theory (TDDFT) [1]. The method is based on Tully's fewest switches trajectories surface hopping (TSH) where the nonadiabatic coupling elements between the different potential energy surfaces are computed on-the-fly as functionals of the ground state electron density or, equivalently, of the corresponding Kohn-Sham orbitals [2].

In this contribution I will also introduce a novel TDDFT-based on-the-fly scheme for the description of nuclear quantum effects using Bohmian trajectories derived from quantum hydrodynamics [3].

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#274 - Electron-phonon interaction and superconductivity in graphene and in intercalated graphite

Francesco Mauri (I) – CNRS, Paris

Graphene represents a physical realization of many fundamental concepts and phenomena in solid state-physics, but in the long list of its remarkable properties a fundamental one is missing, i.e. superconductivity. Here we show how one can create and engineer a superconducting transition in graphewne by adatoms' doping [1].

Density-functional theory calculations show that the occurrence of superconductivity depends on the adatoms' chosen, in close analogy to the case of graphite-intercalated compounds (GICs). However, most surprisingly, and contrary to the case of GICs, Li-covered graphene is found to be superconducting at much a higher temperature with respect to Ca-covered graphene.

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#275 - First principles study of donor wave functions in silicon nanowires

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The localization of the donor electron wave function can be of key importance in various silicon application, since it determines the interactions between neighbouring donors and influences the charge density close to the donor atom. These properties are important in light of applications like nuclear spin qubits [1] based on the hyperfine interaction between electron and nuclear spin [2] or for determining the critical density of metal-insulator transitions [3]. In particular the delocalization is a critical feature when dealing with nanostructures, where the confinement induces a squeezing of the donor wave function.

Using fully ab-initio calculations, we have studied the delocalization of the donor electron wave function along the axis of a nanowire with different orientations and for phosphorus and selenium donors. We show that the shape and delocalization is greatly influenced by the orientation of the nanowire and that a considerably larger value can be obtained for [011] oriented nanowires, compared to [001] and [111] orientations. We also demonstrate that its value can be controlled by applying a compressive or tensile uniaxial strain. As a last result we show the effect of the delocalization on the hyperfine parameters, that can be calculated with projector augmented-wave method (PAW) [4].

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#276 - Structural, electronic and optical properties of PDI-FCN$_2$ crystal

Renato Colle – Università di Bologna

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We present a theoretical and experimental investigation of the crystalline structure of PDI-FCN$_2$ that has been deduced combining experimental XRD data, obtained from powders, with global-optimization algorithms which allow to identify Bravais lattice, primitive cell parameters and space group of the crystal. The XRD spectrum calculated for the proposed crystalline structure very well reproduces the measured XRD data. Our results suggest the triclinic lattice structure, of spatial groups P1 and P-1, respectively, for the crystalline PDI-FCN$_{2-1,7}$ and PDI-FCN$_{2-1,6}$ isomers. In both cases the primitive cell contains a single molecule. On the proposed crystalline structures, KS-DFT cell energy calculations, including van der Waals interactions, have been performed to assign the minimum energy geometrical structure and orientation of the molecule inside the corresponding primitive cell. These calculations evidence the molecular packing that characterizes the strong anisotropy of the PDI-FCN$_2$ crystal. Electronic band-structures calculated for both isomers within the Kohn-Sham density-functional theory indicate that the crystalline P1 structure is an indirect gap semiconductor, while the P-1 structure is a direct gap semiconductor. The electronic band structure calculations on the optimized crystal geometries highlight strong anisotropy in the dispersion curves E(k), which roots at the molecular packing in the crystal. The optical absorption spectrum calculated in RPA approximation from the band structure of the crystalline PDI-FCN$_{2-1,7}$ isomer well compares with the absorption spectrum measured on PDI-FCN$_2$ crystalline film grown on silicon dioxide substrate. Finally, the infrared spectrum of both crystalline isomers has been predicted in harmonic approximation.

#277 - Novel 2D materials for opto-electronics and photo-voltaics

Maurizia Palummo - ETSF, Dipartimento di Fisica, Università degli Studi di Roma "Tor Vergata", Roma

Marco Bernardi, Jeffrey C. Grossman (Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA 02139-4307, USA)

After the discovery of graphene, new emerging two-dimensional materials including layers of BN, hybridized graphene-BN (CBN) and dichalcogenides (MoS_2,$MoSe_2$,WS_2 ect.) have been the focus of strong interest for their tunable opto-electronic properties, their high carrier mobility and the envisaged possibility to use them in photovoltaic devices.
In this talk, I will focus on the electronic and optical properties of CBN hybridized monolayers [1-2] studied by ab-initio density functional theory and many-body perturbation theory (GW and Bethe-Salpeter) calculations.
Then based on our recent first-principles simulations, I will present candidate interfaces and device architectures to implement CBN [3] and other monolayer semiconductors [4] into efficient and photostable excitonic solar cells alternative to those based on conjugated polymers and small molecules.

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#278 - Surface electronic properties and lattice dynamics of group-V semimetals from ab-initio calculations

Davide Campi – Università Milano-Bicocca

Marco Bernasconi (Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca), Giorgio Benedek (Dipartimento di Scienza dei Materiali, Universita' di Milano-Bicocca e Donostia International Physics Center (DIPC), University of the Basque Country (UPV-EHU), San Sebastian/Donostia,Spain)

Recently group-V semimetals Bi, Sb and As attracted a considerable interest at both fundamental and applied level because of their peculiar surface properties and their possible applications in spintronic devices.
These elements present metallic surface states which show a remarkable spin-splitting as a consequence of the strong spin-orbit coupling and the broken inversion symmetry. Moreover in Sb and As the electronic surface states connect in a non-trivial way the valence-like and the conduction-like bands as a consequence of the topologically non-trivial bulk band order that these materials share with the strong 3D topological insulator Bi_xSb_{1-x}.
Recent He atom scattering measurements of Bi(111) surface phonons and the interest in understanding the interplay between electronic surface states and lattice dynamics at surface and in thin films motivated the present study based on density functional perturbation theory (DFPT).
All the three materials, that crystallize in the same bilayer structure, exhibit similar surface phonon dispersions characterized by a wide gap between acoustic and optical modes and the appearance of a surface branch above the maximum of the bulk frequencies. These features were found to be relatively stable with respect to the slab thickness down to a single bilayer despite the important changes that occurs in the electronic structure that cause the transition from a metallic to an insulator character in low dimensional slabs.
In the case of Sb the electron-phonon coupling coefficient have been calculated. We found that the main contribution to electron-phonon interaction involves transitions between surface and bulk states, mostly driven by bulk phonons, in good agreement with the value derived from spin angle-resolved photoemission spectroscopy.

#279 - Atomistic calculation of thermoelectric properties of Si nanowires

Igor Bejenari – Duisburg, Essen University

Silicon nanowires (NW) represent building blocks for nanoscale electronics. They can be fabricated with a very good control of composition, size and shape. For Si NW with a diameter of 5 nm and less, the number of atoms in the NW cross section becomes countable. Therefore, one should take into account electron-phonon interaction, crystalline orientation and quantum confinement to estimate transport characteristics of Si NW in order to predict the performance of nanoscale transistors, sensors and thermoelectric devices. In contrast to the bulk materials conventionally used in thermoelectrics, the nanostructured materials offer a possibility to design thermoelectric devices with an improved efficiency by exploiting the quantum confinement of electrons and phonons on the nanoscale. In this case, a fully atomistic simulation considering both the electron and phonon band structures as well as electron-phonon interaction is required to estimate thermoelectric properties.

We study thermoelectric properties of Si square nanowires with <100> crystalline orientation taking into account atomistic electron-phonon interaction. In our model, facets <010> and <001> are passivated by hydrogen and there are dimers on the nanowire surface. The electronic structure was calculated by using the sp3s*-spin-orbit-coupled atomistic second-nearest-neighbor tight-binding model. The phonon dispersion and density of states were calculated in framework of Brenner's model. Both Rational Functional Optimization (RFO) and Conjugate Gradients were used to calculate relaxation in the atomistic structure. Based on Fermi's golden rule, the electron-phonon scattering rate was obtained by combining the electron and phonon eigenstates. We used a relaxation time approximation to calculate transport characteristics. To obtain the relaxation time, the Boltzmann transport equation was solved by using iteration method.

#280 - Ab initio many-body effects in TiSe$_2$

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H. Cercellier (Institut Neel, CNRS and UJF, Grenoble), M. Holzmann (LPTMC, CNRS and UPMC, Jussieu and LPMMC, CNRS and UJF, Grenoble, ETSF), C. Monney (Research Department Synchrotron Radiation and Nanotechnology, Paul Scherrer Institut, Villigen PSI), P. Aebi (Departement de Physique and Fribourg Center for Nanomaterials, Universite de Fribourg, Fribourg), G. Onida (Università degli Studi di Milano, Dipartimento di Fisica, ETSF), V. Olevano (Institut Neel, CNRS and UJF, Grenoble, ETSF)

TiSe$_2$ is a non -conventional Charge- Density -Wave material, whose ground state is believed to be a coherent exciton condensate called the Excitonic Insulator. DFT calculations give a metallic ground state with top of-valence and bottom-of-conduction too much overlapping. On the contrary experiments predict this system to be a semi-metal or an indirect gap semiconductor, with a very small gap/overlap. More refined ab initio GW calculations predict this system to be a semiconductor with a 0.2 eV gap. In addition they provide a renormalization of the band structure around the Γ point, arising a mexican-hat dispersion as predicted by Kohn in an exictonic insulator.

We will present and discuss excited state properties comparing calculations with ARPES, STS, and EELS measurements.

#281 - An overview on the application of Vis-NIR hyperspectral and THz-TDS imaging methodologies to the investigation of paintings

Marcello Picollo (I) – CNR – Istituto di Fisica Applicata "Nello Carrara", Sesto Fiorentino

Andrea Casini, Costanza Cucci, Lorenzo Stefani CNR – Istituto di Fisica Applicata "Nello Carrara", Via Madonna del Piano 10, 50019 Sesto Fiorentino (FI)), Kaori Fukunaga (National Institute of Information and Communications Technology (NICT), Koganei, Tokyo 184-8795, Japan)

During the past two decades, thanks to the rapid development of solid-state-based sensor technology, digital imaging methodology emerged as one of the most attractive research areas for the non-invasive investigation of paintings and two-dimension artworks. Imaging techniques are currently being used for the conservation of the cultural heritage, not only to support documentation, but also to investigate the material composition of artworks.

Here, a prototype of a hyperspectral scanner based on two prism-grating-prism line-spectrographs, operating in the 400–1700 nm range, was designed and built at the Istituto di Fisica Applicata 'Nello Carrara' (IFAC) of the Italian National Research Council (CNR). The results that can be obtained with this scanner provide useful information, in particular on the identification and characterisation of pigments and dyes, and on the presence of under-drawings, retouching and pentimenti. Moreover, the acquired images in the visible range can be used for high-quality RGB reproductions and colorimetric applications, since the editing program can compute colorimetric images and store them as CIE L*a*b* TIF files. In addition, the data elaboration based on multivariate analysis methods, such as the principal components analysis (PCA) algorithm, makes it possible to reveal hidden details and to map the materials distribution on the painted surface.

Terahertz (THz) Time Domain Spectroscopy (TDS) imaging systems have many applications as a new, non-invasive methodology for investigating various materials. In recent years, THz-TDS technology has also been proposed for the study of artworks in order to identify the different compounds that constitute multilayered painting systems. In principle THz-TDS imaging makes it possible to fill in the information gap between two imaging diagnostic techniques, namely IR reflectography and X-ray radiography, because it provides useful data on the internal physical structure of non-metallic objects without touching the artworks investigated. This non-invasive cross-section image of the object is acquired by extracting the reflected pulse from a particular interface of two media with different refractive indexes. To summarise, THz-TDS imaging technique provides various types of information in the investigation of panel paintings, as follows: a) condition and appearance of the gilding and gold backgrounds; b) information about the chemical composition of some of the pigments; c) extent of surface deterioration; d) stratigraphic analysis of the various materials with the capability to isolate images of the individual layer of interest.

The application of the above described imaging techniques to some specific case studies will be presented.

#282 - The skin of the ancient egyptian mummies: a fascinating source of information on body preservation

Maria Grazia Bridelli – Dipartimento di Fisica e Scienze della Terra, Università degli Studi di Parma

Chiaramaria Stani, Andrea Baraldi (Dipartimento di Fisica e Scienze della Terra, Università degli Studi di Parma), Rosa Boano, Emma Rabino Massa (Dip. Scienze della Vita e Biologia dei Sistemi, Università di Torino)

The Museum of Anthropology and Ethnography of Turin stores one of the most important Egyptian collections of ancient human remains in the world, comprising the heads of 80 mummies, five complete Predynastic (about 5000-3000 B.C.) mummies and 15 Dynastic (about 3000 B.C.- 300 A.D.) mummies. For many years research activities for the management of these specimens were promoted by the Museum staff members for the investigation of the degradation status of organic materials originated from biological tissues of archaeological origin. The studies are of importance to conservators not only from the historic perspective but also for enabling the appropriate conservation treatments and to assess optimal preservation environment. Fourier Transform Infrared (FTIR) absorption spectroscopy is an investigation technique suitable for ancient biological tissue characterization due to its non-destructive character, requiring minimal quantity of the sample and no treatment of the biological system prior to investigation. In the IR spectrum of a human skin the main absorption bands of the biological components such as proteins, lipids, nucleic acids, and carbohydrates, all occurs in the same wave number range (400-4000 cm^{-1}). The Infrared spectrum of a modern skin sample was compared with that recorded on skin fragment of both a Predynastic and some Dynastic mummies. The biochemical modifications recorded reveal a partial alteration of the ancient tissues which have been stabilized by the chemical-physical environmental conditions or embalming treatments and preserved for thousand years. The whole IR spectrum of the tissue reveals traces of these "age-inhibitor" processes: 1) the water OH-stretching band (~3400 cm^{-1}) features are indicative of the twofold role of the dehydration processes, as a result of hot temperatures in the desert or by salt treatment, both contributing to the protein deterioration and determining their conservation; 2) conformational features of the skin proteins can be extracted by monitoring Amide I band (1600-1700 cm^{-1}), primarily arising from the C=O stretching vibrations of the peptide backbone, by deconvolution of such a band in Gaussian components, and by relating the frequencies of the obtained band components to the protein secondary structures. In the mummified samples the Amide I decomposition reveals a decrease in the alpha-helix amount and an increase in the beta-sheet motif, showing different extent in dependence on the post-mortem treatment of the corpses; 3) in the glucid specific spectral range (950-1150 cm^{-1}), in the mummified skin spectra an increase was measured in the glucid/protein ratio with respect to modern skin sample, a spectroscopic marker for the AGE compounds formation as a consequence of the collagen binding to sugars in tissues.

#283 - Fluorescence hyperspectral lidar imaging of the cultural heritage: recent instrumental and application advances

Valentina Raimondi - CNR – Istituto di Fisica Applicata "Nello Carrara", Sesto Fiorentino

Lorenzo Palombi, David Lognoli (CNR – IFAC, Sesto Fiorentino)

Fluorescence lidar imaging has been demonstrated as a useful tool for the diagnostics and documentation of the monumental cultural heritage, with particular reference to the detection and classification of biodeteriogens, characterisation of lithotypes and detection of protective coatings. The technique relies on the use of a low-fluence UV pulsed laser, which is used to remotely excite fluorescence, and a telescope, which is used to collect the signal emitted from the monumental surface. The signal is fed to a proper dispersion, detection and acquisition system and the obtained spectral data are stored for subsequent processing. A computer-controlled scanning system is employed to scan the surface and to acquire hyperspectral fluorescence images. Finally, suitable data processing methods, such as multivariate data analysis, are used to produce false-colour coded thematic maps of the investigated areas.

The technique offers several advantages for the investigation of the monumental cultural heritage, since it can be used to carry out fluorescence measurements on site from distances as far as hundred of metres without the need for scaffolds or lifts. In particular, it can provide an overall assessment of the entire surface investigated and the results can be exploited to address further analytical measurements and/or sampling in specific areas identified on the thematic maps.

This paper briefly outlines the basics about the technique and then focuses on the latest advances and results concerning both instrumental features and applications to the diagnostics and documentation of the cultural heritage. In particular, it addresses the impact on applications of the instrument's upgrade in terms of scan speed, enhanced spatial resolution and field of view of the instrument. It shows recent studies aimed to extend the field of application of the lidar technique to wall paintings and to the classification of microbial communities and finally outlines the potential of a new concept of fluorescence lidar system based on the integration of hyperspectral and fluorescence lifetime spectroscopy, together with imaging capabilities.

#284 - Crystal luminescence and cultural heritage: from pottery authentication to historical buildings dating

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Authentication and dating methods used on Cultural Heritage are based on luminescence emissions of minerals extracted from pottery, bricks, sediments and terracotta artifacts. The most commonly used minerals are quartz and feldspars and the luminescence production is a result of multiple interactions within these imperfect natural crystals extracted from the sample of interest.

Luminescence arises from stimulation, either thermal or optical of minerals that have been previously exposed to ionizing radiation. During exposure, radiation energy is accumulated and stored in crystal lattice defects in the form of trapped electrons. This trapped charge is released during stimulation and the resulting luminescence signal becomes zero.

Thermally stimulated luminescence, thermoluminescence (TL), has been used extensively as a tool in the investigation for authenticity of fired clay such as pottery, porcelain and casting cores of bronzes. In the case of an object which has been excavated under controlled conditions, TL is useful to give a precise historical date.

Currently TL dating is a routine tool in archaeological domain as well as to identify the period of construction of historical buildings. This application is based on the assumption that the manufacture of the bricks used for TL measurements was contemporary to the edification. Of course we consider the hypothesis that no reuse material was used coming from older fabrics. In the past the use of pre-existing material was usual and then particular attention is aimed to the mortar considering that it is prepared just before its use. Investigation on mortars are based on Optically Stimulation Luminescence (OSL) emissions assuming the optical bleaching of minerals during mixture phase.

The different applications of luminescence require a specific methodology depending on the purpose of the work and on the kind of sample. With this aim each step must be optimized starting from sample collection and physical chemical preparation procedure to absorbed dose evaluation and age calculation.

A detailed description of the specific protocols developed at the PH3DRA laboratories to TL authentication and dating of pottery as well as to establish the chronology of historical buildings will be made. Considering different case studies, particular attention will be devoted to some critical points like quantity and amount of sample, the necessary tests choosing the best measurement conditions and the most appropriate procedure.

#285 - Use of a versatile instrument for X-ray radiography and tomography of artworks, precious objects and archaeological materials

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Debora Angelici (Dip.Fisica, Univ.To - INFN To - TecnArt S.r.l. To), Rosa Boano (Dip.Scienze della Vita e Biologia dei Sistemi, Univ.To), Cristina Bortolin (Dip.Fisica, Univ.To), Rosa Brancaccio (INFN -To), Jacopo Corsi (Dip.Fisica, Univ.To - INFN To), Fulvio Fantino (TecnArt S.r.l., To), Novella Grassi (CCR "La Venaria Reale", Torino), Alessandro Lo Giudice, Giorgia Mila (Dip.Fisica, Univ.To - INFN To), Raffaella Navone (RAG TO), Roberto Sacchi (Dip.Fisica, Univ.To - INFN To)

X-ray imaging is now widely used in the Cultural Heritage field because of its non-invasivity and for the high number of information which can be obtained on the inner structure of an object. A new instrument for X-ray radiography and tomography has been developed by the Physics Department of the University of Torino and the INFN (National Institute for Nuclear Physics). It is based on a microfocus X-ray source, a rotary stage and a linear X-ray detector moved by a high precision mechanics. A frame to fix paintings and larger objects is also available, allowing radiographies on large areas. The possibility to change distances among the analysed object and both the detector and the source makes the instrument very versatile, allowing to analyse both small objects (exploiting a high magnification) and bigger ones (analysing large areas). Moreover many parameters, like X-ray energy, current, integration time and distances, can be optimized in real time, allowing to obtain the best configuration in short time.

In this presentation a selection of case-studies will be proposed, showing the potentiality of the instrument on very different kinds of objects and artworks. Painted canvas and panels radiographies will be shown: radiography allows to obtain useful information about the state of conservation, the technique used by the painter (also for authentication purpose) and some basic indication about the pigments (limited to the different radiopacity of various materials).

Another field in which radiography is useful is archaeology: radiographies of earth-blocks can show hidden objects before the micro-excavation and can reveal its state of conservation in an absolutely non-invasive way, allowing to decide if it is suitable to remove it from the earth or not. Moreover they can reveal some details of the hidden objects, for example the presence of different materials or decoration obtained with different thicknesses of the same material.

Also for gemmology digital radiography is very useful and we applied it to pearls. This technique allows to obtain information on their inner structure and so to understand if the pearl is natural or cultured with a solid bead or beadless cultured, discriminating the market value of the pearl.

A third field for which both 2D (radiography) and 3D (tomography) X-ray imaging can give useful information is in the characterisation of objects coming from museum collections. Some examples from artworks and objects from the Anthropological and Ethnographical Museum of the University of Turin will be shown, giving a great number of information on different materials, constructive technique and state of conservation useful both for their valorisation and protection.

This work is part of a larger collaboration research project that involves also the Centro Conservazione e Restauro "La Venaria Reale" and the neu_ART regional project.

#286 - Semi-conductor pigments in 19th C. paintings:time-resolved fluorescence spectroscopy and imaging

Austin Nevin – CNR - Istituto di Fotonica e Nanotecnologie, Milano

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We present the non-invasive study of historical and modern Zn- and Cd-based pigments with time-resolved fluorescence spectroscopy, fluorescence multispectral imaging and fluorescence lifetime imaging (FLIM). Zinc Oxide and Zinc Sulphide are semiconductors which have been used as white pigments in paintings, and the luminescence of these pigments from trapped states is strongly dependent on the presence of impurities and crystal defects. Cadmium sulphoselenide pigments vary in hue from yellow to deep red based on their composition, and are another class of semiconductor pigments which emit both in the visible and the near infrared. We have measured the fluorescence lifetime of historical and modern pigments ZnS, ZnO and Cd-based pigments using both an Optical Multichannel Analyser (OMA) coupled with a Nd:YAG ns-laser, and a streak camera coupled with a ps-laser for spectrally-resolved fluorescence lifetime measurements. For Zn-based pigments we have also employed Fluorescence Lifetime Imaging (FLIM) for the measurement of luminescence. A case study of FLIM applied to the analysis of the painting by Vincent Van Gogh on paper – "Les Bretonnes et le pardon de Pont-Aven" (1888) is presented. The results obtained with both multispectral imaging and FLIM and complementary multivariate statistical analysis of reflectance images allowed the extraction of maps of pigment distribution in the larger painting. Through the integration of complementary, portable and non-invasive spectroscopic techniques, new insights into the optical properties of Zn- and Cd-based pigments have been gained which will inform future analysis of late 19th and early 20th C. paintings.

#287 - Raman scanning device for the analysis of works of art

Gianluca Valentini – Dipartimento di Fisica, Politecnico di Milano

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One of the main issues in conservation science is the extraction, in a non-invasive way, of chemical information from the materials works of art are made of. Raman Spectroscopy has emerged in recent years as a reliable tool for the non-destructive analysis of a wide range of inorganic and organic materials in works of art and archaeological objects. Nevertheless, vibrational spectroscopy techniques, including Raman spectroscopy and the complementary technique called Fourier Transform Infrared Spectroscopy (FTIR) are still mainly limited to the analysis of micro-samples taken from artistic surfaces. This approach severely limits the scope and applicability of vibrational spectroscopy, since microsampling should be avoided as much as possible in valuable masterpieces and is often strictly forbidden. Actually, pointlike Raman devices that can be used in-situ are available and can overcome the microsampling issue. Yet, the heterogeneity and the size of many works of art are challenging even for such devices, since many measurements have to be taken in order to get a reasonable knowledge of the materials artifacts are made of. In addition, the harsh conditions that scientists and restorers have to face on scaffolds, and in most archeological sites make difficult the use of proximity probes, while contact probes are seldom allowed. For the above mentioned reasons, the development of a Raman spectrometer capable to perform the analysis of an area of several square centimeters and working from a safety distance could greatly increase the applicability of this spectroscopic technique. The present paper describes the development of a prototype of Raman scanning spectrometer based on a diode laser, a 2D galvo scanner and a custom optical system. The device can easily map a surface of 6 cm in diameter at a working distance of 20 cm. Moreover, the collecting optics features a depth of field close to 5 cm, which makes the Raman system suitable for the analysis of non-flat surfaces and three dimensional objects. In addition, the overall dimensions and weight of the instrument have been limited in order to make the device transportable and user friendly for in situ measurements. Details on the design of the device and the results of the characterization tests carried out to assess its performances are reported.

#288 - Integrated photonic quantum simulation

Paolo Mataloni (I) - Università Sapienza, Roma

Quantum simulation allows to study various phenomena which are hard to simulate by classical approaches. Relevant examples are given by quantum transport, particle localization and energy transfer, quantum-to-classical transitions and quantum improved computation. Recent examples of on-chip integrated photonics applied to the quantum regime has opened important perspectives bearing great promises for future quantum simulation. Interesting results have been achieved by exploiting the femtosecond laser writing technology to implement the particle quantum walk, which represents one of the most promising resources for the simulation of physical quantum systems.

I will present experiments dealing with quantum walks of pairs of entangled photons realized by on-chip integrated arrays of interferometers and where controlled phase shifts are introduced into each unit mesh of the network. Polarization entanglementhas been exploited to investigate the genuine effect of (bosonic and fermionic) statistics in the absence of particle interaction and to observe Anderson localization in two-particle discrete quantum walks affected by position dependent disorder. Other measurements, dealing with different types of disorder and studying on how the localization of entangled particles is affected by the wave-function symmetry, will be also discussed.

Among the perspectives of optical quantum simulation I will present also the experimental implementation of the so-called boson sampling problem to demonstrate the computational capability of quantum systems and the development of arbitrary integrated architectures based on three-dimensional geometries.

#289 - Optimal control: From superadiabatic evolution to the speed limit

Rosario Fazio (I) - Scuola Normale Superiore, Pisa

Optimal control theory is a very promising candidate for a drastic improvement of the performance of quantum information processing. By exploring its ultimate limit of performance it is possible to show that it coincides with the maximum speed allowed by quantum evolution: The quantum speed limit. I will discuss some paradigmatic cases, a Landau-Zener problem and the dynamics of a system close to a critical point. On the other side it is possible to guarantee robustness by using the superadiabatic evolution initially proposed by Berry. Here I will describe an extension of this method in open quantum systems.

#290 - From classical to quantum nonlinear photonics

Marco Liscidini (I) - Università degli Studi di Pavia

The drive to reduce the size of optical systems has led to a transition from bulk-crystal optics to integrated photonics, with large improvements of conversion efficiencies in second- and third-order classical nonlinear optical processes. While often designed with classical nonlinear optics in mind, photonic structures will also enhance the corresponding quantum nonlinear optical processes. But is there a simple connection between these two types of processes? Can one infer anything about the outcomes of a quantum process from classical experiments? In this talk, I will show that results of classical experiments allow for an accurate description of quantum correlated photon-pair generation, opening a path to move from classical to quantum nonlinear optics in integrated photonic structures.

#291 - Efficient selection of mesoscopic twin-beam states for the optimal production of sub-Poissonian light

Maria Bondani – CNR - Istituto di Fotonica e Nanotecnologie e CNISM, UdR Como

Alessia Allevi, Marco Lamperti (Dipartimento di Scienza e Alta Tecnologia Universita' degli Studi dell'Insubria, Como) Radek Machulka, Vaclav Michalek, Ondrej Haderka, Jan Perina Jr. (RCPTM, Joint Laboratory of Optics of Palacky University and Institute of Physics of AS CR, Palacky University Olomouc, Czech Republic)

During the last decade, the generation of nonclassical states in the continuous variable domain by means of conditional measurements has been extensively investigated for many quantum-optical applications, including quantum information processing, quantum computing and quantum cryptography. In general, the preparation of conditional states exploits the existence of correlations between two modes. When some observable is measured on one of these two modes, the state of the other one is irreversibly modified. From the experimental point of view, the production of nonclassical states by means of conditional measurements has been achieved either at single-photon level by using single-photon detectors or in the low energy regime with some photon-counting detectors. The possibility to extend the experimental results presented so far to a higher-intensity domain is still object of active research. If on the one hand the main limitation to achieve this goal is related to the optimization of the performances of the employed detectors, on the other hand a complete investigation on the properties of the conditional states as a function of the parameters involved in their production is still missing.

Here we present an experimental scheme aimed at producing and characterizing nonclassical photon-subtracted states obtained by performing conditioning operations on a multimode twin-beam (TWB) state generated by a spontaneous parametric down-conversion process in the linear gain regime. This investigation has been carried on by means of a direct detection scheme involving two hybrid photodetectors, which are photon-counting detectors with a linear response up to 100 photons. We report on the systematic study of the nonclassical properties of the TWB state, and in particular of its noise reduction factor, as a function of the experimental parameters (namely the pump mean power and the collection area) and we show that the optimal generation of conditional states with sub-Poissonian statistics strongly depends on the existence of quantum correlations.

The good quality of the experimental result together with the resolving capability of the detectors we used suggest the future

exploitation of our multimode TWB state for the production of sub-Poissonian states optimized to have selected properties, such as a given mean value or a given amount of non-Poissonianity.

#292 - Characterizing the non-classical nature of mesoscopic optical twin-beam states

Alessia Allevi - Dipartimento di Scienza e Alta Tecnologia, Università degli Studi dell'Insubria e CNISM, UdR Como

Maria Bondani (CNR - IFN e CNISM, UdR Como), Marco Lamperti (Dipartimento di Scienza e Alta Tecnologia, Università degli Studi dell'Insubria, Como), Radek Machulka, Vaclav Michalek, Ondrej Haderka, Jan Perina Jr. (RCPTM, Joint Laboratory of Optics of Palacky University and Institute of Physics of AS CR, Palacky University, 17. listopadu 12, 77146 Olomouc, Czech Republic)

The quantum nature of an optical state is a requirement for the exploitation of the state in many applications, such as for quantum information, quantum computing and quantum metrology.

By definition, a state is nonclassical whenever it cannot be written as a mixture of coherent states. In terms of the Glauber-Sudarshan P function, this condition corresponds to either a highly singular or a negative distribution. However, as this kind of representation is in general not connected to any observable quantity, the negativity of the Wigner function of the states is commonly used as nonclassicality indicator for single-mode states.

A different approach is offered by the implementation of direct detection schemes, with which it is possible to have access to the photon-number statistics of the states and to investigate the possible existence of correlations among the components of a multipartite state.

In this work we present the experimental generation of a pulsed multimode optical twin-beam (TWB) state in the mesoscopic photon-number domain, where a sizeable number of photon pairs is produced, and we report on the characterization of its quantumness by means of a direct detection scheme involving two photon-counting detectors.

To demonstrate the correlated nature of the TWB state, we compare three different nonclassicality criteria based on shot-by-shot intensity measurements, namely the noise reduction factor, the Schwarz inequality and a new inequality based on high-order correlations, and we discuss advantages and limits of all of them.

A further investigation based on the measurement of joint signal-idler photocount statistics is also described and a momentum criterion recently introduced is applied to the experimental data.

On the basis of the obtained results, this sort of investigation can be considered as a robust discriminating tool to characterize the quantum nature of optical twin-beam states in different experimental conditions, such as in the case of different mean number of photons and of a variable number of modes.

#293 - Two-photon spectral amplitude resolved in separable Schmidt modes

Alessio Avella - Istituto Nazionale di Ricerca Metrologica, Torino

Marco Gramegna, Alexander Shurupov, Giorgio Brida (INRiM, Torino), Maria V. Chekhova (Max-Planck Institute for the Science of Light), Marco Genovese (INRiM, Torino)

The ability to access high dimensionality in Hilbert Spaces [1, 2] represents a demanding keystone for state-of-art quantum information. The manipulation of entangled states in continuous variables, wavevector as well frequency, represents a powerful resource in this sense. The number of dimensions of the Hilbert space that can be used in practical information protocols can be determined by the number of Schmidt modes that is possible to address separately [3, 4]. For wavevector variables it is possible to filter Schmidt modes losslessly using single-mode fibre and a spatial light modulator [5], but no similar procedure exists for the frequency space.

Aim of this work is to present a method of engineering the spectral properties of biphoton light, emitted via ultrafast spontaneous parametric down conversion, in such a way that the Two-Photon Spectral Amplitude (TPSA), that fully characterizes a biphoton sate [6-8], contains several non-overlapping Schmidt modes, each of which can be filtered in frequency variables without losses. Such TPSA manipulation is operated by a fine balancing of parameters like the pump frequency, the shaping of pump pulse spectrum, the dispersion dependence of SPDC crystals as well as their length.

Measurements have been performed exploiting the group velocity dispersion induced by the passage of optical fields through dispersive media [9, 10], operating a frequency to time two dimensional Fourier transform of the TPSA [11-13]: this returns the possibility to reconstruct the biphoton spectral amplitude through a temporal measurement among the delay between the laser pulse emission (trigger) and the detection times of the two correlated photons.

Exploiting this kind of measurement we experimentally demonstrate the ability to control the Schmidt modes structure in biphoton spectral amplitude by controlling the shape of the pump spectrum.

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#294 - X-entanglement, the non factorable spatio temporal correlation of twin photons

Alessandra Gatti – CNR - Istituto di Fotonica e Nanotecnologie, Milano

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Parametric down-conversion (PDC) is a widely employed source of entangled photon pairs, the key ingredients for several quantum communication and metrology schemes. The popularity of this source is also related to the possibility of generating entanglement in various degrees of freedom of light (polarization, space, time) Depending on the application, traditional approaches have often focused on a single degree of freedom at a time, or even when considering them simultaneously, treated them as independent. However, as for many nonlinear optical processes, PDC is ruled by phase matching, which establishes an angular dispersion relation that links the frequencies and the angles of emission of the generated photons in a non-factorable way. This work will discuss the non-factorability of the PDC state with respect to the spatial and temporal degree of freedom of light, and show how it leads to a peculiar distribution of the relative temporal delay and transverse spatial separations of twin photons, a feature that we named *X-entanglement* [1]. A relevant novelty emerging from the coupling of space and time is the possibility of manipulating the temporal entanglement of photon pairs by acting on their spatial degrees of freedom. In particular, by localizing the twin-photon positions the whole ultra-broad bandwidth of the PDC emission can be accessed, thus achieving an ultra-narrow temporal localizations of biphotons, close to the optical cycle.

After reviewing the key aspects of *X-entanglement*, we shall discuss a setup where the spatio-temporal correlation of twin photons can be reconstructed [2] by means of its inverse process, i.e. sum frequency generation (SFG). We shall conclude by reporting about the esperimental demonstration of the ultranarrow (6 fs) temporal correlation and of the skewed X-type spatio temporal correlation of twin beams recently obtained [3] at the Ultrafast Nonlinear Optics Lab in Como.

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#295 - Nanodevices for cancer diagnosis and/or therapy

Luigi Paduano (I) – Università di Napoli Federico II

Gaetano Mangiapia , Gerardino D'Errico (Dipartimento di Scienze Chimiche, Università di Napoli Federico II), Aurel Radulescu, Henrich Frielinghaus (Jülich Centre for Neutron Science, Garching bei München, Germany), Daniela Montesarchio(Dipartimento di Scienze Chimiche, Università di Napoli Federico II)

Amphiphilic molecules of appropriate design can form a variety of supramolecular aggregates such as micelles, vesicles and inverse bicontinuous cubic phases that may be exploited in several applications such as in medical diagnostic and therapy. The aim of this lecture is to present the update development and improvement of potential tumor–specific supramolecular contrast agents for magnetic resonance imaging (MRI) applications or chemotherapy.

In the field of tumor diagnosis nanodevices based on gadolinium complexes and peptides were prepared [1,2] . In the field of tumor therapy new classes of potential antineoplastic agents based on ruthenium amphiphilic complexes were synthetized and used to form nanoaggregates [3,4] .

Their morphology has been studied in different conditions of pH, temperature and ionic strength by means of small-angle neutron scattering, dynamic light scattering, electron paramagnetic resonance spectroscopy and electron cryomicroscopy. These aggregates are stimuli-responsive can switch from one structure to other depending on the environmental condition. Appropriate literature models were used to be fitted to SANS data with the aim to get the microstructural parameters of the nanoaggregates. In the case of bicontinuous phase a new theoretical model has been proposed to fit the SANS experimental data [5] .

Finally in vitro and in vivo tests, of these nanoaggregates on live cultures of human cancer cells were performed, demonstrating high efficiency of these tools both in diagnosis and therapy [2,3] .

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#296 - QUAFIT: a program to evaluate quaternary structure and heterogeneity of proteins from small-angle scattering

Francesco Spinozzi - Dipartimento di Scienze della Vita e dell'Ambiente, Università Politecnica delle Marche, Ancona

Paolo Mariani (Dipartimento di Scienze della Vita e dell'Ambiente, Università Politecnica delle Marche), Mariano Beltramini (Dipartimento di Biologia, Università di Padova), Claudio Ferrero (ESRF, Grenoble, France)

The new QUAFIT method for determining the quaternary structure of biological macromolecular assemblies by analyzing X-ray or neutron small-angle scattering data is presented [1]. The method is based on the idea that asymmetric monomers, formed by rigid domains of known atomic structure, possibly connected by flexible linkers of known sequence, are assembled according to a point group symmetry. Scattering amplitudes of domains and linkers are calculated by means of spherical harmonics and combined to obtain the form factor of the assembly. In order to avoid any overlap among domains, the "contact distance" between two asymmetric domains is determined as a function of their orientation by a novel algorithm, based on a Stone's invariants. An anisotropic Lennard-Jones potential among domains, written in terms of the contact distances, is included in the merit function to account for continuity and compactness of the whole assembly. QUAFIT allows for the simultaneous presence of oligomerization intermediates as well as of monomers distributed over multiple conformations.

QUAFIT has been tested by studying the structure of hemocyanin from *Octopus vulgaris*, a high molecular weight protein that shows a particular self-assembling pattern, characterized by a hierarchical organization of monomers. The highest molecular weight aggregate is a decamer, the stability of which depends on the chemical-physical characteristics of the solvent. A dataset of small-angle X-rays and neutron scattering (SAS) curves has been recorded under different pH values, buffer compositions, H_2O/D_2O ratios and Hofmeister's salts. In the first QUAFIT study, the structures of the decamer and of the dissociated "loose" monomer have been identified by analysing SAS curves in the most and the least aggregative conditions, respectively. Results are in very good agreement with the structural model derived from electron microscopy observations. Afterwards, all the other curves have been analysed through QUAFIT, by considering heterogeneous mixtures composed of the entire decamer, the dissociated "loose" monomer and all the intermediate dissociation products. QUAFIT has proved to be a method of general validity to describe solutions of proteins that, even after purification processes, appear to be intrinsically heterogeneous [2].

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#297 - Research and development on ³He free neutron counters

Antonino Pietropaolo - ENEA Laboratorio di Tecnologie Nucleari, Centro Ricerche Casaccia, Frascati

The research and development activity on He-free neutron detectors is of strategic importance for neutron sources worldwide due to the lack and high costs of He-based neutron detectors.

In this contribution Gas Electron Multipliers (GEM), radiative capture-based neutron counters are discussed as well as dimanond neutron beam monitors. Tests pefomed on these detectors at reactors and accelerator driven neutron sources will be presented and perspectives will be presented.

#298 - Structural dynamics studies on single floating membranes by neutron and X-ray reflectivity

Valeria Maria Rondelli - Università degli Studi di Milano

Elena Del Favero, Simona Motta, Laura Cantù (Dip. BIOMETRA, Università degli Studi di Milano)

Biomembrane components are unevenly distributed within the aggregated structure. The use of asymmetric model systems is rare, due to the difficulty of realizing artificial membranes with well defined heterogeneous composition and applicable for non-average structural investigation. In collaboration with the ILL in Grenoble, we developed an experimental model bearing forced membrane asymmetry in the form of single floating bilayers, that we investigated by neutron and synchrotron radiation reflectivity. Two coupled different bilayers are prepared by Langmuir-Blodgett/Langmuir-Schaefer technique. We studied the asymmetric phospholipid / cholesterol / ganglioside model system. In fact, gangliosides in real membranes reside in the outer layer, which has been invoked to provide the structural basis for the third-dimension static deformation of membrane portions. Also cholesterol transverse disposition may assume specific arrangement in asymmetric domains [1]. The Angstrom scale of Neutron accessibility coupled with the possibility to play with deuteration, is able to reveal the cross profile of the membrane, while X-ray are particularly sensitive to sugars, components of ganglioside polar head. We experimentally found that the presence of GM1 ganglioside forces asymmetry in cholesterol distribution. Moreover, our results suggest that a preferential asymmetric distribution of GM1 and cholesterol is attained in a model membrane with biomimetic composition, revealing that a true coupling between the two molecules occurs [2,3]. Our model, stable and responsive, is a meaningful mimic of a biological membrane raft and the non-invasive techniques used have the sensitivity needed to probe the structural dynamics resulting from interactions occurring at their surface, such as the interaction with approaching proteins or soluble enzymes. Some example will be presented.

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#299 - Silicon and germanium spintronics

Matthieu Jamet (I) - INAC/SP2M, CEA-Grenoble and University Joseph Fourier

Abhinav Jain, Juan-Carlos Rojas Sanchez, Murat Cubukcu (CEA-UJF), Julian Peiro, Jean-Christophe Le Breton (UMP CNRS-Thalès), Céline Vergnaud (CEA-UJF), Emmanuel Augendre (CEA-LETI), Laurent Vila, Jean-Philippe Attané, Serge Gambarelli (CEA-UJF), Henri Jaffrès, Jean-Marie George (UMP CNRS-Thalès)

In this presentation, I will first review the recent advances in silicon and germanium spintronics. This field of research aims at combining the carrier charge and spin in the same device made of silicon and germanium in order to add new functionalities to nowadays microelectronic devices [1]. The first proposal for a semiconductor-based spintronic device was made in 1990 by Datta and Das: they introduced the concept of spin transistor [2]. Since then, huge effort has been devoted to succeed in the very first step to the development of such a device: electrical spin injection in semiconductors. Indeed many obstacles had to be overcome before creating a non-equilibrium spin population into Si or Ge conduction or valence bands [3]. In this talk, I will discuss about these different issues and show how we could circumvent most of them to achieve spin injection in n-Si and n-Ge at room temperature. In particular, we clarify the exact role of interface states in the spin injection mechanism [4] and show a clear transition from spin accumulation into interface states to spin injection in the Si and Ge conduction bands. For this purpose, we have grown a CoFeB/MgO spin injector on Silicon-On-Insulator (SOI) and Germanium-On-Insulator (GOI). We observe a spin signal amplification at low temperature due to spin accumulation into interface states [5]. At 150 K, we find a clear transition to spin injection in the channel up to room temperature: the spin signal is reduced down to a value compatible with spin diffusion model. In this regime, we could also demonstrate the spin signal modulation by applying a back gate voltage and by spin-pumping at the ferromagnetic resonance of the CoFeB layer which are clear manifestations of spin accumulation in the Si and Ge channels. Finally by setting a temperature difference between Ge and CoFeB we could thermally induce a spin accumulation in Ge due to the tunnelling spin Seebeck effect [6].

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#300 - Super-magnetoresistance effect in triplet spin valves

Francesco Romeo – Dipartimento di Fisica, Università di Salerno e CNR - SPIN

We study a triplet spin valve obtained by intercalating a triplet superconductor spacer between two ferromagnetic regions with non-collinear magnetizations. We demonstrate that the magnetoresitance of the triplet spin valve depends on the relative orientations of the d-vector, characterizing the superconducting state, and the magnetization directions of the ferromagnetic layers. For devices characterized by a long superconductor, the Cooper pairs spintronics regime is reached allowing to observe the properties of a polarized current sustained by Cooper pairs only. In this regime a super-magnetoresistance effect emerges, and the chiral symmetry of the order parameter of the superconducting spacer is easily recognized. Our findings open new perspectives in designing devices based on the cooperative nature of ferromagnetic and triplet correlations in a spintronic framework.

#301 - Spin currents in Ge-based heterostructures

Federico Bottegoni - Dipartimento di Fisica, Politecnico di Milano

A. Ferrari (Dipartimento di Fisica, Politecnico di Milano), S. Cecchi (LNESS-Dipartimento di Fisica, Politecnico di Milano), M. Finazzi, F. Ciccacci (Dipartimento di Fisica, Politecnico di Milano), G. Isella (LNESS-Dipartimento di Fisica, Politecnico di Milano)

Germanium has recently become an appealing candidate for spintronics applications, due to the large spin-orbit interaction, long electron spin lifetimes at the L point of the Brillouin zone and the easy integrability with Si-based electronics. In this context, we studied the properties of spin currents optically injected in Ge-based heterostructures and detected using inverse spin Hall effect (ISHE). We characterized the ISHE signal in diffusive regime, as a function of the initial electron spin polarization, generation depth, doping of the structures and externally applied electric fields.

#302 - Exchange and Rashba interactions in thin film systems

Paolo Moras – CNR - Istituto di Struttura della Materia, Trieste

P. M. Sheverdyaeva (CNR – ISM, Trieste), M. Papagno , D. Pacilé (CNR - ISM, Trieste e Dipartimento di Fisica, Università della Calabria, Arcavacata di Rende (CS)), G. Bihlmayer, F. Freimuth, Y. Mokrousov, S. Blügel (Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany), C. Carbone (CNR - ISM, Trieste)

The Rashba interaction manifests at the surface of a crystal or the interface between crystals with a spin-splitting of the surface or interface electronic states in the k-space ($E_{\uparrow\downarrow},k=E_{\downarrow\uparrow},-k$). Splittings ascribed to the Rashba effect were identified by spin- and angle-resolved photoemission spectroscopy in a variety of low-dimensional systems containing heavy elements. These findings suggest further possible ways to engineer the electronic structure of solids for spintronics applications. In the present talk we will discuss a case where the Rashba and exchange interactions act on the same energy scale. The electronic structure of Ag$_2$Bi-terminated Ag(111)

thin films grown on ferromagnetic substrates display asymmetric bands, where $E_{\uparrow\downarrow},k \neq E_{\downarrow\uparrow},-k$. The experimental results are understood in terms of simultaneous breaking of the time and structural inversion symmetry. Model transport calculations reveal implications of such asymmetry for spin-polarized transport and magnetization manipulation.

#303 - Storing magnetic information in antiferromagnetic tunnel junctions via field-cooling

Edoardo Albisetti - LNESS-Politecnico di Milano, Como

D. Petti (LNESS-Politecnico di Milano), J. Gazquez, I. Fina (ICMAB-CSIC, Spain), M. Varela (Oak Ridge National Laboratory, USA), M. Molina-Ruiz, A. F. Lopeandía (Universitat Autonoma de Barcelona, Spain), H. Reichlová, K. Olejník, V. Novák, T. Jungwirth (Institute of Physics ASCR, Czech Republic), B. Dkhil (Ecole Centrale Paris, France), X. Marti (University of California, USA), J. Wunderlich (Hitachi Cambridge Laboratory, UK), R. Bertacco (LNESS-Politecnico di Milano)

Magnetic tunnel junctions used in modern hard-drive read heads and magnetic random access memories comprise two ferromagnetic electrodes whose relative magnetization orientations can be switched between parallel and antiparallel configurations, yielding the tunneling magnetoresistance effect. Recently [1], large magnetoresistance signals have been observed on NiFe/IrMn/MgO/Pt stacks with an antiferromagnet (AFM) on one side and a non-magnetic metal on the other side of the tunnel barrier. In these devices, the rotation of the AFM moments in IrMn is achieved by the exchange-spring effect of NiFe on IrMn. This is then detected by the measured AFM tunneling anisotropic magnetoresistance (TAMR). This work has experimentally demonstrated the feasibility of a spintronic concept in which the device transport characteristics are governed by an AFM.

Here [2], we demonstrate a new concept for storing magnetic information in distinct resistance states of a tunneling device comprising an AFM/insulator/normal-metal stack, with the auxiliary ferromagnetic NiFe layer removed. The metastable configurations of the AFM moments, which yield the higher and lower resistance states of the ATJ (TAMR=10 %), can be set by cooling the AFM from above the Neel temperature (TN) in magnetic fields with different orientations. We observed a splitting in two different resistance states due to the different orientation of the magnetic field applied during the field cooling process. The stability of the two states with respect to strong external magnetic perturbations was confirmed by the fact that sweeping external magnetic fields up to 3T below the Nèel temperature did not produce any sizeable change in the junction resistance.

After the stack deposition, performed by magnetron sputtering, pillar structures were patterned by optical lithography in order to define the ATJs for electrical measurements. The high quality of the interfaces, the correct layer texturation and the continuity of the MgO insulating barrier over large distances were confirmed by TEM and XRD measurements.

Our approach removes ferromagnets from the design of the spintronic memory structure which allows to exploit the unique features of compensated-moment AFMs, namely the lack of magnetic stray fields and the relative insensitivity in the ordered AFM state to external magnetic fields.

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#304 - Enhancement of electron spin lifetime in GaAs bulks: the benefits of external noise

Dominique Persano Adorno - Dipartimento di Fisica e Chimica, Università di Palermo

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Possible utilization of electron spin as an information carrier in electronic devices is an engaging challenge for future spin-based electronics. However, each initial non-equilibrium magnetization decays both in time and distance during the transport [1]. Because of increasing miniaturization, to avoid too much intense electric fields, the applied voltages are very low and are subjected to the background noise. Hence, it is mandatory to understand the influence of fluctuations on the spin depolarization process in order to guarantee a reliable manipulation, control and detection of information in spin-based devices. In the last decade, an increasing interest has been directed towards possible constructive aspects of noise in the dynamical response of non-linear systems [2]. Previous theoretical studies have revealed that, under specific conditions, the addition of external noise sources to intrinsically noisy systems may induce an enhancement of the dynamical stability of the system, resulting in a less noisy response [3]. Preliminary findings have shown that a fluctuating electric field can strongly modify the spin depolarization length, an essential design parameter in spin-based electronic devices [4].

In this contribution, we investigate the electron spin relaxation process in doped n-type GaAs crystals driven by a fluctuating electric field. A symmetric dichotomous noise and a gaussian correlated noise are used as two different sources of fluctuations. Our findings show an enhancement of the spin relaxation time by increasing the amplitude of the external noise. Moreover, in the case of dichotomous fluctuations, the electron spin lifetime monotonically increases also with the noise correlation time, in contrast with the non-monotonic trend obtained in the case of bulks subjected to a Gaussian correlated noise. The enhancement can be explained in terms of a decrease of the occupation of the L-valleys, where the strength of spin-orbit coupling felt by electrons is at least one order of magnitude greater than that present in the lowest energy valley. Since the spin depolarization process changes in a way that critically depends on the correlation time of the external noise, fluctuations can play a relevant role on controlling and tuning the coherence of spin-relaxation processes. In this view, by using appropriate noise characteristic times, it is possible to select the most favorable condition for the transmission of information by electron spin.

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#305 - Room temperature spin transport in Ge: optical and electronic measurement of the spin diffusion length

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Ge-based spintronic devices have recently deserved great attention, thanks to the compatibility with Si-based electronics, the large carrier mobility, the possibility of optical spin pumping and the opportunity of electrical spin manipulation.

Fe/MgO/Ge spin-photodiodes (spin-PDs) exploit the coupling between the angular momentum of photons and the spin angular momentum of photo-generated carriers to convert the light helicity into a variation of the photocurrent, opening the route to spin-optoelectronics. In a spin-PD, the left/right circular polarization of light is translated into up/down spin-polarization of photo-generated carriers within Ge, that subsequently undergo a spin-dependent tunnelling at the Fe/MgO interface, giving rise to higher/lower transmission (and thus current crossing the device) according to the direction of their spin (i.e. light helicity) with respect to the Fe magnetization.

The first demonstration of the room temperature operation of Fe/MgO/Ge spin-photodiodes has recently been reported by our group [1]: a variation $F=\Delta I/I$ of the photocurrent for opposite orientations of the circular polarization has been obtained for infrared light (λ=1300 nm).

In this work, we report on the efficiency F with respect to the wavelength of light λ, moving from the infrared to the visible range. We found that the maximum of $F(\lambda)$ is located within the visible range ($\lambda \sim$ 540 nm). The trend of $F(\lambda)$ results from the competition between two wavelength-dependent parameters: (i) the initial degree of spin polarization (DSP) created by circularly polarized light in Ge; (ii) the attenuation length of light in the semiconductor compared to the spin diffusion length, which determines the spin-memory loss. In order to explain the trend of $F(\lambda)$, we developed a macroscopic transport model that allows to interpret the efficiency dependence of the spin-PD on the light wavelength and gives access to the spin diffusion length of Ge. Finally, we fabricated Fe/MgO/Ge devices for non-local lateral transport measurements in order to determine the spin diffusion length of carriers when a tensile [111] strain is applied to Ge. We will show whether the strain is effective in increasing the spin diffusion length of carriers by removing the degeneracy of the conduction band minima, according to first principles calculations by Tang et al. [2].

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#306 - Identifying the electronic character and the role of the Mn-derived states in (Ga,Mn)As via HAXPES

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Dilute Magnetic Semiconductors (DMS) have attracted a lot of attention due to the combination of the semiconducting behaviour and ferromagnetism and therefore due to their possible applications in the field of spintronics [1]. The case of (Ga,Mn)As is prototypical: despite the wealth of experimental and theoretical works devoted to (Ga,Mn)As in the last decade, a clear picture of the modification induced in the external shell of the GaAs by the Mn states is still lacking; this is partly due to a profound difference between surface and bulk electronic properties, as cuased by a) the presence of both substitutional (acceptors) and interstitial (double-donor sites) impurities, with opposite contributions to the magnetic properties, and b) off-equilibrium growth conditions and post-growth annealing, strongly influencing the homogeneity of (Ga,Mn)As.

we report valence band and core level HAXPES results, including magnetic sensitive polarization dependent experiments, as a fucntion of both temperature and doping, supported by model calculation, where we clearly observe [2,3]: a) a distinct electronic screening channel in the bulk, hitherto undetected in more surface sensitive analysis, b) an important role of hybridization in mediating the ferromagnetic coupling in (Ga,Mn)As, c) the evolution of the Mn-derived states in the vicinity of the Fermi level as d-like character, and their relationship with the host GaAs band [4] .

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#307

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#308 - Optofluidics as a novel platform for optical sensors

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Optofluidics essentially merges optics and microfluidics at micro and nano scales. This approach permits to realize innovative optical system in which fluids can act as an optical material providing a significantly enhanced performance and functionality that cannot be achieved without this seamless integration. The possibility to guiding and manipulating light through a fluid offers very interesting applications in sensing fields enabling high interaction efficiency between the light and the substance with unprecedented sensitivity and limit-of-detection. In particular, the performances of biological and chemical sensors could strongly benefit from this effective integration between complex integrated microfluidic networks and the optical detection part. To date most of microfluidic sensors employ a separate microfluidic network to prepare and delivery very small sample volumes (femtoliter to microliter) under analysis that is simply connected to the optical sensing part degrading the sensing performances. In other cases, also if an integration has been achieved, the design of optical part has been privileged respect to microfluidic one, sacrificing the feasibility and the final sensitivity of the device. In fact, while microfluidics enable compact systems, recent results show that performances of biosensors can be seriously limited in a fluidic environment by the inefficient analyte transport instead of their intrinsic optical detection capabilities. In this field liquid core waveguides can represent an important component of optofluidic sensor devices and systems. In fact they represent the maximum integration and functionality between waveguides, the key element of the optical structure, and microchannels, the key element of microfluidics.

In this work we show how optofluidics can act as a novel platform for optical sensors. Optofluidic waveguides has been realized using both Silicon and polymer technology. In particular, single mode optofluidic waveguides with low loss has been realized using antiresonant reflecting optical confinement (ARROW). These waveguides can be fabricated using full standard silicon technology or hybrid Silicon-polymer processes. ARROW waveguides have been used in order to realize complex optofluidic devices like Mach-Zehnder interferometers and ring resonators. The advantage of using optofluidic waveguide results in very compact devices with a total length of 2.5 mm and a required liquid volume less than 0.16 nl. Application of polymer based optofluidic sensors to on-line monitoring of organic compounds in drinking water will be also reported.

#309 - Molecular beacon as oligonucleotide nanosensors for intracellular mRNA

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Molecular beacons, molecules capable to turn on or to modify their light emission upon the interaction with well-defined molecular targets, are among the most promising optical intracellular nanosensors proposed in the recent years. They are oligonucleotidic sequences labeled at the two side-ends, with a fluorophore (F1) at one side and a quencher Q (or a second fluorophore) at the other side, characterized by an absorption band overlapping with the F1 emission band. In the absence of the target, these structures have a closed conformation with F1 and Q so closed that in the presence of F1 excitation fluorescence resonance energy transfer (FRET) occurs and no emission is observed. In the presence of the target, these structures open and fluorescence emission is observed since F1 and Q are sufficiently distant that FRET does not take place. Their intracellular internalization must be performed using suitable carriers capable to allow these nanosensors to penetrate the cell membrane and enter the cell.

We describe here the design, implementation and characterization of structured polymethylmethacrylate (PMMA) nanoparticles (NPs) and carbon nanotubes (CNTs) for intracellular mRNA monitoring. PMMA NPs and CNTs were characterized as potential intracellular nanocarriers of the molecular beacon (MB) for the detection of mRNA encoding surviving, a protein member of the inhibitor of apoptosis family, highly expressed in most types of cancer. Atto647N and Blackberry 650 are the MB fluorophore/quencher pair. Hybridization studies with a target sequence analogous to survivin specific mRNA were conducted in vitro, and the MB functionalities, in solution and once anchored to NPs and CNTs, were successfully demonstrated. An increase of fluorescence signal was observed with the increase of the target concentration from 10 to 500 nM, confirming the dependence of the MB fluorescence on the presence of the target also after its immobilization onto the NPs. MB functionality and specificity were also tested in living cells by transfection with a classical lipid agent, lipofectamine, and by confocal microscopy imaging. A fluorescence increase was observed in the cytoplasm after 1 h from the transfection without fluorescent aggregates or fluorescence in the extracellular environment. On the contrary, no fluorescence was observed in transfected cells not expressing surviving.

#310 - Forest of silica nanowires decorated by metal nanoparticles : light trapping at plasmon resonances and biosensing applications

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Forests of inorganic nanowires (NWs) are among the highest diffusive materials to date due to multiple scattering events that the incoming light undergoes from many NWs. The combination of light trapping and absorption resonances of the NW materials is a strategic tool to achieve efficient light absorption in thin-film devices and the solar cells are the most important example. The multiple light scattering can indeed fold the light path many times in a random walk, achieving an efficient light absorption and a consequent drastic reduction of the reflectivity in the NW absorption spectral range. As such, the NWs capture and absorb significantly more photons than an equivalent volume of bulk material.

Our main idea is to develop new plasmonic materials which combine the light trapping properties of white and highly diffusive NWs with the selective absorption resonances of metal nanoparticles (NPs), i.e. the local surface plasmon resonance (LSPR). For white and highly diffusive NWs we intend NWs transparent in the UV-visible spectral range with a large distribution of the diameter, shorter or comparable with the optical wavelengths, in order to assure light scattering at any wavelength in the UV-visible range. A good candidate for this purpose is a forest of silica NWs with diameter ranging from few tens up to few hundreds of nanometers. Hence, we have fabricated disordered silica NW mats and decorated them with Au or Ag NPs by de-wetting metal evaporated thin films. The combination of silica NWs with metal NPs form a plasmonic material characterized by an effective suppression of light reflection at the well-defined frequencies of the LSPR as shown by measuring the integrated total reflectivity. The light trapping properties and the availability of highly dense metal NP ensemble, easily accessible by biomolecules due to the microporous structure of the NW forest, make these materials promising candidates as plasmonic biosensors. For this purpose, we test with success the ability to act as refractive index sensors and to detect biomolecular binding of the Protein A-anti Salmonella bonding.

#311 - Bio-patterned magnetic biosensing platforms with sensitivity below the pM range

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In the last years, magnetic biosensors arrays have emerged as a new promising platform for biosensing. In the magnetic sensing scheme, the target molecule is attached to a superparamagnetic bead and the biomolecular recognition event is detected by the magnetic sensors which are sensitive through magnetoresistance to the fringe field of the magnetic beads. The main advantages of this technique are: robustness, inexpensiveness, integrability in lab-on-chip platforms, and high sensitivity (down to zeptomolar range [1]). In order to achieve high sensitivities, different aspects must be taken into account.

First of all, the working point of the sensor must be carefully chosen. Here we show with a theoretical model and experiments employing sensors based on magnetic tunnelling junctions [2] that, in case of lock-in detection and bead excitation by a small AC magnetic field, the best choice does not correspond to the linear part of the R(H) characteristic where the sensitivity to the external field is maximum. Indeed, the highest sensitivity to the magnetic beads is achieved biasing the sensor in the region of its characteristics where the product between the DC bias field and the second derivative of the resistance with respect to the magnetic field is maximum [2].

Secondly, controlling the beads distribution over the sensor and hence the location of the biological active area is critical for tailoring and maximizing the magnetic signal arising from the biomolecular recognition events. This is a major issue, in order to achieve higher sensitivities, quantification capability, lower essay time and less biological material requirement. To satisfy these requirements a new, straightforward procedure to create patterns of bio- reactive polymer (copoly (DMA-NAS-MAPS)) regions on the sensor's surface using standard photolithography and a lift off procedure has been developed [4]. The effectiveness of the procedure in achieving high specificity and the enhancing the sensor performance is demonstrated comparing different assays of DNA-DNA hybridization with patterned and unpatterned sensors. Through these optimizations, sensitivities down to the pM range have been achieved.

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#312 - Memory effect in gated single-photon avalanche diodes: a limiting noise contribution similar to afterpulsing

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In recent years, emerging applications in which a wide dynamic range is crucial have turned the interest towards Single-Photon Avalanche Diode (SPAD), such as diffuse optical imaging and spectroscopy (e.g., functional brain imaging and optical mammography). In these fields, the use of a fast-gated SPAD has proven to be a successful technique to increase the measurement

sensitivity of different orders of magnitude. However, an unknown background noise has been observed at high illumination during the gate-OFF time, thus setting a limit to the maximum increase of the dynamic range. In this paper we describe this noise in thin-junction silicon single-photon avalanche diode when a large amount of photons reaches the gated detector during the OFF time preceding the enabling time. This memory effect increases the background noise with respect to primary dark count rate similarly to a classical afterpulsing process, but differently it is not related to a previous avalanche ignition in the detector. We discovered that memory effect increases linearly with the power of light impinging on the detector and it has an exponential trend with time constants far different from those of afterpulsing and independently of the bias voltage applied to the junction. For these reasons, the memory effect is not due to the same trapping states of afterpulsing and must be described as a different process.

#313 - Quantum cavity optomechanics with nanomembranes

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A semitransparent thin membrane within a Fabry-Perot cavity is a promising tool for investigating quantum effects in cavity optomechanics. We show recent experimental results demonstrating sideband cooling of a vibrational mode of the membrane [1], and tunable optomechanical induced transparency at room temperature [2]. We also investigate theoretically how to use these devices for manipulating continuous variable quantum information: in particular we show how such a system could be used for interfacing microwave and optical radiation [3], and how robust entanglement between mechanical resonators at remote sites can be created and certified with only local measurements [4].

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#314 - Hydrodynamics of a Fermi gas at unitarity from a time-dependent density functional

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We use a time dependent density functional theory with an extended Thomas-Fermi functional showing that various dynamical properties of the zero-temperature unitary Fermi gas critically depend on the presence of a dispersive gradient term in the equation of state.
First we use a variational approach to get a reliable analytical formula for the quadrupole oscillation frequency, which reduces to the familiar Thomas-Fermi one in the limit of a large number of atoms.
Then, motivated by a recent experiment [1], we simulate the collision between two clouds of cold Fermi gas at unitarity.
At variance with the current interpretation of the experiment, where the role of viscosity is emphasized, we find that a quantitative agreement with the experimental observation of the dynamics of the cloud collisions is obtained within our superfluid effective hydrodynamics approach, implying that density variations during the collision are controlled by the purely dispersive quantum gradient term.
Finally, we study the real-time motion of a microscopic object in a cold Fermi gas at unitarity. We find that the spontaneous creation of singly quantized vortex-antivortex pairs occurs as a critical velocity is exceeded, which leads to a drag between the moving object and the Fermi gas. The resulting force is linear in the velocity for subsonic motion and becomes quadratic for supersonic motion.

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#315 - Quantum correlations in bipartite systems with $1/f^\alpha$ noise

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We address the dynamics of quantum correlations for two non interacting qubits initially prepared in a maximally entangled state and then subject to a classical colored noise, i.e. coupled with an external environment characterized by a noise spectrum of the form $1/f^\alpha$. We investigate two different configurations of the environment: in the first the noise spectrum is due to the interaction of each qubit with an undetermined switching rate, whereas in the second case we consider a collection of Nf classical fluctuators with fixed switching rates. Since environmental noise is introduced by means of stochastic time-dependent terms in the Hamiltonian, we are able to describe the effects of both separate and common environments. We show that environments with the same power spectrum, but different configurations, give raise to opposite behavior for the quantum correlations. In particular, depending on the characteristics of the environmental noise considered, both entanglement and discord display either a monotonic decay or the phenomena of sudden death and revivals. Our results show that the microscopic structure of environment, besides its noise spectrum, is relevant for the dynamics of quantum correlations, and may be a valid starting point for the engineering of colored environments.

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#316 - Single photon emitters in AlGaAs epilayers at liquid nitrogen temperature on silicon substrates

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One of the fundamental ingredients for quantum cryptography and quantum information applications is the fabrication of single and entangled photon emitters. Single photon emitter should produce exactly a single photon on demand, should work not only at cryogenic temperature and should be easy to produce and to integrate on existing electronic devices. In this work, we present the fabrication and characterization of single photon emission from high quality GaAs quantum dots (QDs) by droplet epitaxy (DE) and from impurity centers in AlGaAs layers grown on Si through a thin Ge buffer layer deposited by Low Energy Plasma Enhanced Chemical Vapour Deposition (LEPECVD). The deposition of a thin Ge layer by LEPECVD and subsequent annealing cycles allow for the reduction of threading dislocation density down to few 10^7 cm^{-2}. DE is an intrinsically low thermal budget technique, being performed at temperatures between 200 and 350 °C. This makes DE perfectly suited for the implementation of growth procedures compliant with back-end integration of III-V nanostructures on CMOS. GaAs QDs with a density of few 10^8 cm^{-2} and a mean height of 8 nm are fabricated by DE inside a $Al_{0.3}Ga_{0.7}As$ barrier. Bright and sharp emission lines are observed in a micro-photoluminescence experiment around 700 nm, with pure radiative excitonic lifetime and clear evidence of exciton-biexciton cascade. The achievement of quantum photon statistics is directly proved by antibunching in the second order correlation function as measured with a Hanbury Brown and Twiss interferometer up to T=80 K, thus making the single photon emitter working at liquid nitrogen temperature and compatible with present CMOS technology. The optical quality of the GaAs quantum dots grown on Si substrate is almost comparable with quantum dots directly grown on GaAs substrates. We also show that the epitaxial growth of thin layers of $Al_{0.3}Ga_{0.7}As$ on GaAs buffer layers grown on Si and Ge substrates allows to obtain a single photon source by exploiting the strewn and unintentional contamination with defects of the $Al_{0.3}Ga_{0.7}As$. Very bright and sharp single photoluminescence lines are observed in confocal microscopy. These lines behave very much as single excitons in QDs, but their realization is by far much easier, since it does not require 3D nucleation or spatially selective doping. The photon antibunching is demonstrated by time resolved Hanbury Brown and Twiss measurements. In both cases (GaAs QDs by DE and impuritues in AlGaAs layer) it is clearly demonstrated a new procedure for the integration of high efficient light emitters, based on III-V semiconductors, directly on Si substrates, and opening the route to wide applications to optoelectronics, photonics and quantum information technology.

#317 - Quantum-information processing with hybrid spin-photon qubits

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A quantum computer, like its classical analog, will probably be a hybrid device exploiting the best characteristics of distinct physical systems. In this spirit, several theoretical works have considered the possibility of exploiting fast processing of Cooper-pair boxes (CPB) and long coherence times proper of spin ensembles (SE) [1]. Much work has also recently been done to experimentally achieve strong coupling of high-quality factor coplanar-waveguide resonators with SE [2]. In these schemes, cavity photons are used as a bus to transfer the quantum state from CPB to SE, in which information is stored.

In the present work, we introduce hybrid spin-photon qubits, whose manipulation is achieved simply by tuning the resonance frequencies of planar superconducting resonators to the spin-energy gaps. In this hybrid encoding, each physical qubit is represented by a resonator mode and a SE. An additional cavity mode is exploited as an auxiliary degree of freedom to implement two-qubits gates. We simulate the quantum gates in the elementary unit of a scalable setup, namely two resonators containing different SEs, where each qubit is encoded in the state of a distinct SE-resonator pair. The spin-photon coupling is described by means of a Jaynes-Cummings interaction and photon-hopping is allowed between photons of neighboring cavities. Our scheme allows implementation of arbitrary single- and two- qubit gates with high-fidelity, and its application to an array of cavities enables general quantum algorithms as well as quantum simulators [3] to be implemented. Simulations have been performed assuming fundamental frequencies around 15 GHz and exploiting different harmonics as cavity modes to encode qubits.

The few requisites of the scheme can be fulfilled by a large variety of systems, ranging from diluted transition-metal or rare-earth ions to molecular nanomagnets [4].

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#318 - Nanostructures for silicon photonics

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Silicon nanophotonics is emerging as a new platform for the integration of photonic and electronic devices. Several examples on our recent efforts on monolithic light sources based on silicon nanostructures will be presented and discussed. In particular it will be shown that silicon-on-insulator (SOI) is emerging as an interesting photonic material. The first electrically pumped silicon-on-insulator nano light source, tunable around 1300-1600 nm range and operating at room temperature will be presented. H-related optically active defects are properly introduced into silicon enhancing the electrically driven emission in a photonic crystal nanocavity device. A narrow ($\Delta\lambda = 0.5$ nm) emission line with the highest spectral power density ever reported from any silicon emitter will indeed be presented. Alternatively Er ions are introduced into the nanocavity showing an enhanced emission at 1500 nm with potentials for a population inversion and laser action. Group-IV semiconductor nanowires (NWs) are also attracting interest among the scientific community as building blocks for a wide range of future nanoscaled devices. We show that metal-assisted chemical etching is a powerful technique to obtain nanometer-size high density and low-cost Si NWs with high and controllable aspect ratio. NWs obtained by this technique have exactly the same structure and doping properties of the substrate and present quantum confinement effects. We will show that luminescence is very efficient (in the order of the percent) and tunable with NWs size according to quantum confinement. Light emitting devices based on Si NWs have also been realised, showing the efficient electroluminescence emission at room temperature under low voltage excitation. In addition a giant Raman enhancement within a fractal forest of silicon NWs, due to multiple scattering events. The relevance and the perspectives of the reported results opening the route towards novel applications of Si nanostructures in photonics will be discussed. The results reported in this work have been performed as a collaboration among several people belonging to the University of Catania, CNR-IMM, CNR-IPCF, University of Pavia and St. Andrews University.

#319 - Nanosilicon photonics, a new twist to silicon photonics

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Silicon Photonics is no more an emerging research topics but is an actual technology with commercial products already available on the market. Quantum confinement of carriers or spatial localization of photons allow dramatically enhancing and widening the scope and potential of silicon photonics.
The use of nano-Si in silicon photonics (waveguides, modulators, switches, sources and detectors) is reviewed and discussed. Recent advances of nano-Si devices such as bio-imagers, optical resonators (linear, rings, and disks) are treated. The development of high efficiency light emitting diodes for interchip bidirectional optical interconnects is presented as well as the recent progresses to exploit nano-Si for solar cells. In addition, non-linear optical effects which enable fast all-optical switches are described. On the other hand, confinement of photons to small microresonators allows tuning the photon properties. Here also novel effects are found. Ultra high bandwidth robust optical switches for UDWDM, active suspended microdisk bistable devices, nonlinear optical generations are only few applications where nanophotonics can be appreciated.

#320 - The bright and the dark sides of silicon photonics

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In the last decade, silicon on insulator technology (SOI) has emerged as a leading photonic platform, reaching remarkable results in the extreme miniaturization of integrated optical devices for the generation, manipulation, and detection of the light on small-sized photonic chips. Although device downscaling is a fundamental step towards very large scale of integration, technology maturity is still far from enabling the realization of complex photonic integrated circuits (PICs) integrating hundreds of optical functions. So far the desire to push the performance of single components to the limit, via iterative process modifications, has overridden the search for technological solutions enabling the manufacturing and control of complex on-chip systems.
The slow evolution in the development of large scale integration on-chip systems is the main bottleneck that currently prevents the full exploitation of silicon photonics in many fields of application, such as telecom, optical interconnects, biosensing and quantum information, where new concepts like chip-scale systems, re-configurability, and adaptivity are starting to appear.
The contribution will review the state of the art of silicon photonics devices in the entire scenario of passive functions, modulators, detectors, light sources and packaging. Examples of complex circuits such as tunable delay lines and tunable filters will be discussed in detail demonstrating the inherent potential of the technology for high integration scale, small footprint, low power consumption, low cost, mass production and CMOS compatibility.
However, the way from successful proof of concepts to multifunctional products is long and difficult. The evolution from device level to system-on-a-chip level touches a number of critical issues, such as fabrication tolerances, functional drifts (aging, environmental conditions), mutual crosstalk effects (thermal, optical, electrical), backscatter, undesired nonlinear behaviors (TPA) and more. All these need to be addressed in order to set and maintain the circuit to the desired functionality, in particular the capacity to hitless probe the light in the waveguides and modify the functionality through "green" actuators. Critical points and possible solutions will be presented and discussed.

#321 - Classical and quantum nonlinear optics in silicon integrated devices

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High-quality microring resonators have been fabricated for over a decade in a variety of CMOS compatible platforms [1] and have been recently investigated for their quantum optics potential [2]. As the quantum process of spontaneous four-wave mixing is due to the same nonlinearity as the stimulated process, we show theoretically and experimentally there is a definite relation between the two. This proves that it is possible to predict the results of a proposed quantum experiment from the results of a classical experiment. We also demonstrate, using time correlated measurements, that the signal and idler beams generated in the spontaneous process come in correlated pairs. These results open the way to the emission of heralded single photons and entangled photon pairs from integrated devices [3a,b].

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#322 - Giant Photo Luminescence Emission in Si Grains

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We report the demonstration of giant photoluminescence (PL) emission stimulated by a specific deposition of a newly synthesized material consisting of crystalline grains of silicon.
Although bulk silicon does not emit any photoluminescence, and the crystals with this size do not exhibit neither quantum confinement effects nor gap widening, we have been able to pile up a suitable deposition of nanocrystals where a laser beam with wavelength 632.8 nm can locally produce a high temperature and giant PL radiation emission, with an amplification factor g of 0.14 cm/Watt. The gain of optical functionalities for an indirect band gap semiconductor like Si could represent a huge advancement in the field of optoelectronics and photovoltaics.

#323 - Porous silicon technology a breacktrough for silicon photonics: from packaging to monotithic integration

Marco Balucani – Università Sapienza, Roma

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The concept of Integrated Optics (IO), with the meaning of optical devices and circuits realized in a patterned planar waveguide format, was first described by Stewart Miller in a historic special issue of the Bell System Technical Journal (BSTJ), as long ago as 1969. Miller envisaged an analogous development to integrated electronics with a continuously growing density of integration (Moore's law). However, it turned out, that the growth of integration density in the optical domain was much slower than in electronics. There are several reasons that explain the different rates of development. An important one is that a single material silicon has an almost completely dominant role in integrated electronics, as the base material for more and more complex integrated circuits (IC). The situation in the domain of integrated optics is quite different. There is a wide range of materials used for specific applications. Interestingly, silicon also, in the form of silicon-on-insulator (SOI), has emerged during the last few years as a strong contender for various applications of integrated optics. Due to the high refractive index contrast between waveguide core and its surrounding, SOI waveguides can have an extremely small cross-section with strong mode confinement allowing bending radii even below 5μm. This enables the development of very compact ring resonators and of further devices of unprecedented small size. Nevertheless, standard singlemode fibers (SMF) are very large size compared to silicon photonic (SP) strip or slot waveguides. The typical core diameter size of a standard SMF is approximately 8μm. Thus, coupling light from an optical fiber to a SP waveguide, that is in the submicron range dimension, becomes a quite difficult task. The high difference in the dimensions between the fiber and the waveguide causes a high mismatch between their optical modes. Due to this mismatch, a coupling structure is needed to adapt a wide fiber to a narrow silicon waveguide improving the coupling loss. Typically, a direct butt coupling between a SMF (mode field diameter MFD=10 μm) and a SP waveguide (MFD <1 μm) leads to more than 20dB insertion loss. The insertion loss between an optical fiber and a SP circuit is definitively a big issue as it is directly linked with performances such as the link reach, the signaling rate, the receiver sensitivity, and so on. Moreover, in order to be compatible with functions for FTTx or WDM applications for instance, a good coupling structure is also required to be broadband and polarization insensitive. Furthermore, considering the packaging cost, the footprint of a coupling structure must be kept small and have sufficient alignment tolerances.
The present work refers to porous silicon technology that will be partially or fully oxidized to modulate refractive index from 1,20 to 2,40 realizing a suitable impedance adapter for SMF optic to SP allowing very low loss (i.e. < 0,5 dB), mechanical stable, large bandwidth (i.e. > 100 nm) and polarization insensitive SMF to SP optical coupling package. A new breakthrough technology is presented showing how is possible to realize monolithic integration of SP devices and IC within the same silicon wafer and an easy way to realize slot plasmonic waveguides.

#324 - What about magnetic reconnection?

Francesco Pegoraro (I) – Università di Pisa

The transformation of magnetic field energy into particle energy (both thermal and kinetic) is a fundamental process in magnetized plasmas. It occurs in different physical plasma regimes. These range from laboratory experiments in controlled fusion research, to space and solar plasmas, to the extreme electromagnetic fields of astrophysical objects such as the magnetosphere of neutron stars, to plasmas produced in the laboratory by ultrafast and ultraintense laser pulses. This energy conversion occurs through the onset of processes of *magnetic field line reconnection*. In these processes more conventional energy transformations, common to most physical systems, concur with *features of magnetic field topology* that are specific to magnetized plasmas in creating a fascinating, but complex, nonlinear and nonlocal dynamics.

In this presentation, after recalling some of the fundamental features of magnetic reconnection (and of its inverse process in which plasma thermal anisotropy generates magnetic fields through the onset of the Weibel instability), I will address some open problems presently under investigation and emphasize how similar physical questions are encountered in all the different plasma regimes and configurations where magnetic reconnection can occur.

#325 - Plasma self-organization in a magnetic confinement system

Susanna Cappello (I) - CNR - Consorzio RFX, Padova

Plasmas in fusion research for energy production offer intriguing challenges for physicists, involving the difficulties often summarized under the subject of "complex systems". In this presentation we provide a survey of the advancements and open issues developed in the Reversed Field Pinch activity in Padova, at Consorzio RFX. The RFP configuration relies basically on currents flowing in the plasma itself in order to produce both the confining magnetic field and plasma heating. This character can be used to describe the difference with respect to the leading toroidal magnetic configurations in present fusion research, the Tokamak and the Stellarator. This character is also at the basis of a phase transition which sees the system living either in a magnetically disordered phase or developing a helical (kinked) pattern, which can favor the formation of confining ordered structures. The transition to similar ordered helical regimes provides a possible path to the development of confinement system based on plasma self organization. The helical self-organization process was firstly anticipated in magneto-fluid modeling since the 90ties (3D nonlinear numerical simulations), and then observed in larger experiments, in particular in RFX-mod, when pushing plasma currents to higher values: experimentally, such a helical state corresponds to improved plasma confinement. Present research focuses on how to best exploit the "natural" tendency toward helical regimes. On the one hand, feedback techniques applied to a net of magnetic coils at the plasma boundary are considered in order to comply with or to stimulate the process. On the other hand, techniques to treat the plasma facing materials in order to avoid too dense and cold plasmas at the edge are under development. The integration of different disciplines (physics of complex systems, engineering, material science) and activities (theory and numerical modeling, experimental phenomenology and diagnostics) is part of the challenge in our research activity.

#326 - Perspectives for inertial fusion

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The quest for demonstrating ignition and gain in Inertial Confinement Fusion [1] has come to a crucial point, where the long awaited proof of principle of this approach to fusion still fails to arrive. We present the status of this field of research, both at the international [2] and european level [3], focussing on the standard approach and on the new strategies in laser fusion.

The path ahead is also indicated, highlighting some of the key points in the design of a fusion reactor. The recent results obtained by our group on target design for shock ignition [4], optimization of direct-drive irradiation schemes [5], and energy and laser wavelength scaling models are illustrated [6].

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#327 - Resonant and non-resonant ponderomotive effects in laser-matter interaction

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A general expression of the ponderomotive force of a laser beam at relativistic intensity is derived in an arbitrary sytem of reference from an adiabatic invariant. The appearance of hyteresis of a free particle is eludidated and its relevance for laser-particle accelration is presented. The ponderomotive concept is then generalized to particles with internal degrees of freedom and particles in a static magnetic field; the connection with level shifts (e.g. Stark effect) in atoms is established.

In a second part it is shown that a whole variety of resonant poneromotive effects in intense laser-matter interaction (stimulated Brillouin and Raman effect, two plasmon decay, others) as well as non-resonant phenomena (self-focusing, modulational instability,

stationary plasma density structures and plasma flow variations; above threshold field ionization) is driven by ponderomotive action. The usefulness of such a unified picture is illustrated by specific examples from intense laser-matter interaction. Finally, the limits of the pondereomotive concept as a secular force most clearly appear when it is applied to non-monochromatic light beams or when transitions to particle trapping start dominating.

#328 - Nonlinear dynamics of Alfvèn modes in tokamaks investigated by phase-space numerical diagnostics

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Numerical simulation results obtained by hybrid MHD-gyrokinetic simulations for Alfvén modes in tokamaks are presented, with emphasis on diagnostics conceived for the analysis on nonlinear dynamics.

To get information about the behaviour of resonant particles and the connection of such behaviour with mode saturation, we follow a set of test particles evolved in the fields computed in self-consistent simulations. Particles are initialized with different radial positions (around the mode localization) and given values (the same for all particles) of the two constants of motion, M (magnetic momentum) and $C=\omega P_\varphi - nE$ (with ω being the observed mode frequency, n the toroidal number of the mode, P_φ the toroidal component of the particle momentum and E the particle energy). Particle coordinates are collected at each time ($t=t_j$) particles cross the equatorial plane ($\vartheta=0$) at its outmost radial position. The wave phase seen by the particle at those times is $\Theta = \omega t_j - n\varphi_j + 2\pi j(m-k)$, with m being the poloidal number of the mode and k the order of the resonance. At each time step, a marker is plotted for each test particle in the (Θ, P_φ) plane, referred to the last crossing of the equatorial plane by that particle. During the unperturbed motion, markers drift in Θ, while maintaining constant P_φ. In the nonlinear phase, P_φ varies (e.g. because of the radial $\mathbf{E}\times\mathbf{B}$ drift), giving rise to two kinds of trajectories for the markers: passing and trapped ones. The evolution of the resulting phase-space structures is analized in connection with the flattening of resonant particle density profile and saturation process. The relevance of *resonance detuning* and/or *radial decoupling* is discussed.

#329 - Non-linear plasma physics and current drive at density required for a tokamak thermonuclear reactor

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The most efficient method for driving off axis non inductive current in tokamaks is based on coupling, by means of antennas built by a phased array of rectangular waveguides, microwave power of several GHz to tokamak plasmas. This power feeds lower hybrid (LH) plasma waves capable of producing the lower hybrid current drive (LHCD) effect [1]. LH waves propagate in density plasmas that satisfy the cut-off condition: $\omega_{pe}>\omega 0$ (where $\omega 0/?\pi?$ is the operating frequency of the RF power source). The properties of LH modes of being slow and quasi-electrostatic waves enable momentum transfer from waves to plasma electrons, which contributes to the plasma current.

For long time the LHCD effect was observed to occur only in experiments operating at low plasma density (up to line averaged value $n_{e\_av} \sim 0.4\times10^{20}$ m^{-3}) with quite peaked radial profiles, i.e., in conditions that are far from those required for a thermonuclear fusion reactor experiment. The penetration of the coupled LH power to plasma core appeared problematic, indeed, at higher densities occurring, in particular, at the periphery of plasma column, although quasi-linear theory expects LH waves to be fully propagating at high density [2].

Modelling results identified non-linear wave interactions with the plasma edge as cause of penetration failure of the coupled LH power to plasma core, under relatively low local electron temperature [3]. Consequently, operations producing relatively high electron temperature at the periphery of plasma column were expected to solve the problem of LHCD at high density. Experiments performed on FTU (Frascati Tokamak Upgrade) have validated indeed these theoretical predictions, thus enabling assessing a new method for LHCD at reactor-graded high plasma density [4].

New data from modeling and experiments will be discussed here, which further support the conclusion that ENEA-Frascati has assessed a change of paradigm for driving current in tokamak plasmas, by externally launching microwave power.

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#330 - Nanostructured tungsten films exposed to high-flux deuterium plasmas for nuclear fusion research

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We present an experimental investigation on the relation between the nano-structural properties of W films, deposited by Pulsed laser Deposition (PLD), and deuterium (D) retention arising from exposure to high-flux deuterium plasmas.

W coatings have been recently adopted to cover plasma facing surfaces of first walls in thermonuclear fusion machines (i.e. Tokamaks) [1]. Neutrons, particles, e.m. radiation deeply change first wall material properties during machine operation, inducing modifications at the nanometric level, like vacancies, defect formation and nanocrystalline growth [2]. The dependence of deep diffusion in metals on particle fluxes and radiation damage is largely unknown and requires further research also because of the lack of knowledge of the influence of materials properties at the nanoscale on macroscopic behavior.

To investigate this issue we deposited by PLD nanostructured W coatings and characterized them by high resolution SEM, XRD and EDS [3]. Thanks to the flexibility of PLD it is possible to study a wide range of coating compositions, structures, growths and morphologies, by changing the process parameters. The coatings are dense, non-porous and exhibit different crystalline structures, ranging from highly crystallographic oriented with columnar structure to "amorphous like" structure with a high level of nm defects (crystalline domain size less than 2 nm). We exposed the films to high-flux ($>10^{24}$ $m^{-2}s^{-1}$) D plasmas in the divertor simulator Pilot-PSI, to investigate the deuterium retention and erosion properties. Surface temperatures below 520 K and between 600-950 K were adopted, to investigate the effect of vacancy migration during D implantation. Thermal Desorption Spectroscopy measurements show that retention properties are highly influenced by nanostructure and disorder. The measured retention levels are similar or even much higher than the highest measured in pre-damaged W. Surface morphology changes, like bubble formation and nano-crystalline structures, were found.

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#331 - High energy resolution XAS and XES - applications in catalysis and materials science

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X-ray absorption and emission methods provide numerous advantages for in depth studies of chemical systems [1]. While EXAFS (extended X-ray absorption fine structure) delivers a detailed picture of the geometric structure around a X-ray absorbing center, [1] X-ray emission methods are able to reflect the electronic structure: HERFD-XANES (high energy resolution fluorescence detection X-ray absorption near edge structure) resolves details of the prepeak structure caused by transitions to the lowest unoccupied states (LUMO) [2] , while valence-to-core or $K\beta_{2,5}$-XES complementary reflects the highest occupied states (HOMO) [3]. Core-to-core or $K\beta_{1,3}$-XES complements these pieces of electronic structure by making the total spin at the metal center accessible [4] . Taken together, the mentioned hard X-ray methods present a powerful toolbox to answer dedicated questions in catalysis and material science. Selected applications in sustainable chemistry will be presented with the example of iron-catalyzed CO oxidation and photocatalytic water reduction, which opens the chance of introducing sustainable chemistry to the emerging field of X-ray free electron lasers. This is also relevant for the last topic to be presented, namely the investigation of spin-cross over processes by XAS and XES, which requires time-scales from minutes to femtoseconds.

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#332 - Coherent diffraction imaging project at FERMI@Elettra: present status and research opportunities

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The high transverse coherence and peak brightness of ultra-short SASE-FEL pulses have already demonstrated the extraordinary potential for coherent diffraction imaging (CDI) in a single shot experiment before the radiation damage of the sample is manifested [1]. The limitations imposed by the partial longitudinal coherence of SASE-FEL for getting selective chemical information using single shot resonant (R-) CDI, should be overcome by the seeded FEL sources, as FERMI@Elettra [2]. This opens unique opportunities for single-shot R-CDI experiments with access to elemental and/or magnetic structure of morphologically complex targets using the energy tunability and multiple (circular or linear) polarization of the fully coherent seeded FEL pulses.
The measurement station for CDI, operating at the DiProI beamline of the FERMI@Elettra, is designed to meet the requirements for performing a wide range of static and dynamic studies and has been already commissioned using both synchrotron and FEL radiation [3,4]. This presentation will report the first CDI measurements illustrating the performance of the measurement station in single-shot CDI and the advent of tunability and multiple polarization of the FERMI pulses in resonant magnetic scattering at Co M-absorption edges. Finally, the unprecedented opportunity offered by FERMI@Elettra source to performe jitter-free pump-probe experiments using both infrared laser and EUV/Soft-Xray pulses will be presented.

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#333 - N K-edge Time Resolved X-ray absorption of the ZnOEP films

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Optical excitation in porphyrin derivative complexes leads to a complex relaxation dynamics which involves various transient states with a wide range of lifetimes (10 fs to 10 ns and beyond), the atomic structure of which is different from the one of the ground state. The properties of transient states are often studied with UV–VIS pump and probe (P&P) techniques. However, these techniques lack structural resolution and are not element sensitive; instead, TR-XAS can probe the structure of transient states with structural and elemental sensitivity.
We present the study of the relaxation dynamics of Zinc octaethylporphyrine (ZnOEP) molecular thin films performed by time resolved X-ray Absorption Spectroscopy (TR-XAS), at the BACH Beamline, TRex facility of ELETTRA.
The N K-edge TR-XAS spectra of ZnOEP measured with 2 ns time resolution show the presence of a transition with a long decay time of about 20 ns.
Spectra simulation by MXAN (static and Time resolved version) code are in progress. Preliminary analysis indicates a structural

distortions of the macrocycle following optical excitation in the Soret band with a dynamics in the scale of tens of ns time. In particular a modification of the Zn – N bond lengths (and extraligands) is hinter by our results.

#334 - dd Excitations in a Ni-based metal-organic framework: comparison between rixs and optical spectroscopy

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We identify the dd excitations in the metal−organic framework CPO-27-Ni [1] by coupling resonant inelastic X-ray scattering (RIXS)[2] and UV−vis spectroscopy, and we show that the element selectivity of RIXS is crucial to revealing the full dd multiplet structure, which is not visible in UV−Vis. Combininig calculations using crystal-field multiplet theory and density functional theory it is possible to reproduce the RIXS spectral features, crucially improving interpretation of the experimental data. We obtain the crystal-field splitting and magnitude of the electron−electron interactions and correct previously reported values. RIXS instruments at synchrotron radiation sources are accessible to all researchers, and the technique can be applied to a broad range of systems [3].

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#335 - EUV transmission and reflection measurements at Fermi@Elettra

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The FERMI@Elettra FEL1 free-electron-laser generates subpicosecond pulses at variable photon wavelengths (20-65 nm range) [1] which can be used to raise the temperature of solid specimens by exciting a large fraction of the electrons. In fact, wavelength and intensity of the Fermi@Elettra FEL pulses are suitable for an efficient ultrafast heating of most bulk-like dense samples. The TIMEX end-station, developed through a collaboration between the University of Camerino and Sincrotrone Trieste, [2,3] has been conceived to investigate metastable and/or excited states of matter under extreme conditions.
In the present communication we shall present some of the first results obtained during the initial beamtime sessions as well as the design and present status of the end-station. In particular, selected experiments aimed to measure the saturable absorption of ultra-thin films as a function of fluence for different photon wavelengths will be discussed also in light of previous results and of new theoretical modelling [4] approaches. Results of extreme ultraviolet (EUV) reflectivity measurements on selected mirrors for increasing fluence and different photon wavelengths will be also discussed. [5] The relevance of these studies for investigation of matter under extreme conditions up to the warm dense matter regime will be discussed.

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#336 - The L23VV Auger spectrum of Cu(001)-p(2x2)S studied by Auger-photoelectron coincidence spectroscopy

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An accurate determination of the electron correlation energy has always been a relevant issue for many branches of material science and solid state physics. Indeed, it plays a crucial role in the determination of physical and chemical properties in a wide class of materials presenting very interesting characteristics, for example: superconductivity, giant and colossal magnetoresistence, ferro- or antiferromagnetism. In spite of its relevance, not many experimental methods are available to investigate this quantity.
We measured the Cu(001)-*p(2x2)*S L2VV and L3VV Auger line shapes by means of Auger PhotoElectron Coincidence Spectroscopy. Measuring the LVV Auger electron distribution in coincidence with 2p1/2 and 2p3/2 photoelectrons we succeeded in separating the two overlapping spectra and to measure the line shape of each considered decay. We found out that the two Auger transitions, though shifted in energy, display an identical line shape that cannot be described by the self-convolution of the single particle density of states, while it is very well described within a Cini-Sawatzky (CS) approach [1,2]. A fit to the APECS data using the CS line shapes obtained with different correlation energies superimposed to a Shirley-type integral background indicates that the most reliable value for the valence band hole-hole correlation energy, here used as a free parameter, is $U = 0.3 \pm 0.1$ eV. This is the

first time that the CS theory is successfully used in conjunction to experimental APECS line shape to determine the amplitude of the Coulomb interaction of two valence band holes in a system where it is very close to zero.

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#337 - Local disorder in doped ceria: from low temperature to operating conditions

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In recent years, doped ceria compounds have attracted increasing attention as electrolytes for application in Solid Oxide Fuel Cell devices, thanks to their high performance at intermediate temperature (500-700). In cerium oxide, ionic conductivity is driven by the presence of oxygen vacancies, introduced for charge balance after doping with a lower valent cation. With increasing doping concentration the oxygen diffusion is impeded, probably because of the formation of aggregates that trap oxygen vacancies. Their nature is though still under debate.

Owing to the close interplay between transport properties and local structure, an accurate description of the defects on the atomic scale is of the utmost importance for understanding the mechanisms at work in doped ceria.

To this purpose both X-Ray Powder Diffraction (ESRF, ID31 beamline) and Neutron Powder Diffraction (ILL, D20 and D4 instruments) studies were performed. The average and local structure was determined employing both the conventional Rietveld analysis and the Pair Distribution Function (PDF) technique. The local structure of doped samples differs from the average one [1]. The investigation of doped samples up to very high doped systems revealed a continuum of structural evolution, both long range and locally and allowed us to determine a fingerprint of disorder in the PDF patterns. The local structure determined through XRPD PDF is consistent with the formation of dopant-rich droplets embedded in a fluorite-like matrix [1,2], whilst NPD PDF highlight the O distortions induced by vacancies [3].

Different dopants affect in a similar way the local structure of doped ceria, but differ in the magnitude of the induced distortion. The latter, as determined by XRPD or NPD, matches the trends of ionic conductivity observed in the literature. The above mentioned studies were performed at low temperature, which is the best experimental condition for a crystallographic study aimed at unravelling static disorder. In order to fill the gap with real operating conditions, XRPD PDF were collected at high temperature under air and reducing atmosphere. The doping-induced distortions are retained even at high temperature and are magnified when doped ceria is subjected to a reducing atmosphere [4].

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#338 - Investigation on structural and electrical modifications in Bi-2212 whiskers exposed to synchrotron nano-beam radiation

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Among the family of high-temperature superconductors (HTSC), $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) is widely studied material both for fundamental research and for applications. In the latter respect, this compound attracts significant attention because of the alternation of superconducting and insulating planes that form its layered structure and represents a series of intrinsic Josephson junctions, which can be exploited for the fabrication of electronic devices such as voltage standards, THz emitters/sensors [1] and micro-SQUIDs [2]. Spaceborne applications of this kind have the potential advantage of using passive cooling only, but in this case the presence of cosmic radiation is an issue [3]. Therefore the response of this material to harsh working conditions has to be carefully investigated. To this purpose, we exposed two high quality single-crystal Bi-2212 whiskers with electrical contacts to hard X-rays (17.1 keV) at the ID22-NI beamline of ESRF, Grenoble. We used the nano-beam (space resolution= 117x116 nm^2) both to age the crystals and to monitor their structural homogeneity and the modifications induced by the synchrotron radiation by means of in-situ acquisition of XRF maps and XRD frames, respectively. Electrical modifications were recorded by measuring ex-situ R versus T curves in a four point configuration both for the pristine samples and after each stage of damaging.

In spite of the limited thickness of the crystals (about 2 μm), we could retrieve c-axis values of the samples in different points between the voltage contacts by using a grazing incidence configuration. The c-axis length, obtained from the Bragg equatorial reflections, increases with the dose in all cases. Correspondingly, an increase of the mid-point transition temperature and of the in-plane resistivity is observed with increasing the dose. These phenomena can be explained by a change in the doping regime from overdoped to nearly optimally doped, as already verified for by other studies [4].

We were also able to measure the value of the c-axis length just below a voltage contact and verified that an alteration is induced in the crystal by the proximity of the silver layer. The high value of the c-axis indicates an oxygen depletion of the near-surface Cu-O planes due Ag deposition on the surface. The local variation of oxygen content leads to the creation of a new phase in the sample, that can be associated to a secondary transition clearly visible in the resistivity curves.

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#339 - State of the art and perspectives of inorganic photovoltaics

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Inorganic materials dominated the PV market from the beginning. PV devices based on silicon are the most common solar cells currently being produced and it is mainly due to silicon technology that the PV has been growing by 40 % per year over the last decade. Cost, sustainability and environmental issues are at the core of the PV silicon based industry activities. An additional step in the silicon solar cell is on-going and it is related to a further efficiency improvement through defect control, device optimization, surface modification, nanotechnology approaches.

Inorganic thin film PV technologies have been under development in the last decades as a low cost alternative to bulk c-Si. Incidentally, this technology is the most suitable for Building Integrated Photovoltaics and for large-scale production since the module is the final stage of an in-line process that does not require the assembly of discrete smaller cells. In the frame of inorganic thin film $Cu(In,Ga)Se_2$ (CIGS) solar cells is one of the most promising in terms of the efficiency record (20.3 %), nearly reaches the one of Si solar cell and of stability. Despite the promise of CIGS thin-film and also of CdTe photovoltaic technologies with respect to reducing cost per watt of solar energy conversion, these approaches rely on elements that are either costly and/or rare in the earth's crust (e.g. In, Ga, Te) or that present toxicity issues (e.g., Cd), thereby potentially limiting these technologies in terms of future cost reduction and production growth. The new material Cu_2ZnSnS_4 (CZTS), in which indium and gallium are replaced by the readily available elements zinc and tin, is very promising in terms of reduced cost and sustainability but an intense research activities to optimize the growth process and the material quality are still necessary before transferring the device on the market. In the MIB-SOLAR center of UNIMIB, a new method for chalcogenide thin film (CIGS) deposition on glass and flexible substrates has recently been developed, in collaboration with a small enterprise. Up to now the process has been optimized for CIGS films with a thickness of around 2 micron, obtaining a cell efficiency of 14 % on glass and 8.3 % on flexible stainless steel substrate, respectively, in less than 3 years of activity. In the last year we started a new activity regarding CZTS thin film. Two main growth depositions (sputtering and sol gel methods) are under investigation and testing.

This article points out the most important advances and current technologies related to inorganic PV devices. In the meantime the most challenging and promising strategies acting to increase the ratio between the efficiency and the cost of inorganic solar cells, developed in our laboratory will be described. Some novel concepts under development in MIBSOLAR centers, which could have an important role in the future of PV will be also described.

#340 - Approaching 4n2 classical limit in metal-free and ultra-thin crystalline silicon solar cells

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Light trapping has produced a significant efficiency gain in crystalline silicon (c-Si) solar cell performances over recent decades. However the need for cost reduction, that requires less raw materials and low-cost processes, calls for more advanced optical schemes to not sacrifice the conversion efficiency. We present an experimental approach that maximizes absorption in metal-free and ultra-thin c-Si wafers. Our light trapping scheme involves low cost and industrially scalable processes such as black silicon (b-Si), random pyramids and dielectric distributed Bragg reflector (DBR) for four different bulk thicknesses (80, 100, 140 and 190 µm). Particularly, black silicon (b-Si) as front texture strongly enhances light in-coupling in a broad wavelength range due to its high aspect ratio, while random pyramids at the back side (BS) can effectively interact with light at long wavelengths. Our wafers were coated on both sides with thermal SiO_2 to achieve state-of-the-art passivation of front and back side textures. In addition, by fabricating a dielectric DBR formed by six pairs of $a-SiN_x:H$ / $a-Si:H$, we implemented an omni-directional and metal-free reflector at the rear side of our structured wafers.

Independently from bulk thickness, we found that measured absorptance achieved with dielectric DBR back reflector on textured BS was extremely close to the one obtained with the same textured BS but coated with Ag and even higher than that obtained with Ag-coated flat BS. The implied photo-current related to our metal-free advanced light trapping scheme was found to be up to 98.0 % of the one calculated from the classical $4n^2$ limit. Moreover, attractive electronic properties were measured for our ultra-thin wafers. Combination of these effects resulted in an increase of predicted conversion efficiency while decreasing the wafers thickness. Extrapolated conversion efficiency for wafers thinner than 80 µm shows that the optimum for the proposed light trapping scheme lies between 40 and 60 µm with a potential conversion efficiency above 22 %.

#341 - Photoluminescence study of chalcopyrite based PV absorbers

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The development of photovoltaic (PV) absorbers other than silicon proper for thin films based devices has become fundamental in the last decades to reduce the manufacturing costs. To raise the competitiveness of the second generation (thin films based) modules, rare elements should be avoided in all layers of newer solar devices. For example, elements such as indium and gallium in Cu(In,

Ga)Se$_2$ (CIGS) constrain the further development of CIGS-based cells, although they had already shown to attain efficiencies over 20% [1,2].

A possible alternative to CIGS is Cu$_2$ZnSnS$_4$ (CZTS), where more abundant and less expensive elements like Zn and Sn are used in place of In and Ga [3]. CZTS, whose most stable crystalline form is kesterite, has a direct band gap of 1.4-1.5 eV and high absorption coefficient (over 10^4 cm^{-1}) [4]. The low formation energy of many of the acceptor defects present in the CZTS matrix lead to an intrinsic p-type character, in particular attributed to the Cu$_{Zn}$ antisite [5].

CZTS can be synthesized through solid state chemical reactions of ZnS, Cu$_2$S, and SnS$_2$. Investigations on the phase diagram of the system demonstrated that secondary phases are likely to occur due to the rather small existence region of CZTS as single phase [6]. This work will report the study of the structural and optical properties of CZTS thin films grown by sulfurization of stacked metal precursors. The metal stacks were prepared both by sputtering and chemical methods. Both the presence and the nature of point defects have been investigated in these CZTS samples by above and below bandgap excited photoluminescence. Broad emissions centered at 1.3, 1.23 and 0.85 eV were observed at low temperature for the above bandgap excitation process, while broad bands at 1.075 eV and 0.85 eV were detected at low temperature for the below bandgap excitation process. Radiative transitions involving point defects related levels determined by first-principles calculations (i.e. levels associated to Sn$_{Cu}$, V$_{Zn}$, V$_S$, Cu$_{Sn}$, V$_{Sn}$, Sn$_i$ [5]) were proposed to be responsible for the observed emissions. Such a comparison between theoretical data and experiments is mandatory to deepen the limited current knowledge on defect levels in CZTS.

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#342 - Plasmonic metal nanoparticles for thin film solar cells

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Over the past few years metal nanoparticles (NPs) have attracted considerable interest due to their ability to strongly enhance electromagnetic fields and their potential applications in thin film photovoltaics [1, 2]. When the size of a noble-metal particle, such as Au or Ag, is reduced to the few nanometer range, it can sustain Localized Surface Plasmon Resonances (LSPR), collective oscillations of free-electrons resulting from the interaction with the incident light, which dramatically influence the NPs optical properties. The LSPR strongly depend on the material of the NPs, their geometrical parameters (size, shape) and the surrounding medium. Thus, metal nanoparticles should be properly designed in order to reduce as much as possible the parasitic absorption inside their material while allowing high light scattering [3].

In this work, plasmonic nanostructures are fabricated with a self-assembly method and incorporated in the rear side of a-Si:H solar cells, so that the NPs interact only with light that is not absorbed during the first pass through the absorber cell material. In this way, a plasmonic back reflector (PBR), composed of a flat silver mirror and a layer of Al-doped ZnO (AZO) with embedded metallic NPs, is constructed. Such PBR can redirect the light at angles away from the incidence direction and consequently increase its optical path length in the solar cell. The aim of the present study is twofold. First, we provide an insight into the correlation between the structural and optical properties of self-assembled NPs, and second we experimentally demonstrate that self-assembled NPs based PBR can provide light trapping performance comparable to state-of-the-art random textures in a-Si:H solar cells.

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#343 - Engineered disorder for light-trapping in thin-film solar cells

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Strong light-trapping is crucial to obtain highly efficient thin-film solar cells, thus a number of different light-management strategies have been explored. On the one hand, ordered photonic structures can provide an efficient light-trapping in narrow wavelength intervals, but it is also known that broad-band absorption enhancement requires the introduction of a certain amount of disorder in the structures. On the other hand, randomly rough interfaces are intrinsically broad-band scatterers and appear to be particularly promising. Yet, the description of a realistic rough interface is complicated, which makes the study and the optimization of devices challenging and computationally demanding.

In our approach, we are able to efficiently describe the optical properties of state-of-the-art rough substrates by means of only two statistical parameters: the root mean square of height and the lateral correlation length. The simplicity of this strategy allows us to drastically reduce computational cost in the view of a better understanding and optimization of light management in thin-film solar cells with rough interfaces [1].

In this contribution, we demonstrate that the Lambertian limit of absorption can be obtained in a structure with a properly optimized

roughness. We study this by considering solar cells made of different materials to investigate the role of size and nature (direct/indirect) of the energy band gap in the optimization of light-trapping. Finally, we suggest the possibility of combining rough interface with a diffraction grating, which gives a significant absorption enhancement also for a relatively small roughness.

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#344 - Self-organised nanopatterning of thin film amorphous silicon solar cells featuring broadband light trapping

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We exploit Ion Beam Sputtering (IBS) for producing nanostructured glass, semiconductor and TCO interfaces endowed with enhanced vertical dynamic in order to mimick the broad-band light-trapping functionality of bio-mimetic interfaces. The high aspect ratio nanoscale features are formed recurring to defocused IBS through a self-organised sacrificial Au stencil mask assisted by simultaneous co-deposition of gold atoms from an auxiliary Au atom source; in this way it is possible to significantly enhance the vertical dynamic range of the nanostructures up to 250 nm [1].
The presence of high aspect ratio sub-wavelength features results in a progressive transition of the refractive index from the value of air to that of the substrate (index grading) analogous to that observed in the corneas of nocturnal moths [2]. Large angle diffuse light scattering (Haze) is instead induced by surface corrugations with lateral size comparable or bigger than light wavelength [3]. The potentiality of the patterned glass substrates in promoting broad-band photon harvesting is demonstrated by comparing the performance of thin film amorphous silicon solar cells grown on the nanostructured glass templates with that of reference devices grown on flat glass [1].

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#345 - Quantum dot intermediate-band solar cell grown by droplet epitaxy

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Quantum dot intermediate band (IB) solar cells have been proposed in order to increase the efficiency of traditional solar cells and immediately attracted a lot of attention and research since the time they were first proposed. The IB introduces an extension of the absorption coefficient of the semiconductor to lower energies, allowing a more thorough collection of the solar spectrum, via a two-step absorption of low-energy photons. Quantum dot (QD) structures are good candidates for IB solar cells, because their confined energy levels can overlap and form a miniband in dense arrays and the position of these levels and bands can be tuned varying the size and spacing of the QDs. The IB working mechanisms have been demonstrated for InAs QDs in GaAs, and many efforts are devoted to reduce the problems due to strain, and defect nucleation increasing carrier escape.
Droplet epitaxy (DE) is a molecular beam epitaxy technique that allows for the growth of quantum dots of materials lattice matched to the barrier and the removal of the wetting layer. DE makes possible to indipendently control density, size and shape of the nanostructures. Densities as high as some 10^{11} cm^{-2} per layer have been reported and potentially a large number of layers can be stacked because the system is strain-free. Being a strain-free technique, there are virtually no defects in DE-grown materials. By tuning the size of the QDs it is obviously possible to change the position of the IB, and by tuning their aspect ratio the high energy states of the QDs can also be tuned in order to have a small electron-phonon coupling with the barrier. The lack of defect and wetting layer states can greatly reduce thermal escape of carriers from the IB, leaving photon-induced transitions the dominant ones, as requested by IB theory. For these reasons DE is a good candidate for the realization of QD-IB solar cells.
We demonstrate the key working principle of IB materials, that is the production of sub-gap two-photon photocurrent, with $Al_{0.3}Ga_{0.7}As$ solar cells containing GaAs QDs grown by DE. Measurements show that the shape of the two-photon photocurrent signal is different from the VB-CB photoresponse, indicating clearly that a two-photon process involving the QD levels is taking place. The two-photon signal response is in good agreement with the PL spectrum of the QD samples, that lets us easily understand the position of the energy levels of the system.

#346 - Structural, electrical and optical properties of nanostructured Ta-doped TiO$_2$ produced by PLD

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The field concerning transparent conducting oxides (TCO) has recently been attracting much attention in the research for an alternative material to indium tin oxide (ITO) and for the development of oxide nanostructures for advanced light trapping or novel photoanodes for 3rd generation photovoltaic applications.
Nanostructured anatase TiO$_2$, due to its large surface area, high chemical stability in reducing atmosphere, low toxicity and ideal

position of the conduction band edge, is a key material in many applications including photocatalysis, water splitting and Dye Sensitized Solar Cells (DSSC). For such applications, a hierarchically organized TiO_2 in the form of a nano-tree forest can lead to interesting results in light harvesting, charge collection and transport [1]. Interestingly, it has been recently discovered that charge transport properties of anatase TiO_2 can be strongly enhanced by means of doping with Nb^{+5} (NTO) [2], or Ta^{+5} (TaTO).

We here present the synthesis and characterization of TaTO thin films by nanosecond Pulsed Laser Deposition (PLD). We exploited the deposition process at room temperature, followed by a vacuum ($p < 4x10^{-5}$ Pa) annealing to obtain single phase oxygen deficient anatase films, as the coordination between substitutional Ta and oxygen vacancies plays a key role in the conductive behavior. We investigated the effect of oxygen partial pressures during the deposition process and we were able to obtain compact (0.1-2 Pa range) and nanoporous-nanostructured (5-15 Pa range) thin films with a tree-like architecture. The role of the annealing temperature (350-550°C range) on the electrical properties (Van der Pauw, Hall) of compact TaTO films was analyzed as well. The best results were obtained for deposition in oxygen pressure of 1 Pa coupled with a vacuum annealing at 550 °C. The resistivity obtained for a 185 nm TaTO film is $1.2x10^{-3}$ Ωcm, with a mean transmittance in the visible range of 75%. Transmittance can be enhanced by reducing the thickness of the TaTO thin films without strongly affecting the resistivity. Exploiting such approach it is possible to realize a fully TiO_2-based photoanode by the synthesis of a graded structure, i.e. a large surface area, nanoporous film on top of a compact TaTO electrode, in view of application in DSSC or hybrid solar cells.

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#347 - Characterization of archaeometallurgical artifacts through neutron diffraction and neutron imaging techniques

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Use of neutron diffraction and neutron imaging techniques in archaeometry represents one of the most important research achievements, in recent years, for non-destructive characterization of metal artifacts. These techniques, originally developed for bronze archaeological findings, have received renewed momentum when applied to more recent steel artifacts of historical origin.

Owing to the peculiar properties of thermal neutrons, like their penetration power and their consequent ability to gather information on the microscopic properties of thick metal samples, these neutron-based techniques allowed to experimentally access the average bulk microstructure of archaeological and historical objects without having to resort to sampling, or even to surface cleaning.

Thanks to the wavelength range of thermal neutrons, the diffraction techniques could be effectively applied to measure the sample microscopic structure at the atomic level and to quantitatively derive its phase composition, averaged over a sample volume of several cubic centimeters. In addition, Bragg peak analysis, carried out using the most recent achievements in the Rietveld refinement techniques, allowed to obtain, from a detailed investigation of the peak shape, precious hints on the most likely thermal and working processes carried out on the artifact, which is representative of the skill level reached by a particular civilization.

Last, but not least, neutrons can be used in a similar way to X-rays, though with a much higher penetration power in metal samples, to obtain radiographic and tomographic images which reveal the interior of bulk metal objects in an almost absolute non-invasive way.

In this presentation we will show a panoramic view of the various archaeometry problems that were dealt, and often solved, using these neutron-based techniques by the CNR-ISC neutron research group working in close collaboration with some Museums and Public Institutions with whom we have built a well established and proficuous collaboration.

#348 - Digital X-ray radiography of paintings

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The impact of digital technology in X-ray imaging cannot be overemphasized and all effects on the field of Cultural Heritage are still far to be fully evaluated. Here is a little sample of the existing applications.

The digitization at 12, 14 or 16 bits/pixel offers the widest gamut of information on the inner composition of the target artwork. Digital images are ready for elaboration, even as simple as assembling a complete view of a large painting by stitching or enhancing contrast of an individual detail.

Multi-image processing is the ultimate choice in digital elaboration. Tomographic sections, for instance, are obtained by a parallel processing of a sequence of similar X-ray projections. Logarithmic subtraction of radiographs, obtained from narrow-band radiations braketing the K-edge absorption of a chemical element, maps that particular element among any other, in a painted layer.

Some of these techniques, using facilities at the Department of Physics and Earth Sciences, INFN Research Unit and TekneHub Laboratory at Ferrara University are reported. Applications of instruments and methods like 2D scanner, 3D rotational tomography, K-edge differential radiography to ancient and modern paintings are described and shown.

#349 - Neutrons and music: imaging investigation of ancient flute musical instruments

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A set of nine musical instruments coming from the 'Fondo Antico della Biblioteca del Sacro Convento' in Assisi, Italy, were investigated by imaging techniques. The historical and scientific interests in the knowledge of ancient instruments motivate an intense research effort for the characterization using non-destructive and non-invasive techniques. X-ray and neutron tomography/radiography were applied to the study of composite material samples containing wood, hide and metals. The study was carried out at the NEUTRA beamline, PSI (Paul Sherrer Institute, Switzerland). The measurements were dedicated to studying: the internal structure of the samples, position of added materials like metals, the wood fibre displays, deformations, presence of adhesives and their spatial distribution to give information about construction methods and guide the restoration process.

#350 - Phase sensitive mm-wave and Terahertz imaging for art conservation studies

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At the ENEA Center of Frascati different Free Electron Laser (FEL) sources are available, emitting in the spectral region between 0.1 and 0.8 THz. The peculiar characteristics of such sources make them a useful tool for studies in the field of art conservation. Radiation in the sub-mm/THz region has the capability of penetrating through dielectrics, while it is strongly absorbed and reflected by water and metals. Being the emission frequency very low, the irradiation does not produce ionization of the sample. The peculiar

temporal characteristics of the FEL pulses avoids the risk of heating the sample under investigation, keeping a low average power (about a mW) while the peak power is very high (about 1 kW). The high transmission through dielectric materials has demonstrated to be useful to look through layers of gesso or other materials, covering a painting or a fresco. An imaging tool, working in reflection, has been set up, and it is now able to perform scans of small areas (50x50 mm^2) of paintings, obtaining a THz image also through gesso. Moreover the system has been studied with the ability of detecting the phase change caused by the reflection of the radiation by the sample. By means of a simple mathematical model it is possible to use this phase measurement to obtain information about the optical properties of the sample, obtaining the real and imaginary part of the refraction index at the radiation frequency. This capability has been exploited in order to optimize the contrast between different pigments in the sample, thus obtaining a good THz image.

Based upon the experience acquired in laboratory experiment, a new portable system is being designed, able to perform scans on larger areas (1000x1000 mm^2) directly on site, thus allowing its use for frescoes and samples that cannot be delivered to a laboratory. Other mm-wave and THz sources are under study to verify their possible application in this field.

#351 - A study of surface optical properties for characterizing the cleaning process of paintings

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Restoration refers to the removal of surface dirt and discoloured varnish layers, the treatment of the support, the replacement of missing portions imitating the original, or building up fragments of sculpted or moulded areas of an artwork. A painting can be built up in transparent or semi-transparent glazes, which can be partially or totally opaque due to adverse conditions such as lighting, heating, fluctuations in temperature, exposure to direct sunlight which can cumulatively create the need for restoration. Over many years the transparency of the varnish will become clouded and discoloured often resulting in a picture being viewed as if through an amber or even brown filter. These effects on the varnish layers aren't the only results of the ageing process. Cracks which appear in the most extraordinary formations, apparently on the surface, are also caused by a number of complex interactions between the support, the primer and the pigment layers.

"Cleaning" is a process of carefully identifying the cause of any deterioration or discolouration and then removing or treating these layers. The skill of the restorer is not only to understand the techniques and media used by the artist, but also to recognize what beauty lies beneath the veils of many years of neglect or adverse conditions. Surface cleaning is then one of the most important and sometimes controversial stages of the conservation process: it is an irreversible process that generally results in substantial physical changes of the object surface, raising thus a series of questions regarding aesthetics, the potential loss of historical information, and the ability to control the cleaning process adequately. Decisions have to be made regarding partial or complete removal of varnish: technical considerations include selection of a method that allows a great deal of control in the cleaning process, so that undesired layers can be removed without damaging the underlying ones by means of traditional cleaning methods, including mechanical or chemical removal.

In this work we present a study of the optical properties of painting surfaces for the characterization of the cleaning process. Analyses were carried out by means of laser micro-profilometry and confocal microscopy.

Measurements were carried out on a few paintings which are under repair at the Opificio delle Pietre Dure in Florence. Selected areas were surveyed with the two above mentioned techniques and results were correlated.

#352 - Luminescence spectroscopy: an investigative tool for art materials

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UV-Visible luminescence measurements have been largely used in the last two decades for cultural heritage diagnostics [1]. In particular, over recent years, fibre optics and electronic miniaturizations have facilitated the design and set-up of compact portable equipment which can be used in-situ as powerful non invasive investigative tools. Very often such instrumentation is not commercially available and so their setup and optimization covers a wide part of the research activity. Steady-state and time-resolved emission spectroscopy techniques are informative for fluorescent organic and inorganic materials used in artworks production. In particular for organic dyes, knowledge of their electronic spectroscopic properties often represent the only feasible way in order to obtain their identification in a completely not invasive manner. Moreover, UV-VIS reflectance, which is an interesting investigative tool itself, can be efficiently coupled with luminescence information providing the corrected emission spectrum of a luminescent painted layer. Through the conversion of the total reflectance spectra into Kubelka-Munk values, the emission spectrum can be corrected from physical self-absorption phenomena, providing a higher specificity to luminescence experimental data. Fluorophores with similar emission spectra can be distinguished by measuring fluorescence decay lifetimes. In order to apply all these techniques together, namely reflectance spectroscopy, steady-state and time resolved luminescence spectroscopy, obtaining information from the same point of whatever artwork, a compact portable instrumentation has been assembled and optimized [2]. As it always happen for scientific investigations, the spectroscopic characterization of fluorophores present in an artwork, do not only provide analytical answers but often permit surrounding chemical interactions to be investigate and acknowledged. Coupling the information obtained with further spectroscopic techniques, such as Infrared and Raman, allows reasonable hypotheses concerning ageing and degradation pathways of the examined target to be proposed [3-4].

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#353 - Microwave dielectrometry for the diagnostics of wall paintings

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As well known, the deterioration of wall paintings due to the presence of moisture is a very widespread problem. The moisture content is related to the capillary rise of water from ground through the walls, water condensation on the surface of the wall paintings, or infiltration of water cause by the rain. Water is the main source of damages: the process of water evaporation through the surface could bring to the detachment of the painted layer and/or to the whitening due to the precipitation of salts (efflorescence) conveyed by water itself. A system for an early detection of the presence of water under the wall painting surface could be decisive for avoiding such kind of damages. A non-destructive and fully portable tool based on microwave dielectrometry has been realized and is described in this paper. The system allows the sub-surface measurement of the moisture content and the detection of salts on wall paintings and on any type of porous material. The measurement system consists of an evanescent-field resonant sensor, a network analyzer, and a proper numerical code dedicated to the control of the system and data elaboration. The method has been validated by measurements performed on conditioned samples caught from different porous materials (plaster and stones). Extensive tests have been performed in order to verify the effectiveness of the system in quantifying the moisture content and salt content. In-situ investigations on wall paintings and comparison with others method demonstrated the usefulness of the method as a reliable diagnostic tool for investigating the wall paintings conservation status.

#354 - Ab-initio computational methods for the calculation of optical properties applied to cultural heritage

Adriano Mosca Conte – Università degli Studi di Roma "Tor Vergata", Roma

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We have recently set up a non-invasive and non-destructive method to evaluate the level of degradation of ancient paper artifacts. It combines reflectance measurements with theoretical ab-initio simulations on cellulose. The analysis of the experimental and calculated optical spectra allows to identify and quantify the oxidized groups induced by ageing in paper. This chemical information can be extremely useful to plan restoration strategies.
Furthermore this method, being non-invasive, can be even applied to those ancient documents whose uniqueness and fragility require special care.
After having described in details the theoretical and experimental approaches we use, I will show the results of our investigation on the famous Leonardo Da Vinci's self-portrait and suggest how our analysis can orientate future restoration and preservation strategies.

#355 - Terahertz quantum cascade laser: a powerful metrological source across the far-infrared

Miriam Serena Vitiello (I) –CNR - Istituto Nanoscienze e CNR - Istituto Nazionale di Ottica, Firenze

Quantum Cascade Lasers (QCLs) witness how materials engineering can actually forge objects that, with conventional technologies, could never exist. Being fully designed from scratch, they represent a powerful testing ground for fundamental properties relying on the quantum nature of the device. These devices are then a powerful testing ground for the fundamental physical parameters determined by their quantum nature.

Despite the cryogenic operation temperatures ($\leq$ 195 K), QCLs working in the far infrared have now a realistic chance to deeply impact technological applications, thanks to the high output power (>100mW), the quite broad operating frequency range (1.2 - 4.7 THz), the tunability of nearly 10 % of the emission frequency, the coherence and the compactness. Frequency- and phase-stabilized, high-power and reliable, solid-state terahertz sources can indeed find application in a large number of fields spanning from far-infrared astronomy and high-precision molecular gas spectroscopy, to high resolution coherent imaging and telecommunications, providing the carrier wave for broadband wireless links. To address such application requirements, high frequency stability ultra-narrow and ultra-stable sources are almost mandatory.

Recent results on the analysis of the frequency noise features of Terahertz Quantum Cascade Lasers (QCLs) will be discussed, together with their potential in polarization spectroscopy experiments addressed to high sensitivity molecular detection. Highlighting the key role of the gain medium engineering, we demonstrate that properly designed semiconductor-heterostructure lasers could unveil the mechanisms underlying the laser intrinsic phase-noise, revealing the link between the device quantum properties and its quantum-limited linewidth.

In addition, novel experimental approaches aimed to the phase-locking of 2.5 THz QCLs to a free-space comb, generated in a $LiNbO_3$ waveguide and covering the 0.1–6 THz frequency range will be presented. The described approach paves the way to novel metrological-grade terahertz applications, including high-resolution spectroscopy, measurement of the absolute frequency and manipulation of cold molecules.

#356 - Integrated optical devices for single cell manipulation and analysis

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In recent years an impelling demand has arisen for the development of miniaturized devices for trapping and manipulation of single biological cells. Trapping devices can be usefully combined with microfluidic circuits that are becoming increasingly important for chemical, biochemical and biological analysis, as they allow reproducing complex phenomena on a micro- or sub-micro scale.

Here we report on our recent work concerning innovative optofluidic devices in which single cell analysis and manipulation is performed by means of on-chip integrated tweezers.

Two different approaches are presented. In a first approach, cell trapping and manipulation is obtained through optical waveguides integrated in microfluidic chips. The chips are fabricated in a fused silica glass substrate by exploiting femtosecond laser micromachining technique that ensures extreme flexibility and accuracy.

The delivery of the samples in the trapping region is accomplished through a controlled flow in a microfluidic channel. We will show that this approach allows the design and fabrication of optofluidic devices able to accomplish single cell stretching, which is a reliable method for measurement of cells' mechanical properties. In addition an integrated cell sorter is demonstrated which enables sorting and recovery of single cells selected on the basis of their fluorescence response or of their morphology.

In the second approach presented, on chip cell manipulation and analysis is obtained by means of optical fiber tweezers. Tweezers are fabricated by means on a new approach based on the two-photon lithography technique and can be successfully employed to gently trap and manipulate without physical contact single cells. In addition, the device results as a handy tool, fully compatible with the microfluidic set-up, that can be easily enriched with additional optical functions aiming at the realization of a multipurpose device for analysis and sensing of the trapped cells.

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#357 - Photonically enhanced polymer optofluidic chips

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Over the last few decades, various micro total analysis systems (µTAS) –also called lab-on-a-chip, miniaturized, or optofluidic analysis systems– have been developed, which integrate different chemical processes (sample pre-treatment, mixing, chromatographic, or electrophoresis separation) on a single chip. In these systems, a good molecule detection is one of the biggest challenges. To this end, optical techniques are often used, to measure the absorbance , fluorescence or molecular fingerprint of molecules. Fluorescence measurements are very sensitive and selective, but in general an extra sample preparation step is required to

label the often non-fluorescent molecules with a fluorescent dye. Absorbance measurements are less sensitive but do not need this extra labelling step. The latter also holds for Raman spectroscopy, a technique which very recently has been gaining ground in label-free detection and identification of species. To overcome the drawback that the scattered signals are very weak, the combination with optical trapping can be made and immobilization of the species at the Raman interrogation zone can be established.

Up to now, only classical microscopes are sufficiently sensitive to detect small amounts of molecules in the nanoliter detection volumes on the chip. These instruments are, unfortunately, too big and too expensive for integration in portable devices. Therefore, there is a large demand for efficient, small and robust optical detection units. At VUB different micro-optical detection systems were developed used for fluorescence and absorbance measurements in microfluidic channels as well as first prototypes for on-chip Raman spectroscopy. In this work we have used plastic micro-optical components and optical fibers to develop such integrated miniaturized detection units. For each system we present the complete development process from optical design, to fabrication and proof-of-concept demonstration. For all detection systems we have created designs with a high sensitivity but yet with a relatively simple layout to ensure their manufacturability and robustness.

By focusing on microminiaturization and integration, we were able to remove the free-space optical hardware needed in conventional bench-top microscopic systems such that a significant size reduction of the detection systems and a first step towards the development of multifunctional, low-cost, portable, robust, and, ultimately, disposable lab-on-a-chip systems was realized.

#358 - Advanced light scattering methods for studying supramolecular inhomogeneities in H-bonded liquids

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H-bonded liquids can be considered as mediums that have supramolecular heterogeneities, the existence of which is proved by static and dynamic laser scattering (M.Sedlak, 2006). Percolation model and concept of supramolecular inhomogeneities were successfully applied to describe inelastic light scattering spectra of amorphous media (S. Alexander, 1989).

The structure of H-bonded liquids can be presented as an infinite cluster whose cavities contain clusters of lower dimensions, small groups of bond molecules and separate molecules.

The low-frequency region of inelastic light scattering spectrum is shown to reflect fractal features of structure in H-bonded liquids. Low-frequency inelastic scattering in liquids occurs on thermal vibrational excitations. Owing to thermal disorder the vibrational excitations are damped and behave mostly similar to those in amorphous media. Vibrational excitations which have wave length larger than the correlation length do not feel fractality of the medium and therefore their dispersion remains linear. This transition wave length corresponds to the crossover frequency. Vibrational excitations with lower frequencies are damped acoustic phonons and with higher – fractons.

The effective vibrational state density of some H-bonded liquids was measured by the Raman scattering technique. The existence of the liner region in low-frequency spectral range for reduced intensity in log-log scale proves the fractal percolation clusters model to be valid in case of such medium. The concentration dependencies of the linear region's slope for different solutions are in good agreement with the behavior of other physicochemical parameters that depend on the H-bond network structure.

 Previously, it was showed that the light scattering by acoustic phonons is accompanied by 1/f fluctuations of intensity and the law $S(f) \sim 1/f^{\alpha}$ reflects the phonon energy fluctuations. Light scattering in the liquid systems occurs on phonons localized at inhomogeneities. In this work fluctuations of light scattering in H-bonded liquids have been investigated. We found that the index α depends on the type of liquid and solution concentration. We consider two mechanisms of 1/f - process forming: fluctuations of phonon energy and fluctuations caused by dynamical inhomogeneities, predicted by percolation model. Thus, they represent Brillouin-Mandelstam scattering and Rayleigh one correspondingly. The α variability can be explained by different contributions of the both scattering mechanisms, which form an overall picture of low-frequency fluctuations of scattering light intensity in complex liquids. Our work provides new experimental evidences for existence of supramolecular inhomogeneities in hydrogen-bonded liquids.

#359 - Scale-free optics in programmed dipolar glasses

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In rapidly-cooled photorefractive disordered ferroelectric crystals (KTN:Li), the glassy response supports a light propagation regime in which diffraction is cancelled without scale-dependent constraints ("scale-free optics") [1]. The phenomenon, which, in principle, supports high-resolution imaging, has the limitation of requiring that the disordered crystal be equilibrated at its specific room-temperature Curie point (T_C), which is strongly sample dependent. In one given sample, we use dynamic cross-over caused by non-monotonic thermal trajectories to change and program the critical equilibration temperature for which the scale-free response is activated [2]. For compositionally different samples, cross-over is implemented to make two crystals, which have notably different responses at equilibrium ($\Delta T_C \approx 4°C$), have the same scale-free response at the same equilibration temperature [3]. Our results turn scale-free-optics from a sample-dependent effect to a programmable optical response, an example of how disorder can be used to design a material with a desired characteristic.

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#360 - Temperature dependence of photorefractivity in iron doped lithium niobate and its polaron - based interpretation

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Light - induced charge transport phenomena are a subject of major interest in such a technologically important optical material as lithium niobate is. The microscopic interpretation of these phenomena relies essentially on two descriptions. The best known one is based on a band transport picture, similar to the one used in semiconductor physics. The other one, more recent, is based on the concept of polaronic charge carriers, i.e. electrons or holes self localized at a given site thanks to a dynamic deformation of the surrounding crystal lattice. This description appears to be more physical and several authors are nowadays addressing to it. In any case a satisfactory description of this scenario is still missing, partly because of the lack of precise experimental data on the subject. A consequence of light induced charge transport is photorefractive effect, i.e. a semi permanent modulation of the crystal refractive index caused by inhomogenous illumination. This effect is caused by a light induced charge redistribution giving rise to strong local fields, which alter the refractive index via electro optic effect. Photorefractivity is therefore one of the best ways to study light induced charge transport in lithium niobate.

In this work we develop the original approach of studying the temperature dependence of the photorefractive effect as a way to obtain fundamental information on the microscopic processes responsible for charge transport in lithium niobate. We present here an experimental analysis carried out in the range between 100°K and 450°K. The results are interpreted considering a thermally activated polaron hopping conduction.

#361 - Optical waveguides fabrication in single-crystal diamond using focused ion microbeams

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In this study, we use for the first time direct ion-beam writing to create buried light waveguides in single crystal diamond [1]. Linear waveguides are fabricated using 3 MeV H+ implantations with a scanning ion beam microprobe, thus increasing the refractive index in buried layers or micro-channels in a controlled manner and allowing wave guiding beneath the surface. Waveguide characterization is performed by means of direct laser coupling. A phase-contrast microscopy technique is also adopted: the interference between guided modes and the un-guided light makes it possible to extract, in the phase domain, information about the field amplitudes of the modes which propagate in the waveguides. The experimental data are also compared with the results of Finite Element Model (FEM) simulations. Experimental and numerical results illustrate the wave guiding properties of the fabricated structures.

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#362 - Direct measurement of competing quantum effects in the melting of heavy water

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Even at room temperature, quantum mechanics plays a major role in determining the quantitative behaviour of light nuclei, changing signicantly the values of physical properties such as the heat capacity. However, other observables appear to be only weakly affected by nuclear quantum effects (NQEs): for instance, the melting temperatures of light and heavy water differ by less than 4 K.

Recent theoretical work has attributed this to a competition between intra and inter molecular NQEs, which can be separated by computing the anisotropy of the quantum kinetic energy tensor.

The principal values of this tensor change in opposite directions when ice melts, leading to a very small net quantum mechanical effect on the melting point. This work reports the direct experimental observation of this phenomenon, achieved by measuring the deuterium momentum distributions n(p) in heavy water and ice using Deep Inelastic Neutron Scattering (DINS). Results from the experiments, supplemented by a theoretical analysis, show that the anisotropy of the quantum kinetic energy tensor can also be captured for heavier atoms such as oxygen.

#363 - In situ powder neutron diffraction of microwave-induced reaction of TiCon D20 beam line at ILL

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Microwave (MW) assisted processing are essentially different from conventional thermal processing: in the latter, energy is transferred to the material through convection, conduction and radiation of heat from the surface of the material inward, while MW energy is delivered directly to materials through molecular interaction with the electromagnetic field [1]. Further, MW heating is the transfer of electromagnetic energy to thermal energy: it is energy conversion, rather than heat transfer.

This gives many advantages when using MWs for processing materials: rapid/volumetric heating and better quality of products; selective heating of materials and new materials production; economically viable and ecology friendly processes [2].

In this talk we will present results on the synthesis of MW-induced titanium carbide (TiC) from elemental powders.

The reaction took place in a single mode MW cavity entirely developed in house and the formation of TiC has been observed, for the first time, by means of *in situ* powder neutron diffraction on D20 beam line, at ILL.

We found that MW heating promotes the formation of this compound in seconds, thus significantly reducing power consumption with respect to conventional heating. Temperature measurement, intermediates formation, sequential refinement strategy, together with sample environment implementation will be discussed.

Further MW applications to other compounds will be briefly showed.

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#364 - Electrostatic self-assembly investigated by time resolved SANS

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Self-assembly is an effective method to produce complex macromolecular structures that can respond to external triggers. Recently we have introduced an electrostatic self-assembly approach for the formation of well-defined and responsive supramolecular nano-objects in aqueous solutions. Building blocks are polyelectrolytes and multivalent organic counterions: depending on building block architecture, aggregates with varying shapes, such as spheres, cylinders, vesicles and networks, can be formed [1]. In this framework, pH-responsive systems, in which pH changes can be used to reversibly switch between nano-assemblies and building blocks, have been built [2,3,4]. Furthermore, it has been shown that light, a noninvasive stimulus, can offer the possibility for new functional nanostructures, in particular by triggering the size of electrostatic self-assembled supramolecular particles [5,6].

It is clear that detailed structural characterizations by different techniques as SANS, SAXS, static and dynamic light scattering, AFM, UV-VIS spectroscopy, as well as thermodynamic studies, are necessary to assess driving forces and structural control in the self-assembly process and to derive particle size, shape and distribution [7].

In order to study the self-assembly process directly on the beam, we have recently developed a new SANS cell (now installed on D11 instrument at ILL) that allow us to mix solutions containing the different molecular building blocks in a very fast, uniform and reproducible manner. Several time-resolved experiments have been performed and the different mixing modalities exploited. The systems analyzed are nano-particels made of PAMAM dendrimers generation 4 and organic divalent dyes such as Ar26. This system is pH switchableas the dendrimer charge is pH dependent: HCl was added using the mixing cell. It is then possible to follow the growth mechanism that is induced when charging the dendrimer initiates electrostatic assembly formation. First results have shown a different structure depending on the pH of the solution.

Indeed, going deeply inside the self-assembly process dynamic is of foundamental importance to understand the growth process and to help the design of new nanoparticles.

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#365 - Peculiar and normal dynamics of hydrogen-bond liquids: a neutron scattering and simulation study of methanol

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Methanol is a hydrogen-bond liquid of fundamental importance in pure and applied physics and chemistry, particularly in mixtures with water, and innumerable papers deal with its properties. Yet, the fundamental aspects of microscopic dynamics, even in pure methanol, have not been clearly elucidated so far. The study of the collective dynamics is hindered by the weakness of the acoustic excitations, which has led to the erroneous conclusion that sound modes propagate only in a surprisingly narrow range of small wave vector values. New, accurate, molecular dynamics simulations joint to neutron Brillouin scattering measurements reveal, however, a different situation, reported in this paper. We have determined energy and damping of the acoustic modes in the whole range between the hydrodynamic regime, where the fluid can be viewed as a continuum, and the regime where the excitation wavelength decreases down to the order of intermolecular distances. Methanol is shown, for the first time, to feature the "normal" viscoelastic behaviour characterizing the dynamics of a large variety of liquids, including the arrest of sound mode propagation in the vicinity of the peak of the static structure factor. In addition to this first result, however, the presence of a second excitation with lower frequency, smaller damping and negligible dispersion is displayed. The translational intermolecular dynamics emerging from this study classifies methanol as a fluid having properties similar to those of water, where the presence of a double excitation is a long standing result although its interpretation has remained controversial for long time. However, this study provides a further quite remarkable result, namely the fact that the low-frequency mode seems to be present in the single-molecule dynamics as well. This opens a wide space to further research work, in two directions: one is a better understanding of the effect of hydrogen bonds in the microscopic molecular motions; the other is the problem of the presence of inelastic components, i.e. of characteristic frequencies, in single-particle fluids dynamics.

#366 - High time resolution neutron reflectometry for understanding atmospheric chemical reactions

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Aerosols attract more and more the attention of the scientific community, because their impact on the Earth's radiative balance and on cloud formation is still largely unknown. A key feature for aerosol behaviour is the presence of organic material both in the bulk and at the surface. The understanding of the ageing of organic films on atmospheric aerosols is still incomplete. We present a surface study of the oxidation kinetics of pure and mixed films of oleic acid (OA) and stearic acid (SA) by nitrogen oxides. While bulk studies suggest that OA is more reactive than SA due to the presence of unsaturation, its surface reaction scheme and related kinetic parameters to feed into atmospheric models are missing. Films at the air-water interface of a Langmuir trough, contained in a new miniaturised reaction chamber were exposed to the oxidant and the material loss at the surface during the reaction is followed by neutron reflectometry (NR). The FIGARO instrument optimisation for low-Q data acquisition results in a time resolution as high as 1 s. The reaction chamber has been developed and tested at ILL, it is suitable both for NR and for ellipsometry, giving the possibility to obtain complementary information on the same system.

The oxidants were produced *in-situ* by a well established procedure. A range of concentrations have been accessible by tuning the conditions of the reaction between O_3 and NO_2. We measured the concentrations off-line trough UV-Vis and FTIR spectroscopy and we optimised the reaction conditions to obtain reproducible values. The thermodynamic behaviour of the organic films were previously investigated by isotherms and Brewster angle microscopy. A lifetime of the OA surface layer was shown to be at least two orders of magnitude shorter than that of the SA surface layer. The rate coefficients are used to refine the surface reaction schemes involved. We also found that 10 % surface coverage remained even at long reaction times for OA. Oxidation of recompressed films is discussed to determine the nature of the residual material (products vs reoriented reactant). Lastly, the oxidation by nitrogen oxides of mixed OA/SA films has been studied for the first time to measure the relative reaction rates of the components in more realistic model systems.

So far, we used completely deuterated molecules to gain information on the rate coefficient, in the future we intend to selectively deuterate the molecules in order to study the mechanism of the surface reaction.

#367 - Optofluidic chips fabricated by femtosecond laser micromachining

Roberto Osellame (I) – CNR - Istituto di Fotonica e Nanotecnologie, Milano

A lab-on-chip (LOC) is a device that squeezes onto a single glass substrate the functionalities of a biological laboratory. They are becoming the most powerful tools of analytical chemistry with a broad application in life sciences, biotechnology and drug development. The next technological challenge of LOCs is direct on-chip integration of photonic functionalities for sensing of biomolecules flowing in the microchannels. Femtosecond lasers are powerful tools for volume microstructuring of transparent materials. Optical waveguide circuits can be directly written without any photolithographic process and exploiting unique three-dimensional capabilities in defining the circuit layout [1,2]. In addition, femtosecond-laser irradiation of fused silica followed by chemical etching in HF solution allows the manufacturing of directly buried microfluidic channels, due to the enhanced (by up to two orders of magnitude) etching rate of the irradiated material with respect to the pristine one. This opens the possibility of using a single femtosecond laser system for the production of optical circuits and their possible integration with a microfluidic channel network [3]. Femtosecond-laser micromachining is thus particularly suited for the integration of optical waveguides (or more complex photonic devices such as splitters and interferometers) with a microfluidic network [4]. Applications that will be discussed range from novel microfluidic circuits, integration of fluorescent [5] and label-free [6] detection in capillary electrophoresis microchips, as well as fabrication of biochips for single-cell analysis [7].

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#368 - Droplet based microfluidics

Giampaolo Mistura (I) - CNISM e Dipartimento di Fisica e Astronomia G. Galilei, Università di Padova

Digital or droplet-based microfluidics is a rapidly growing interdisciplinary field of research combining soft matter physics, biochemistry and microsystems engineering. It involves the generation and manipulation of discrete droplets in microdevices. This technology produces highly monodisperse droplets in the nanometer to micrometer diameter range, at rates of up to twenty thousand per second. Unlike standard continuous-flow systems, droplet-based microfluidics allows for independent control of each droplet, thus generating microreactors that can be individually transported, mixed, and analyzed.
Here we present the results of extensive experimental and numerical studies where the wetting and dynamic properties of water droplets can be passively regulated by suitable geometric and chemical patterning of the surfaces. Spreading of a drop is determined by the pinning of the contact line to the post edge. Posts of different shape can then induce significant anisotropies in the drops and morphological transitions. Sliding of drops on inclined surfaces exhibits a rich phenomenology (pinning, stick-and-slip, uniform sliding...) that depends on the chemical pattern of the substrate. In addition, we will show preliminary data on the motion of droplets driven by surface vibrations.

#369 - Introducing purely hydrodynamic networking mechanisms in microfluidic systems

Andrea Zanella – Dipartimento di Ingegneria dell'Informazione, Università di Padova

Andrea Zanella, Giampaolo Mistura, Andrea Biral (Università di Padova)

Microfluidic is a multidisciplinary field with practical applications to the design of systems, called Lab-on-a-Chip (LoC), where tiny volumes of fluids are circulated through channels with millimeter size and driven into structures where precise chemical/physical processes take place. One subcategory of microfluidic is droplet-based microfluidic, which disperse discrete volumes of fluids into a continuous stream of another immiscible fluid, which act as droplet carrier. Droplets can then be moved, merged, split, or processed in many other ways by suitably managing the hydrodynamic parameters of the LoC. A very interesting research challenge consists in developing basic microfluidic structures able to interconnect specialized LoCs by means of a flexible and modular microfluidic network. The aim of this paper is to exploit the properties of droplet-based microfluidics to realize purely hydrodynamic microfluidic elements that provide basic networking functionalities, such as addressing and switching. We define some simple mathematical models that capture the macroscopic behavior of droplets in microfluidic networks and use such models to design and analyze a simple microfluidic network system with bus topology. Experimental tests to validate mathematical and simulation results are ongoing.

#370 - Femtosecond-laser-fabricated microfluidic chip for thermophoresis separation

Francesca Bragheri – CNR - Istituto di Fotonica e Nanotecnologie e Dipartimento di Fisica, Politecnico di Milano

Tommaso Zandrini, Roberto Osellame (CNR – IFN, Dipartimento di Fisica, Politecnico di Milano) Eleonora Secchi, Matteo Contino, Matteo D. Alaimo, Stefano Buzzaccaro, Roberto Piazza (Dipartimento di Chimica, Materiali e Ingegneria Chimica, Politecnico di Milano)

The development of efficient microfluidic separation methods requires the design of novel and flexible approaches. A key figure of merit to assess the performance of a specific separation device is its selectively. To this aim, usual methods such as electrophoresis or

dielectrophoresis are not suitable to discriminate between solutes which, although functionally distinct, are similar in terms of size and charge. Selectivity could be better achieved by exploiting effects whose underlying physical mechanisms depend on specific particle/solvent interactions [1]. One of the most promising phenomena able to meet this goal is thermophoresis, which refers to particles transport driven by thermal gradients. Recently proof of concept chips made by PDMS proved to be effective in selectively separate colloidal particles using thermal gradients, anyway the temperature drop across the PDMS layers limits the achievable thermal gradient [2]. In this work we propose a new microfluidic device fabricated in fused silica by femtosecond laser micromachining followed by chemical etching (FLICE) [3]. The application of this fabrication technique to thermophoresis allows reducing the distance between adjacent microchannels and obtaining higher thermal gradients thanks to the use of fused silica as substrate. In addition the FLICE approach, although it produces channels that are presently limited in length to a few millimeters, has some distinct advantages: by using the laser beam as a pen it allows the creation of directly buried channels which do not require sealing with a cover glass and straightforward fabrication of channels with different cross sections and 3D geometries. Critical aspects of the application of this technique to thermophoretic separation, such as the roughness of the microchannel walls and the uniformity of the cross section along the whole length of the channel, have been tackled.
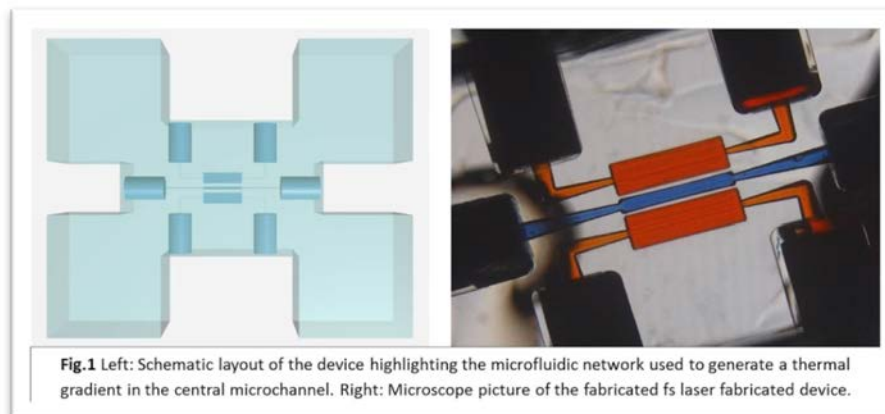
Fig.1 Left: Schematic layout of the device highlighting the microfluidic network used to generate a thermal gradient in the central microchannel. Right: Microscope picture of the fabricated fs laser fabricated device.

Figure 1 shows the schematic layout (left) and a microscope picture (right) of one of the fabricated microfluidic devices. Thermal characterization of the chips and preliminary fractionation results in fs laser fabricated devices will be shown.

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#371 - Optical manipulation of charged microparticles in polar fluids

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Giuseppe Pesce, Giulia Rusciano (Dipartimento di Fisica Università degli Studi di Napoli, Complesso Universitario Monte S. Angelo)

We report on a systematic study of the response of a charged micro-particle confined in an optical trap and driven by electric fields. The particle is embedded in a polar fluid, hence, the role of ions and counter-ions forming a double layer around the electrodes and the particle surface itself has been taken into account.

We analyse two different cases: i) electrodes energised by a step-wise voltage (DC mode) and ii) electrodes driven by a sinusoidal voltage (AC mode).

The experimental outcomes are analysed in terms of a model which combines the electric response of the electrolytic cell and the motion of the trapped particle. In particular, for the DC mode we analyse the transient particle motion and correlate it with the electric current flowing in the cell. For the AC mode the stochastic and deterministic motion of the trapped particle is analysed either in the frequency domain (Power Spectral Density, PSD) or in the time domain (Auto Correlation Function, ACF).

Moreover, we will show how these different approaches (DC and AC modes) allow us, assuming predictable the applied electric field (here generated by plane parallel electrodes), to provide accurate estimation (3 %) of the net charge carried by the micro-particle. Viceversa, we also demonstrate how, once pre-determined the charge, the trapped particle acts as a sensitive probe to reveal locally electric fields generated by arbitrary electrode geometries (in this work wire-tip geometry).

#372 - Sliding droplets on chemically heterogeneous surfaces: a lattice Boltzmann study

Mauro Sbragaglia – Università degli Studi di Roma "Tor Vergata", Roma

Matteo Pierno, Silvia Varagnolo, G. Paolo Mistura, D. Ferraro, P. Fantinel (Università di Padova), G. Amati, L. Biferale (Università degli Studi di Roma "Tor Vergata", Roma)

Mesoscopic Lattice Boltzmann Numerical simulations are used to investigate the principles underlying some experimental observations for the motion of small viscous droplets sliding on flat surfaces decorated with a periodic pattern of strips alternating hydrophobic and hydrophilic areas. Depending on the surface properties and control parameters, a jerkily motion featuring an evident stick-slip dynamics is observed. This is possible because of the pinning-depinning transition of the contact line at the wetting defects,

which causes additional energy to be stored in the non-equilibrium configuration of the droplet and viscous dissipation to be localized in time.

#373 - Tunable microfluidic dye laser : coupling high quality factor microcavities with liquid crystals orientational properties

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The development of simple and low cost miniaturized fabrication methods has been very important for the advancement of microfluidics technology. Although planar micro-fabrication approach based on photolithography is well established and is suitable for surface micro-fabrication, multilayer and multistep processes including stacking and bonding substrates are required to form true three-dimensional (3D) microstructures.

An innovative, simple and maskless technique is the femtosecond laser micromachining, which allows a 3D fast prototyping thanks to its inherent ability to fabricate buried microstructures. Taking advantage from ultrashort-pulse laser, it is possible to realize surface (ablation) or internal (nanocracks) modification of the transparent materials or a high localized photo-polymerization of sensitive polymeric materials, in the focus of the laser beam. Since both the microfluidic channels and waveguides in glass can be fabricated by the same tool on the same substrate, it is easy to create monolithic optofluidic chips which are free of misalignment or vibrations during operation. After the volume laser irradiation, the optofluidic circuit is obtained by chemical etching removing the laser modified areas.

Here, we report an investigation on novel optofluidic microlasers with the goal of exploiting liquid crystal orientational properties for laser tuning. DBR (distributed Bragg reflector) lasers has been fabricated by combining the direct pulse laser writing with the holographic litography methods to realize high quality factor microcavities within microfluidic chips. In order to obtain cavities working on the first order of diffraction of Bragg gratings in the visible range, high spatial resolution (> 6000 lines/mm) holographic lithography has been required. Two Bragg reflectors have been recorded close to the dye recirculation microchannel in which are located two empty "basins" previously filled with the photopolymerizable mixture through a microfluidic circuit. An integrated broad band fibers optic completes the microcircuit design in order to monitor the Bragg reflection efficiency and outcouple the light emitted.

Two different configurations have been investigated in order to get tuning driven by liquid crystal orientational properties. In the first one, liquid crystal is mixed with the dye active material using liquid crystal reorientation by external fields. In the second one, liquid crystal is used in a second channel or in the Bragg gratings realized by composite materials.

#374 - Assembly and manipulation of nanophotonic elements in a fluid: towards reconfigurable photonic structures on a chip

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Madhavi Krishnan (Department of Physical Chemistry - Universität Zürich (UZH))

The ability to trap an object—whether a single atom or a macroscopic entity—is of fundamental importance in a wide range of fields e.g., quantum optics, soft condensed-matter physics, biophysics and clinical medicine. A number of sophisticated methodologies have been developed to overcome the randomizing effect of Brownian motion on an object in solution, however stable trapping of nanometer-sized objects remains challenging. Optical tweezers are widely used traps [1,2] but the relatively high incident laser power needed can cause substantial local heating and limit the parallelization of the process. We recently showed that a fluidic slit with appropriately tailored topography is able to electrostatically trap and levitate nanometer-size charged objects in solution without external intervention, and independently of the particle mass and dielectric function. The stiffness and stability of such an electrostatic trap can be easily tuned by adjusting the system geometry and the solution ionic strength [3]. Here we show that tailoring the 3D morphology of the trap allows single metallic nanorods trapping and permits their orientation in parallel and in high density arrays. The angular trapping stiffness of individual nanorods was measured exploiting the scattered light intensity (iSCAT). In particular, by carefully quantifying the optical scattering contrast of each single particle, we could determine that while rods trapped in circular traps hardly show any optical anisotropy, rods trapped in a cigar-shape traps strongly scatter only linearly polarized light that is parallel to the trap long axis. The angular orientation of each single rod has been deduced by the collected scattering light contrast. Taking into account the angular offset owing to noise in the measurement, we observed strong anisotropy in rod orientation thus demonstrating the achievement of highly directional angular trapping [4]. Importantly, the principle we describe can be easily extended to nano-objects of arbitrary shape. Further, we show that external fields, e.g. optical or electrical fields, may be coupled to the trap to toggle the state of individual nanophotonic elements, raising new prospects for reconfigurable photonic devices and optomechanical manipulation at the nanoscale.

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#375 - Oxide Nanowires for opto-electronics and energy harvesting

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Recent achievements at SENSOR Lab in preparation of Metal Oxide Nanostructures for opto-electronics and energy harvesting will be reviewed. Oxides represent the most diverse class of materials, with properties covering almost all aspects of material science and physics in areas including oxide electronics, superconductivity, ferroelectricity, magnetism, and more:
• Metal oxide Nanowires NWs and TiO_2 nanotubes (NTs) as n- and p-type semiconductor chemical sensors for artificial olfaction: quasi one-dimensional metal oxide nanostructures have several advantages with respect to their traditional thin- and thick film counterpart.
• ZnO NWs on p-GaN for Light Emission. ZnO has recently gathered great interest for lighting applications due to its wide bandgap (3.37eV) and large room temperature exciton binding energy (60 meV). ZnO NWs-based light emitting diodes (LEDs) have been recently proposed as promising candidates for the next generation of blue/near-UV light sources. Vertically aligned ZnO NWs are grown on p-GaN thin film on sapphire and their photoluminescence, electroluminescence and preliminary electrical characterization are presented for the as-fabricated LED structures.
• Metal oxides for energy harvesting:
o ZnO NWs, TiO_2 NTs, hybrid and hierarchical MOX networks, MOX nanoparticles as host for carbon-based nanostructures provide functional scaffolds for fabrication of photoanodes to be applied in third generation photovoltaics. A careful engineering of MOX structures enables the assembly of high performance devices. An overview of the application of wide band gap semiconductor MOX nanostructures for dye- and quantum-dot sensitized solar cells will be presented, together with the full analysis of devices functional performances.
o Thermoelectical properties of ZnO(n) and CuO(p) NWs for micropower generation: ZnO(n) and CuO(p) NWs have been investigated with the aim to build thermoelectric devices based on NW arrays for energy harvesting and potential use in low-power portable electronics and sensor systems.

#376 - Fully integrated all-solid-state electrochemical sensors on micromachined platforms: a new type of gas sensors

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A new fabrication route for producing fully integrated cross plane potentiometric micro sensors based on a thin ion conducting membrane are presented as relevant alternative to the actual huge market ceramic devices like lambda sensors or all-solid-state electrochemical devices for oxidizing gases detection such as CO_2, NO, NO_2 or SO_2 or for reducing gases such as CO, H_2 or hydrocarbons. It is based on the properties due to the nanoionic characteristics in very thin solid electrolytes.
The proposed procedure successes in combine silicon industrial micro fabrication processes with the use of nanometric thin films of Ytria Stabilized Zirconia (YSZ) as solid electrolyte for manufacturing novel silicon based electrochemistry sensors. An all-solid-state electro chemical cell is usually constructed by combining a membrane of solid electrolyte (ionic conductor) with a pair of electrodes (electronic conductor). For the past three decades, various electrochemical gas sensors have been developed or proposed. Those sensors are classified into potentiometric and amperometric sensors, and the former group is further divided into equilibrium- and mixed-potential types. All of them constitute nowadays the broader market of gas sensors and, hence, these gas sensors have been explored extensively by using conventional as well as unconventional solid electrolytes. Here, taking benefits of the ionic conduction in electrolyte films at the nano level, we report on a new generation of fully integrated solid state electrochemical gas sensors. The main highlight of this cross plane configuration is related to the enormous reduction of the electrolyte thickness. YSZ membranes of 200 nm are used, leading to a drastic drop of the working temperature and thermal mass of the active area of the device. This new paradigm opens the way for the fabrication of reliable, low cost, low consumption and rapid electrochemistry gas sensors. A detailed discussion will be reported on fully integrated lambda sensors based on a Nernst behavior. It was introduced in sixteen's using bulky zirconia devices and applied to cars. However, due to its cost, it is much less used for many other combustion control applications as, for example, domestic boilers. Now, with this novel approach many other applications become open defining a huge potential market requesting high reliabilities but with much less expensive costs.

#377 - Large frame ring laser gyroscopes

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Large frame ring laser gyroscopes provide precise measurements of local frame rotations induced by earthquakes, tides, local tilts of the terrestrial crust and even by the wobbling of the axis of the planet [1]. A ground based experiment aimed at measuring the Lense-Thirring effect with an array of laser gyroscopes has been recently proposed [2]. The project foresees the construction of a tri-axial gyroscope for the measurement of the Earth's rotation vector with a precision better than 10^{-9}. This goal requires a strict control of

all the systematics connected to the to the nonlinear dynamics and to the geometrical scale factor of the laser cavity.

We present the results of comprehensive experimental tests of the Lamb's semiclassical theory of ring lasers obtained by operating the "G-Pisa" gyroscope with the laser plane oriented almost perpendicularly to the local North direction. In this configuration, the Earth's rotation contribution to the Sagnac frequency is less sensitive to the orientation error, and a more precise estimate of the systematics coming from the laser dynamics can be achieved. Cavity losses and the corresponding dissipative Lamb parameters are monitored by observing the single beams intensity modulation at the Sagnac frequency while the gain parameters are identified by a dedicated spectroscopic analysis of the plasma dispersion function. The adopted methods and the improvements of the ultimate performances of the G-Pisa apparatus, obtained with the application of a Kalman filter algorithm, will be detailed.

We will also describe a dedicated apparatus, presently under construction, for the complete control of the geometrical scale factor of the ring laser. The experimental setup, named GP2, consists in a ring laser with a side length of 1.65 m equipped with a tridimensional control system of the mirrors positions. It is foreseen a diagnostic system dedicated to the stabilization of the absolute length of the two cavity diagonals forming two crossed Fabry-Pérot resonators. The experimental results concerning the stabilization of two identical linear cavities to a He-Ne-I2 frequency standard will be presented together with the simulation of the automated system for the control of all the geometrical parameters of the ring resonator.

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#378 - Luminescence chemical sensitivity of surface InP quantum dots

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We investigated the photoluminescence (PL) sensitivity of epitaxial surface InP quantum dots (QDs) grown on In0.48Ga0.52P buffer layer lattice matched to GaAs substrate towards methanol vapours. Such QDs show a broad-band near-infrared emission ranging from 750 to 865 nm dependent on their dimensions. Quantum dot exposure to solvent vapours determines an intensity enhancement while peak energy and band shape of the luminescence are not affected by the solvent vapours. The effect depends on solvent concentration and it is always fully reversible. The PL relative change and the concentration are linear in a limited range (up to about 20000 ppm). It was found that for molecules presenting a strong permanent dipole moment like methanol and ethanol a high PL enhancement has been observed, while the effect of less polar solvents like acetone and chloroform is quite low. Interestingly we demonstrated that the system response can be correlated (with linear law) with the effective surface area of the QDs, as estimated by a statistical analysis of the atomic force micrograph images of our samples. The results indicate that the phenomenon involved in the InP QD sensitivity is a genuine surface phenomena. A possible explanation can be the capability of polar adsorbates to saturate non-radiative surface defect states. Such results are promising for the development of integrated miniaturized optical chemical sensors and lab-on-chip devices which can be easily fabricated by well-established III-V semiconductor technology.

#379 - Analyte discrimination in Langmuir - Blodgett porphyrin films

Claudio Goletti - Università degli Studi di Roma "Tor Vergata"

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We have studied the controlled adsorption of volatile molecules on porphyrin Langmuir−Blodgett films deposited onto the surface of a glass substrate at increasing thickness (2, 4, 6, 8 monolayers). The modification of the film optical anisotropy has been measured in real time by optical spectroscopy, namely reflectance anisotropy spectroscopy (RAS), during the exposure of the sample to controlled mixtures of two or three different gaseous analytes. The modification of the experimental RAS line shape with respect to the signal measured before exposure is the sum of the variations produced by single analytes. This shows that the qualitative and quantitative identification of gases and vapors in gas sensing experiments is possible. Listing in a library the responses of the sensing layer to single analytes, the deconvolution of the components of the mixtures is possible, exploiting the excellent sensitivity of RAS for a new kind of optical gas sensor.

#380 - A case study of the optimization of a nanoporous material for sensing applications

Paolo Bettotti – Laboratorio di Nanoscienze, Dipartimento di Fisica, Università di Trento

Nanoporous materials are actively investigated because of their possible application on a wide range of technologies spanning filtering, sensing and catalysis, to cite a few.

Good control over their nanostructure is a formidable task and it is of fundamental importance to tailor and control their properties. Porous Silicon is a nanostructured material known since several decades. Still it is actively investigated because of the high tunability of its optical, electrical, thermal and mechanical properties.

The fine details of the porous structure largely determine the final properties of the device. Thus fabrication processes that permit to pre-determine the details of the samples are required to obtain high quality and reproducible devices.

During the presentation I will show three aspects of the use of nanoporous materials for sensing and analytical applications:

- In recent experimental results we obtain high sensitivity optical sensors based on a polarimetric approach. Using simple free

standing porous membranes refractive index sensibility of about 10^-6 was achieved. I will show to which extent the details of the structure determine the final sensitivity.

- The role of the mass transport in free standing nanoporous materials will be discussed as regards to the nonspecific signal. This is a somewhat underestimated issue as many papers exploit nanopores to capture analytes but most often they do not discuss the role of the aspecific signal that comes from a poor washing (removal) of both unwanted and unbound molecular species. Porous Silicon permits to fabricate both supported and free standing samples with exactly the same structure. Because the latter enables flow through experiments a comparison among the two types of samples can be made. From this comparison we can precisely determine the "real" sensitivity of the porous sensor.

- Finally I will describe the activities envisioned within a recently funded FIRB project that aims to develop an analytical platform to study dynamics and reactivity of DNA molecules in confined volumes.

#381 - Refractive index and temperature characterization of a hybrid optical fiber LPG-FBG configuration

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Grating based sensors (long period gratings and Bragg gratings) have been intensively studied for various physical and chemical sensing applications, such as strain, temperature and refractive index, due to their high resolution and sensitivity, fast response, compactness, low costs. Although sensors based on fiber Bragg grating (FBG) and long period grating (LPG) configurations are both sensitive to different parameters, such as temperature and refractive index, the optical sensing principles are based on different mode – coupling mechanism: in the former the light coupling takes place between the forward and the counter propagating core modes; in the latter between the fundamental core mode and a discrete set of forward propagating cladding modes that make the LPG sensitive both to the external refractive index (RI) and temperature.

One of the major drawbacks associated with the grating based sensors is the inability to distinguish wavelength shifts produced by the cross sensitivity between RI and temperature.

In this work a hybrid configuration based on a cascade of a single LPG and a single FBG was proposed as a sensor in order to discriminate, simultaneously, the RI and temperature of different aqueous solutions.

The FBG was designed to be both spectrally located on one edge of the LPG and physically positioned behind the same LPG. In order to obtain a probe, the optical fiber was also cut after the fiber Bragg gratings.

In this way the FBG reflected amplitude change depends on the variation of the LPG transmission spectrum with both the surrounding refractive index and temperature modification, while the reflected wavelength shift is only due to the changing of the aqueous solution temperature.

The RI value was so obtained by measuring the variation of the optical power reflected and subtracting the contribution of the wavelength shift due to the temperature variation.

The results showed that the proposed configuration can be used for simultaneous measurement of temperature (from 21°C to 28°C) and the surrounding refractive index over a range of 1.33 to 1.40 RIU.

#382 - Thick film technology for chemical sensors

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In the last decades, big effort has been put to develop higher performance sensing units, fostered by the need for modern societies to monitor gases, i.e., pollutants, malodours, dangerous leaks. With this aim, chemoresistive sensors grabbed the attention of researchers and investors with respect to other techniques because sensors can be fabricated cheaply and are very compact and low-power consuming. In spite of these positive features, there are drawbacks that can be summarized by the so-called "3S-rule", i.e., sensitivity, selectivity, stability, a sort of mandatory direction toward which research must be addressed. We will focus here on one of the main techniques for preparation of chemoresistive sensors, that is thick-film. Thick-film deposition normally relies on screen-printing, which is one of the oldest forms of graphic art reproduction known to mankind. A typical thick-film screen consists of a finely woven mesh of stainless steel, polyester, or nylon, mounted under tension on a metal loom. The thick-film paste is transferred on the top surface of the stencil, and a squeegee traverses the screen under pressure. Normally the pastes contain organic solvents that are needed to achieve the correct viscosity and glass frit. The organic compounds are sacrificial ingredients that completely disappear during the thermal processes (drying at about 150-200°C) carried out onto the films. Then, further annealing is needed, called firing, during which the glass melts, the powders sinter and the film becomes a solid composite material. The function of glass is for binding the film to the substrate and to keep the particles together. Firing is performed in a furnace at a temperature ranging typically within 500-900°C through proper ramping of the temperature, after which the film becomes firmly attached to the substrate. In the case of films for gas sensing, the firing serves also for structural and morphological stabilization and to determine grain size and other film properties. Through screen printing technique, the sensing film, interdigitated contact and heater element are deposited on the same substrate (alumina or silicon micro hotplate). The deposited layer depends on specific parameters, such as dimension of the particles in the functional phase, screen mesh number, tension on the wires constituting the screen, hardness and speed of the rubber blade, distance between the screen and the substrate (snap-off).

#383 - THz quantum cascade laser quartz enhanced photo-acoustic sensor

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Quantum cascade Laser based THz-sensing involving molecular fundamental rotation transition absorption is an emerging technology that would allow sensitive detection of trace gas for a variety of applications such as environmental air quality monitoring, medical diagnostics, homeland security, quality and process controls. However, the need of the use of low-noise cryogenic bolometers (spectral dependent, expensive and bulky) limits its application. Quartz-enhanced photo-acoustic spectroscopy (QEPAS) technique uses a commercially available mm sized piezoelectric quartz tuning fork (QTF) as a resonant acoustic wave transducer and exhibits the following advantages: immune to environmental acoustic noise, operation at room temperature, capable of analyzing trace gas samples of ~1 mm^3 in volume, large dynamic range (~10 orders of magnitude of the acoustic signal). In particular, photoacoustic spectroscopic detection scheme dispenses with wavelength dependent photo detector, it is thus applicable to any spectral region where suitable excitation source is available. This feature is especially attractive for gas sensing in the THz electromagnetic spectral region where cryogenic cooling is still required for high-performance optical detectors.

We report here on the development of a QEPAS sensor employing a 3.93 THz QCL and custom-made QTF [1]. Standard photolithographic technique was used to etch the custom QTF, starting from z-cut quartz wafer. Chromium/gold contacts have been deposited on both the QTF sides. The overall QTF dimension was 3.3 cm x 0.4 cm x 0.8 cm; each prong was 2.0 cm long and 2.5 mm wide. The gap between the prongs was ~1 mm. The QTF first flexion resonance falls at f_0 ~ 4246 Hz and atmospheric pressure we measured a Q factor of 9930. For our QEPAS THz sensor demonstration we selected methanol as target gas molecule and we focus on its rotational absorption line falling at 131.054 cm^{-1}, with line-strength $S=4.28 \times 10^{-21}$ cm. QEPAS spectral measurements were performed by slowly scanning the laser wavelength while applying a sinusoidal modulation to the QCL current at the QTF resonance frequency f_0, and detecting the QTF response at the same frequency using a lock-in amplifier. Stepwise concentration measurements were performed to verify the linearity of the QEPAS signal as a function of the methanol concentration. For these measurements the system was operated in the locked mode, i.e., with the QCL frequency set to the center of the selected methanol absorption line. An Allan variance analysis allows us to determine the best achievable sensitivity of the QEPAS sensor. The calculated normalized noise equivalent absorption coefficient NNEA is 2×10^{-10} $cm^{-1}W/Hz^{1/2}$ (1σ), comparable with the best result obtained with mid-infrared QCLs [2] .

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#384 - Interferometric TEM characterization and theoretical investigation of the structural and electronic properties of graphene membrane

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The nowadays capabilities of modern low-voltage aberration-corrected Transmission Transmission Electron Microscopes (TEMs) and Scanning Transmission Electron Microscopes (STEMs), in terms resolution of the imaging techniques and of the associated spectroscopy techniques, allow for the investigation of a wide range of properties in graphene-based materials, with atomic sensitivity and resolution. Among these investigations, we can find the morphological aspects (shape, dimensions, thickness), as well as the structural ones (crystalline habits, edges, defects, strain), and the physical and chemical properties (doping, functionalization) of the systems under analysis, [1-5], making these instruments, and related techniques, as mandatory tools for the investigation of graphene-based materials.

In this contribution we will report an overview of the capabilities of the modern TEM-based techniques in retrieving information on the structure of graphene [6] and graphene-based materials [7], with particular focus on the so-called *interferometric techniques* (e.g. Geometric Phase Analysis and Electron Holography) capable to map in-plane and out-of-plane deformations and displacement fields [8] as well as electric and magnetic fields in the graphene membranes [9].

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#385 - A new approach for elaborating and designing plasmonic substrates for spectroscopy enhancement and high contrast imaging

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The limitation for fabricating molecular plasmonic substrates is due to the drastic requirement of controlling, on large areas in a reproducible way, a well-defined spacing between metallic nanostructures and molecules: their mutual interaction is indeed governed by the local topography of the electromagnetic field. A strategy to design and fabricate hybrid metallic-dielectric substrates for optical spectroscopy and imaging is proposed, based on an original technique, low energy ion implantation beam synthesis (LE-IBS) for the wafer-scale fabrication of Ag nanocrystals (Ag-NCs) planar arrays embedded in silica and silicon nitride layers on a silicon substrate. By coupling this technique to micro fabricated stencils used as templates, we precisely control the size, density, and location of silver nanoparticles embedded in dielectrics (silica or silicon nitride) thin films on silicon. By coupling ballistic simulations and Transmission Electron Microscopy (TEM) observations we showed that sputtering and diffusion effects are the limiting phenomena for the control of the size, position and volume amount of NCs. Concerning NC stability, we demonstrate that post-annealing process strongly limits silver oxidation, which otherwise excludes the use of Ag NCs on free surfaces. Different architectures consisting of three dimensional patterns of metallic nanoparticles embedded in dielectric layers are hence conceived to simultaneously exploit the optical interference phenomenon in stratified media and localized surface plasmon resonances on metal nanoparticles. These structures are based on a simultaneous control of opto-electronic properties at 3 scales (3S) (~ 2 / 20 / 200 nm) and along 3 directions (3D). Elastic (Rayleigh) and inelastic (Raman) scattering imaging assisted by simulations were used to analyze the optical response of these "3S-3D" patterned layers. The reflectance contrast is strongly enhanced when resonance conditions between the stationary electromagnetic field in the dielectric matrix and the localized plasmon resonance in the silver nanoparticles are realized. These novel kinds of plasmonic-photonic architectures are reproducible and stable, they preserve flat and chemically uniform surfaces, offering opportunities for the development of efficient and reusable substrates for optical spectroscopy enhancement (like SERS) and high contrast imaging.

#386 - Interaction forces at the nanoscale: new insights and new perspectives with the force feedback microscope

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Since its invention the AFM has been increasingly used for studying condensed matter at the nanoscale. The capabilities of the AFMs have been constantly improved both from the instrumental and theoretical point of views [1, 2]. However, despite the many efforts produced, some limits have still to be overcome. Here we address to two historical issues and we show how they can be overcome by a new AFM called Force Feedback Microscope (FFM)[3].

1)On one side, we address the problem of the so-called "jump to contact". The mechanical instability of the AFM probe that occurs when the force gradient exceeds the cantilever stiffness leads to the impossibility to perform "non-contact AFM" especially in liquid media where standard dynamic techniques are not efficient because of the cantilevers low Q-factors. The FFM measures interaction force curves without jump to contact in any environments. This is possible thanks to a feedback loop that keeps constant the distance between the probe and a reference point counteracting any force acting on the tip. As a consequence, both the force acting on the tip and the tip position can be independently measured. We present interaction force curves at the solid/liquid and solid/air interfaces without jump to contact, even in presence of capillary forces [3].

2)In addition we address the problem of measuring the viscoelasticity of soft samples. Elastic and dissipative interactions have been subject of an intense investigation in the last years [1], mainly in the frame of soft condensed matter. The emerging Multifrequency techniques provide viscoelastic properties from the single proteins to the living cells. However, the investigation is limited because intrinsically restricted to the cantilevers eigenmodes, while it has been shown that viscoelasticity can vary of several orders of magnitude over the frequency spectrum [4]. Here we present the imaging capability of the FFM on biomolecules (DNA and proteins) and the spectroscopy capability on PC12 living cells in physiological conditions. In addition, we show how the energy involved in the interaction between the AFM tip and the sample is in the order of magnitude of the thermal energy.

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#387 - Ghost Particle Velocimetry: 3-D flow visualization using standard bright-field microscope

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The increasing complexity of microfluidics chips and their widespread diffusion in academic and company research labs calls for plain, low-cost, and practical methods to quantitatively monitor the fluid flow in these devices. A well established technique is Particle Imaging Velocimetry (PIV), where the fluid is seeded with small particles and a 2D velocity field is obtained by tracking the individual particle motion. Individual tracking, however, requires particles large enough to be optically resolved, which therefore perturb the flow over spatial scales that, in microfluidics, may be comparable to those of the investigated structures. Micro-scale Particle Imaging Velocimetry (μPIV) overcomes this limitation calculating the velocity field by cross-correlating images of small fluorescent tracers that do not need to be individually resolved. However μPIV instrumentation requires a rather expensive optical setup, usually including a pulsed laser source synchronized with a high resolution fast CCD camera [1]. Here, we propose a new technique, which we dub "Ghost Particle Velocimetry "(GPV), exploiting as in μPIV sub-resolution tracers, but with the main advantage of requiring just a standard bright-field microscope with Kohler illumination, with no need for expensive sources and further customization [2]. Besides providing a very good resolution of the transversal (in-plane) flow field, the technique allows for an appreciable resolution along the optical axis, yielding 2D sections of the flow pattern separated by about 20 μm. In addition, it has not strong requirements concerning the optical properties and concentration of the tracers. The method relies on a promising combination of standard microscope imaging with novel ideas that widely extend the potential of a well-established intensity correlation technique, Dynamic Light Scattering (DLS) [3]. As an example of the great potential of GPV, we present measurements of the 3D velocity field in complex microfluidic geometries.
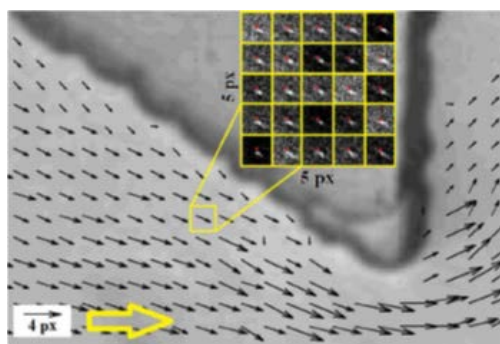
Correlation maps and flow reconstruction around a simple obstacle in a microfluidic channel. The flow direction is shown by a yellow arrow.

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#388 - An electric force microscopy investigation of sub-superficial graphite microchannels in diamond

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The possibility of fabricating sub-superficial graphitic microchannels in diamond offers several promising opportunities in the fields of cellular bio-sensing [1] and particle radiation [2]. In this work we present a study by means of Electrical Force Microscopy (EFM) and of Scanning Kelvin Probe Microscopy (SKPM) of sub superficial graphitic microchannels fabricated in single-crystal diamond with a novel ion beam lithographic technique [3]. The buried (0,5 ; 1 and 1,5 μm from the sample surface) microchannels were fabricated by direct ion writing with a 600 keV He^+ microbeam at the AN2000 accelerator of the INFN Legnaro National Laboratories. Variable-thickness masks were employed to allow the channels endpoints to emerge for surface contacting. Subsequently, the samples were annealed for 1 hour at a temperature of 900 °C, to induce their full graphitization from an amorphized phase. Finally, they were electrocally contacted at their emerging endpoints by thermally-evaporated Cr-Au film. Our study is focused on both the buried channel and on the endpoint where the channel emerges at the diamond surface. The local resistivity of graphite channel was studied performing SPKM in presence of current flow, while trapped and induced charges on the diamond layer above graphite channels were investigated by means of EFM.
The local contact potential of the area where the channel emerge on the surface was studied by means of SPKM. In this way we took high resolution images of the graphite conductive area on the insulating diamond surface.
The results provide useful insight on the charge transport and trapping mechanisms, with significant implications for future fabrication of all-carbon graphite/diamond devices, both in the fields of cellular biosensing and radiation detection.

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#389 - Visualizing electron correlation in molecules using a scanning tunneling microscope: an ab-initio prediction

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Scanning tunnelling spectroscopy (STS) visualizes electron states in both extended systems and nano-objects, such as quantum dots or molecules. Whereas extended quantum states are insensitive to electron number fluctuations, an energy gap opens each time a new electron is injected by the STS tip into a nano-object. This gap originates from the interaction of the next incoming electron with the others already present in the system. Under this Coulomb blockade condition, STS maps the wave function modulus of the electron injected by the tip into the nano-object. The obtained image is routinely interpreted as the atomic-like or molecular [1] orbital of the added electron, that experiences the mean field of the other electrons already populating the system. A fundamental question is whether features of the tunnelling map may appear due to electron-electron correlation beyond mean field [2].
In this work [3] we demonstrate that the STS images of single planar molecules with metal centres predicted by ab initio many-body calculations differ qualitatively from their uncorrelated counterparts. We find in the STS maps resolved at the Fermi energy that correlation alters significantly the spectral weight around the metal atom. This change may be experimentally quantified by contrasting the altered STS images to those of substituted molecules unaffected by correlation that are used as benchmarks.

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#390 - Femtosecond speckle diffraction with coherent electron pulses: dynamics of local order in polycrystalline nanostructures

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We report for the first time the use of ultrafast coherent electron packets with an energy of 30 keV for speckle diffraction, combined with radiofrequency technology [1], to retrieve time-resolved information on the local symmetry of polycrystalline homoligand gold nanoparticles. Hidden local symmetries within disordered systems have recently been classified by means of coherent x-ray scattering intensity correlations around a Debye-Scherrer ring, in the static speckle diffraction pattern of a colloidal glass [2, 3]. We show that a similar approach based on ultrafast electron diffraction can be used to investigate the undisclosed local properties of nanostructured thin films with fs-time resolution, owing to the high cross-section of electrons for interaction with matter and their smaller sample damaging ability [4].

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#391 - WO$_3$ single crystal nanorods from PLD-grown amorphous-like W thin films

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Here we present a new method of synthesis for WO$_3$ single crystal nanorods, which grow at the surface of amorphous-like W thin films, produced by Pulsed Laser Deposition (PLD) [1]. During the PLD process, a large atomic fraction of oxygen (18-72%) can be adsorbed in the film volume, in dependence on growth parameters. After a post-growth annealing step in vacuum at moderate temperatures (around 500°C), WO$_3$ nanorods are formed at the surface, in correspondence to specific values for the average O$_2$ content.

Tungsten oxide WO$_3$ nanorods are promising candidates for a vast range of applications including lithium-ion batteries, catalysts, electrochromic materials and sensors, and can be obtained by several different technological recipes. They grow at the surface of metallic W foils or thin films thermally annealed (700 C-1600 C) either in Ar or in O$_2$ atmosphere [2]; differently, a WO$_3$ source can be directly evaporated onto a hot substrate (800°C) in the presence of NH$_3$ or of a mixture of Ar and H$_2$. Finally, nanorods can be formed by exposing oxidized W films at 900 °C in vacuum or in H$_2$ and methane atmosphere [3].

Yet, the mechanism of formation of WO$_3$ nanorods is not fully understood, since nanorod growth takes place even in the absence of any external catalyst. For tungsten oxidation to end up with the formation of nanorods, a proper combination of oxygen concentration, temperature and duration of the annealing and surface features at the nanoscale must properly match.

We investigated nanorods formation by varying the O$_2$ concentration inside the film and the annealing time and temperature. The stoichiometry and crystallinity of oxide rods has been checked by Raman Spectroscopy. By Scanning Auger Microscopy, a depth profiling of the oxygen concentration in the PLD films and of its evolution induced by thermal annealing is made. In this way, both the role of the annealing in modifying locally the O$_2$ concentration and the specific conditions of film composition at surface, which lead to the nucleation and growth of WO$_3$ rods, are better clarified, in view of a complete mastering of the nanorods growth technique.

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#392 - Does the dynamics of metallic and insulating liquids really differ? A "golden" answer from neutrons and simulations

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The knowledge about the microscopic dynamics of a fluid at equilibrium has, in the years, been increased by neutron or X-rays spectroscopic investigations of liquid metals. Indeed, these are the emblem of "simple fluids", notwithstanding basic differences from rare-gas liquids, such as the existence of an electron gas, the high sound velocity (around and above 2000 m/s, typically), and the greater, sometimes naked-eye, visibility of collective modes in the $S(Q,\omega)$ spectra, even at wave vectors near the position of the maximum in the static structure factor. Experimental evidences that the mentioned visibility of longitudinal acoustic modes is not so peculiar of liquid metals were found only in recent years, when similar features were also observed in insulating liquids and in comparable Q ranges. However, studying monatomic systems like liquid metals remains a main route to the core of collective dynamics in liquids. We present here a recent neutron study of a metal still unknown from the dynamic point of view: liquid gold. Experimental difficulties, mainly related to the high melting temperature and the considerable neutron absorption of gold, turned out to be not critical and allowed a first neutron Brillouin scattering experiment ($0.6 < Q < 1.6$ Å^{-1}) on the BRISP spectrometer at the Institut Laue-Langevin (ILL) in Grenoble. The measurement had golden issues in many respects since it provided clean inelastic spectra rarely gifted by neutron scattering. The quality of the data thus allowed a significant comparison with recent ab initio simulations performed by the ILL Computing for Science group. The agreement found between simulation and experiment justified the further analysis of liquid gold dynamics at the higher Q-values probed by simulations (up to 7 Å^{-1}) and led to conclude that the relevant dynamic features of the system, or of other liquid metals such as cadmium, do not substantially differ from those of insulating liquids, like methane and carbon dioxide. A very different opinion has long been wide-spread in the scientific community.

#393 - Thermodynamic and structural properties of model fluids interacting through microscopic competing interactions

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We present theoretical predictions and simulation results concerning thermodynamic and structural properties of model fluids interacting through competing microscopic interactions, constitued by a short-range attractive well, next to a hard repulsive core, followed by a smooth, long-range repulsive tail. For a suitable choice of potential parameters, the static structure factor S(Q) displays a secondary low-Q peak, also experimentally observed in colloidal suspensions and protein solutions, and explained in terms of the formation of equilibrium clusters in the homogeneous fluid. We show that the threshold temperature for the onset of clustering (for fixed, relatively low, densities) depends weakly on the width of the attractive well and on the height of the repulsive barrier; a much stronger dependence on the repulsion range is instead observed. Evidence is also presented for the existence of small simultaneous jump discontinuities of several thermodynamic and structural properties under physical conditions close to the onset of particle clustering. The discontinuities thus provide a signature of the transition from a homogeneous fluid phase to a locally inhomogeneous cluster phase. Upon appropriate thermodynamic conditions, the microphase separation terminates, at sufficiently low temperatures, with a phase transition into an ordered-pattern fluid. The limits of stability of the microseparated phase are identified by a drastic, diverging-like, increase of the low-Q peak, as the temperature drops. The behavior of S(Q) in the disordered-pattern phase suggests that different morphologies of the ordered patterns should be expected, depending on the ratio between the strengths of competing interactions.

#394 - The quantum nature of the OH stretching mode in ice and water probed by neutron scattering experiments

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The OH stretching vibrational spectrum of water was measured in a wide range of temperatures across the triple point, 269 K $<$T$<$ 296 K, using Inelastic Neutron Scattering (INS), and the hydrogen projected density of states, the proton momentum distribution and mean kinetic energy, $<E\_K>$, were determined for the first time. We found that the value of $<E\_K>\_OH$ is nearly constant as a function of T, indicating that quantum effects on the OH stretching frequency are weakly dependent on temperature. In the case of ice, ab initio simulations, using non local van der Waals functionals, provided $<E\_K>$ values in agreement with INS experiments. We also found that the ratio of the stretching to the proton total kinetic energy, $<E\_K>\_OH/<E\_K>$, increases in going from ice to the liquid at ambient conditions and then to supercritical water. This ratio exhibits a minimum in the metastable liquid phase indicating the presence of hydrogen bonds stronger than in ice, contrary to the accepted view of supercooled water as exhibiting weaker hydrogen bonds than ice.

Overall the present study on the microscopic quantum dynamics of water and ice strongly suggests that the generally accepted picture of relatively weak H-bonds in supercooled water, in the presence of tunneling or anharmonic potentials, may need to be reconsidered. We suggest that the large difference between the momentum distributions of normal and supercooled water, may stem from correlated protons motion in the ground state of supercooled water with an as- sociated quantum coherence length, for example due to the presence of microcrystallites of ice dynamically forming and disappearing, or to the simultaneous presence of O-O shortening and hydrogen bond bendings.

#395 - More is different: the effect of biomolecules on hydration water

Daniele Fioretto - Dipartimento di Fisica, Università di Perugia

Lucia Comez (Dipartimento di Fisica e CNR - IOM c/o Dipartimento di Fisica, Università di Perugia), Laura Lupi (Dipartimento di Fisica, Università di Perugia), Assunta Morresi, Marco Paolantoni, Paola Sassi (Dipartimento di Chimica e Centro di Eccellenza sui Materiali Innovativi Nanostrutturati (CEMIN), Università di Perugia)

Water in biological matter experiences a quite complex environment, being in contact with hydrophilic and hydrophobic surfaces and with charged moieties that interferes with the cooperative rearrangement of the hydrogen bond network. The resulting dynamical perturbation is here investigated by light scattering experiments, on systems of different nature and complexity, including small hydrophobic and hydrophilic [1] molecules, amino acids, dipeptides [2] and proteins [3]. Our results, complemented by neutron scattering investigations, suggest that a reductionist approach is not adequate to describe the dynamics of water in aqueous solutions of bio-relevant molecules: A significant increase of the dynamical retardation and extension of perturbation occurs when increasing the chemical complexity of the solute [4].

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#396 - Adiabatic freezing of supercooled liquids: a maximum-entropy analysis

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The decay of a supercooled liquid to equilibrium usually begins with the rapid (i.e., adiabatic) growth of the solid, which heats the system up to the equilibrium freezing temperature (recalescence). Only later will solidification be completed through the exchange of energy with the colder bath. We use standard thermodynamics to anticipate the immediate outcome of the recalescence stage, assuming it to be a near-equilibrium solid-liquid coexistence state. Two different systems were investigated: a mean-field fluid and water, in two different virtual experimental settings, i.e., under isobaric and isochoric conditions, respectively. We computed the final temperature, pressure, and fraction of solid as a function of undercooling and of the amount of foreign gas which may be possibly present in the vessel. The calculation was then repeated under the more realistic hypothesis of a non-zero cost of the interface between solid and liquid. In this case, we identify the condition when the onset of solidification inevitably occurs at the wall in contact with the bath.

#397 - Magnetic fluids: an x-ray spectroscopy characterization

Silvia Nappini – CNR – Istituto Officina dei Materiali, Laboratorio TASC, Basovizza

Silvia Nappini, Federica Bondino (CNR -IOM, Laboratorio TASC, Trieste), Alessandro Barla (CNR-ISM, Trieste), S. Dal Zilio, D. Borin, V. Toffoli M. Lazzarino (CNR -IOM, Laboratorio TASC, Trieste), P. Baglioni (Università degli Studi di Firenze)

Magnetic nanoparticles (MNPs) have been studied because of their unique properties and wide applicability in many different areas, such as fabrication of electronic components for the information storage, magnetic cards, recording devices. Recently MNPs gained a new interest also in biomedical sciences, since, when properly functionalized and dispersed in aqueous environment, they represent a promising alternative approach for drug delivery, hyperthermia, magnetic resonance imaging (MRI), tissue engineering, biosensing, biochemical separations, and bioanalysis.

An important step for the application of MNPs in biological environment is the evaluation of the chemical and magnetic behaviour of the MNPs in liquid solution. To this purpose a cell for liquid consisting of two Si_3N_4 membranes resistant to UHV conditions and transparent to x-ray photons was developed at IOM-CNR which allows soft x-ray spectroscopy experiments in liquids.

In this work we present the first measurements, performed in liquid, carried out at BACH beamline at Elettra. The effect of hydration, surface charge (related to the pH of the solution) and citrate coatings on the electronic structure of $CoFe_2O_4$ NPs was evaluated by x-ray absorption spectroscopy (XAS) of the $L_{3,2}$ edges of Fe and Co, and the K edge of O. X-ray magnetic circular dichroism (XMCD) measurements, performed during the commissioning of the new cryomagnet installed on BACH beamline, on a dry film of NPs show a strong magnetic dichroism at low T under high magnetic field.

#398 - Undercooling and crystal nucleation in germanium

Adriano Filipponi - Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi de L'Aquila

A. Di Cicco (CNISM, Scuola di Scienze e Tecnologie, Sezione di Fisica, Camerino (MC)), E. Principi (Sincrotrone ELETTRA, Strada Statale 14, 34149 Basovizza, Trieste)

Spontaneous crystal nucleation in metastable undercooled liquids is a spectacular phenomenon occurring when the system finds its way to overcome the interface free energy barrier and leading to recalescence and macroscopic crystallization.

This phenomenon has recently attracted a novel interest especially in IVth group elements [1] characterized by a strong polymorphism in the liquid phase related to the competition between covalent and metallic bonding and resulting in low-density and high-density liquids.

The nucleation phenomenon can be described by a non-homogeneous Poisson process characterized by a temperature dependent rate I(T). Several experimental approaches have been developed by our group which include repeated pyrometric experiments on single specimens and related data analysis techniques [2] or the usage of an x-ray probe on multiple droplet samples.

A central issue in the data interpretation is what information can be gained by an experimental determination of I(T): the physical measurement that can be performed at the lowest possible temperature in the metastable state, and whether the Classical Nucleation Theory is adequate for the complex fluid cases under consideration.

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#399 - In-situ measurements of the wetting properties of individual micro and nanopartciles at liquid-liquid interfaces

Lucio Isa – Swiss Federal Institute of Technology, Zurich

Nanoparticles (NPs) at fluid interfaces are central to a rapidly increasing range of nanotechnological applications, including drug delivery [1], functionalized NPs for uptake through biological membranes [2], emulsion stabilization [3] and the fabrication of nano-composite materials [4]. Considerable experimental and theoretical efforts have been devoted to the study of micro- and nanoparticle adsorption, assembly and dynamics at fluid interfaces [5]. Despite this, many features of wetting at the single-nanoparticle level remain unresolved. Follwoing our recent realization of an approach based on freeze-fracture and cryo-scanning electron microscopy, which allows true single-nanoparticle contact angle measurements down to the 10-nm range [6], we report here its application to a variety of challenging systems, including soft microgels [7], highly hydrophobic silica nanoparticles [8] and the investigation of surfactant adsorption on emulsion double inversion [9]. All these examples demonstrate the importance of nanoscale characterization to guide and control the properties of materials.

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#400 - Superintense laser-plasma interactions: relativistic condensed matter physics

Andrea Macchi (I) – CNR - Istituto Nazionale di Ottica, Pisa

Plasmas produced by superintense (>1018 W/cm^2) laser pulses provide the only example of high-density, relativistic many-body system which can be studied on a laboratory scale. New regimes and applications are now accessible thanks to the advances both in ultrashort (~10 fs), high-contrast laser pulse technology and in target manufacturing. At the same time the development of proton probing techniques allows to study the nonlinear electromagnetic dynamics and self-organization of plasmas with picosecond resolution. This talk will highlight some recent results, including the light pressure boosting of ultrathin targets for novel ion accelerators, the excitation of surface plasma waves in the relativistic regime ("high-field plasmonics"), and examples of electromagnetic dynamics imaging by proton beams such as ultrafast charging of laser-irradiated targets and generation of multi-megagauss magnetic fields.

#401 - Physics of magnetically confined thermonuclear plasmas

Fulvio Zonca (I) - Associazione EURATOM-ENEA sulla Fusione

S. Briguglio, G. Fogaccia, A.V. Milovanov, G. Vlad (Associazione EURATOM-ENEA sulla Fusione, C.P. 65-00044 Frascati), L. Chen, X. Wang (Institute for Fusion Theory and Simulation, Zhejiang University, Hangzhou 31007, P.R.C.)

Energetic particles in the MeV range in thermonuclear plasmas of fusion interest are produced by (D-T) fusion reactions as well as by external heating and current drive systems. They are not only intended to provide the dominant power density in burning plasmas, but also play a crucial and very peculiar role as they act as mediators between different spatiotemporal scales and related fluctuating phenomena. Long time scale behaviors, due to the interplay of fast ion induced collective effects and plasma turbulence, are addressed in the framework of burning plasmas as complex self-organized systems. In this work, two important issues will be discussed in particular: (i) the role of "nonlinear equilibria" that dynamically evolve on characteristic (fluctuation induced) turbulent "transport" time scales, which are generally of the same order of the nonlinear time scale of the underlying fluctuations; (ii) the coherent nonlinear dynamics of structures in the energetic particle phase space, by which secular resonant particle transport can occur on meso- and macro-scales. To elucidate these aspects, theoretical analyses are presented together with numerical simulation results. Meanwhile, with the aim of addressing problems of common interest with neighboring research areas, the general underlying formulation of nonlinear Schrödinger equations with complex integro-differential nonlinear terms will be introduced.

#402 - Energy and wavelength scaling of shock-ignited inertial fusion targets

Stefano Atzeni - Dipartimento SBAI, Università Sapienza, Roma e CNISM

Alberto Marocchino, Angelo Schiavi (Dip. SBAI, Università Sapienza, Roma e CNISM), Guy Schurtz (CELIA, Universitè de Bordeaux 1, France)

Shock ignition is an approach to direct-drive inertial confinement fusion (ICF) in which the stages of compression and hot spot formation are partly separated. The fuel is first imploded at lower velocity than in conventional ICF. Close to stagnation an additional intense laser spike drives a strong converging shock, which contributes to hot spot formation. Shock ignition shows potentials for high gain at UV laser energy below 1 MJ, and could be tested on the National Ignition Facility or Laser Megajoule. Due to the lower implosion velocity, issues related to hydrodynamic instabilities are relaxed. On the other hand, the interaction of the laser spike with the plasma occurs in a regime where parametric instabilities are expected to become relevant. In shock ignition, separation of the stages of fuel compression and hot spot creation introduces some degree of design flexibility. A lower implosion velocity can be compensated for by a more intense ignition pulse. Flexibility increases with target (and driver) size and allows for a compromise between energy gain and risk reduction. Having designed a reference ignition target, we have developed an analytical model for (up)-scaling targets, and for estimating target gain, as a function of laser energy and parameters related to hydro- and plasma-instabilities. Detailed 1D simulations confirm the model and generate gain curves, while 2D simulations show how different design options affect robustness to asymmetries caused by laser nonuniformities and target mis-positioning. The previous results apply to UV ($\lambda = 0.35$ μm) laser light. We also show that our scaling model can be used in the design of targets driven by green laser ($\lambda = 0.53$ μm). 1D simulations show that gain in the range $100 - 200$ can be obtained for total green light laser energy in the range $1.5 - 3$ MJ, while operating in the same laser-plasma regime as the UV-driven targets.

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#403 - Study of parametric instabilities and supra-thermal electrons generation in shock ignition relevant regime

Federica Baffigi - CNR - Istituto Nazionale di Ottica, Pisa

G. Cristoforetti, P. Koester, L. Labate, L. A. Gizzi (CNR-INO, Pisa), F. Consoli, R. De Angelis (EURATOM-ENEA sulla Fusione), L. Antonelli, M. Richetta (Università " Tor Vergata", Roma), D. Batani, G. Folpini, Y. Maheut, G. Malka, P. Nicolai (CELIA, Université Bordeaux 1, France), Y. J. Rhee (Nuclear Data Center, KAERI, Korea and CELIA, Université Bordeaux 1, France), J. Badziak, T. Chodukowski, Z. Kalinowska, P. Parys, T. Pisarczyk, M. Rosinski, J. Wolowski (Institute of Plasma Physics and Laser Microfusion, Warsaw, Poland)

Strong shock-waves in solids lead to the generation of warm dense matter. Such a high energy density plasma has applications in several fields, including astrophysics and inertial confinement fusion (ICF). One way to drive intense shocks in solids is through laser ablation which is capable of generating pressures as high as 100 Mbar. Recently, this topic is being revisited, because shock is regarded as a possible way to achieve ignition of fusion burn in a pre-compressed ICF capsule. This so-called shock ignition (SI) is very promising for the accessible target and laser parameters required and also for the potential high energy gain achievable. In the SI scheme of ICF, the compression phase is separated from the ignition phase. At a few hundred ps before maximum compression the target is additionally irradiated by a 300-500 ps duration laser pulse at higher intensity (1016 W/cm^2) to generate a strong, converging shock wave. The spherical shock wave is further amplified due to the geometrical convergence, capable of rising the plasma temperature and density to the ignition conditions for fusion in the central hot spot.

A series of experiments aimed at investigating the generation of intense shock-waves in the laser-ablation regime envisaged for shock ignition was conducted at the PALS laser facility in Prague. The experiments were performed in a planar geometry and the shock was launched in a pre-heated multilayer target with the main laser beam (λ=438 nm) focused at an intensity up to 1016 W/cm^2. A long scale plasma was created before the arrival of the main laser pulse using an auxiliary beam (λ=1315 nm) and the timing between the two beams was varied. A phase plate was used on both beams in order to ensure a homogeneous intensity profile in a large focal spot. A set of diagnostics was used for the characterization of the laser-plasma interaction, the generated fast electrons and the shock wave. Spectroscopy and calorimetry of the scattered radiation are the key tools for the investigation of the laser plasma interaction regime. Evidence of harmonic and half-harmonic emission, a signature of parametric instabilities such as Stimulated Raman Scattering and Two Plasmon Decay, clearly shows that a strongly non-linear regime is reached in our experiment. Both these instabilities can result in the production of supra-thermal electrons. In addition, X-ray measurements with a CCD working in single-photon regime are presented. Kα emission from a Cu layer inside the multilayer target, as well as the high energy X-ray spectrum, give information about the fast electron energy and conversion efficiency.

The identification of all these effects and their weight in the energy balance ultimately affect the efficiency of the shock wave generation. These are currently among the fundamental open questions concerning the shock-wave generation with intense laser pulses.

#404 - Low-frequency oscillations in a RF-generated electron plasma in a Penning-Malmberg trap

Bruno Paroli - Università degli Studi di Milano

Muhammad Ikram, Giancarlo Maero, Roberto Pozzoli , Massimiliano Romé (Università degli Studi di Milano)

A low-density (10^6 - 10^7 cm^{-3}) electron plasma column confined in a Penning-Malmberg trap can be lost radially due to the growth of the unstable m=1 diocotron mode (i.e. the radial displacement of the plasma column). The instability can be induced by a number of mechanisms (e.g., resistive-wall dissipation [1], presence of positive ions [2,3]). We experimentally observe that an electron column (of total charge about 1 nC) can be produced by a low-power RF excitation which triggers a Fermi-like heating mechanism [4] and a consequent ionization of the background gas. In these conditions, a dynamical equilibrium is reached within few seconds where the axial losses are balanced by the continuous ionization, and the column can remain for hours on a stable radial offset even in presence of a significant resistive dissipation. A newly-observed and peculiar feature of this regime is the occurrence of low-frequency (LF) oscillations (in the Hertz range) modulating the m=1 diocotron mode amplitude and phase. We have studied experimentally these oscillations by means of pulsed and sinusoidal electric perturbations under different resistive dissipation conditions. The charge balance in the plasma column has been evaluated and both the low- and high-modulation depth regimes have been investigated through the correlation between the oscillation's phase and the total trapped charge. The main interest of this subject is understanding the role of the LF oscillations in determining the dynamics and stability of the plasma column.

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#405 - The Future of Elettra and FERMI

Giorgio Paolucci (I) – Elettra -Sincrotrone Trieste S.C.p.A.

The last five years have seen major developments taking place at the Italian synchrotron radiation facility Elettra in Trieste. The homonimous fourth generation light source has been successfully upgraded to operate routinely in top-up mode for users, greatly improving the stability of the source and substantially increasing the time-averaged brightness. New beamlines and experimental stations for x-ray fluorescence, structural biology and diffraction under high pressure are being added to the 23 operating beamlines. A new seeded free-electron laser facility, FERMI, including FEL-1 and FEL-2 sources operating in the extended ultraviolet and soft-x-ray range, respectively, came on line, with three beamlines and experimental station currently open to users on FEL 1, and three more under construction. We will review the current performance of Elettra and FERMI and describe our development plans for the future.

#406 - ESRF status and upgrade program

Pantaleo Raimondi (I) – European Synchrotron Radiation Facility, Grenoble

On Behalf of the ESRF Accelerator and Source Division

The Machine Operations and the status of the Upgrade Phase I will be given.
It will also be described the Phase II Upgrade Project aimed at a significant decrease of the Strorage Ring Horizontal Emittance, in order to increase the brightness of the source and its coherent fraction by a factor up to 100.

#407 - The European X-ray free-electron laser facility: status report

Massimo Altarelli (I) - European XFEL, Hamburg

The European XFEL facility, under construction in the Hamburg region, with financial support of 12 European countres including Italy, is going to generate up to 27 000 ultrabright and ultrashort x-ray pulses (brightness $>10^{32}$ ph/s/mm^2/mrad^2/0.1 % BW, pulse duration from a few fs to >100 fs) in the photon energy region between the C K-edge and ~ 25 keV. When it starts operation in 2016, it will operate a superconducting 17,5 GeV Linac, three undulators and six experimental stations for users. A summary of the status of the construction project shall be given; some examples of experiments made possible by the new facility, and of the accompanying instrumentation developments shall be described. In particular, the exploitation of the very high repetition rate, typically more than two orders of magnitude larger than that of competing facilities, is an important challenge.

#408 - The SwissFEL project

Luc Patthey (I) - Paul Scherrer Institut, Villigen

The Paul Scherrer Institute is running a third generation synchrotron source (SLS) and is planning the construction of a X-Ray Free Electron Laser (SwissFEL) facility, which will produce 20 fsec pulses of coherent x-rays in the wavelength range 0.1 to 7 nm, with extremely high peak brightness. These characteristics will provide opportunities for new experiments in chemistry, solid state physics, biochemistry and materials science. The lecture will present the most important achievements of synchrotron-based research and also focus on novel applications with the SwissFEL facility, the description of the fundamental aspects of the facilities, as well as the challenges to be tackled.

#409 - The DAFNE-light synchrotron radiation facility

Antonella Balerna – Istituo Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati

DAΦNE is a 0.51 GeV e^+e^- collider, where a routinely circulating current over 1 A provides a very high photon flux in an energy range from the IR to soft x-rays. Due to its unique characteristics DAΦNE is also used in dedicated and in parasitic mode for synchrotron radiation applications. In the DAΦNE-Light synchrotron radiation facility there are three beamlines already operational and two new XUV ones ready for commissioning. Two of the existing beamlines, the soft x-ray (DXR-1) and the UV (DXR-2) ones have one of the DAΦNE wiggler magnets as synchrotron radiation source, while the third beamline (SINBAD) working in the infrared region collects the radiation from a bending magnet. The two new bending magnet XUV beamlines will cover the energy range from 30 eV to 1000 eV. A short description of the DAΦNE-Light facility will be given and some recent scientific results will be shown.

#410 - Hybrid Photovoltaics

Giuseppe Gigli (I) – Università del Salento e CNR- Istituto Nanoscienze, National Nanotechnology Laboratory

The exploration of innovative materials and device architectures is constantly fostering our solar conversion research activity, aiming at low cost and highly efficient solutions.

From conceptually new mesostructured solar cells, based on self-assembling hybrid perovskites, to full inorganic bulk heterojunction solar cells based on versatile nanocrystals, we have been exploring viable routes for an effective market impact of third generation photovoltaics.

Our vision is based on solution processable materials and low temperature cell manufacturing, matching the requirements of existing technologies, for large-scale device production at reasonable production costs. Furthermore we pursuit the implementation of such solar converting components into multifunctional devices, an example we conceived on this line, is a photovoltachromic cells integrating both photovoltaic and photoelectrochromic functionalities, targeting building integration.

#411 - Dye solar cells: from basic research to industrialization

Aldo Di Carlo (I) - Center for Hybrid and Organic Solar Energy, Università "Tor Vergata", Roma

Among all the organic and hybrid organic-inorganic solar cell technologies, dye solar cells (DSCs) have demonstrated the highest conversion efficiencies and a mature research and development plan. Compared to traditional photovoltaics (PV), DSCs have several advantages, such as low dependence on angle of light, colors and transparency, which make DSCs very appealing for innovative applications of PV such as building integration photovoltaics.

In this presentation, the efforts made to improve efficiency of small area cells and to scale-up this technology up to modules and panels will be discussed. The relation between transparency and efficiency will be shown for several dyes and for co-sensitized devices. Results will outline the strong interplay between TiO_2 thickness, dye/dyes dipping time and the absorbance profile of the dye/dyes. Particular emphasis will be given to the stability of the cells in relation with properties of materials used in device fabrication. The effect of bias stress tests, studied with resonant micro-Raman spectroscopy, will be discussed and the mechanism of thiocyanato (SCN-) loss will be reported.

#412 - Bi_2S_3 colloidal nanocrystals for non-toxic solar cells

Daniela Marongiu - Dipartimento di Fisica, Università di Cagliari

Feipeng Chen, Roberto Piras, Mauro Aresti, Michele Saba, Francesco Quochi (Dipartimento di Fisica, Università di Cagliari, Complesso Universitario di Monserrato, 09042 Monserrato (CA)), Mauro Mureddu, Carla Cannas, Anna Musinu (Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari, Complesso Universitario di Monserrato, 09042 Monserrato (CA)), Andrea Mura, Giovanni Bongiovanni (Dipartimento di Fisica, Università di Cagliari, Complesso Universitario di Monserrato, 09042 Monserrato (CA))

In the last few years the research on new materials for low-cost non-toxic solar cells has met rapid advances; in particular, solution-processed inorganic solar cells based on colloidal nanocrystals have attracted great interest. Thin films made of colloidal semiconductor nanocrystals seem promising due to their easy and low-cost processability. The best efficiencies in solar cells based on colloidal nanocrystals have up to now been achieved by employing heavy metal chalcolgenides, such as PbS, PbSe, CdSe and CdS. In order to avoid hazards to human health, benign, non-toxic materials need to be considered; among them, Bi_2S_3, with a direct-bandgap of 1.3 eV, ideal for solar cells, appears as a good candidate. Up to now, the few Bi_2S_3-based solar cells that have been demonstrated also employed either Pb or Cd chalcogenides, such as nano-heterojunction solar cells based on n-type Bi_2S_3 nanocrystals and p-type PbS quantum dots [1] or in hybrid solar cell [2]; none of them is entirely made by non-toxic inorganic materials. In this work we investigated the growth kinetics and the optotelectronic properties of Bi_2S_3 nanocrystals. Bi_2S_3 colloidal nanocrystals, with dimensions ranging between 5 and 20 nm, have been obtained by mean of a synthetic route employing oleic acid as the capping ligand and toluene as the final solvent. After achieving control and reproducibility in morphology, size and crystallographic properties of nanocrystals, we focused on the transport properties of a device based on a thin film grown layer by layer. The thin films have been obtained by dip coating the solution on the substrate, followed by a ligand exchange procedure for which the electrically insulating oleic acid is partially or completely replaced by a shorter-chain capping agent such as ethanedithiol, thus increasing the film conductivity.

Current-voltage measurements on the films have shown a high photocurrent with significant variations depending on the nanocrystals dimensions and the study of a FET device in dark and under illumination conditions have demonstrated the existence of mid gap states due to the presence of critical nanocrystal surface defects which can be controlled by a specific surface treatment during the post-deposition processing. Trap states were also investigated with ultrafast optical spectroscopy, providing the knowledge base to control optoelectronic properties of Bi_2S_3 nanocrystals and realize solution-processable, entirely inorganic and non-toxic solar cells.

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#413 - Nanostructured Al-doped ZnO grown by pulsed laser deposition as a transparent conducting oxide for advanced photovoltaics

Paolo Gondoni - Dipartimento di Energia, Politecnico di Milano

Piero Mazzolini (Politecnico di Milano e IIT), Valeria Russo (Politecnico di Milano), Carlo Enrico Bottani, Andrea Li Bassi, Carlo Spartaco Casari (Politecnico di Milano e IIT)

Transparent Conducting Oxides (TCOs) have been intensively studied as compact transparent electrodes in energy conversion and optoelectronic devices. Recently, however, their application to Hybrid and Organic Photovoltaics (HOPV) has raised the need for new functional properties, such as large effective surface area, light scattering and trapping, compatibility with polymer substrates. One means to achieve and control these properties down to the nanoscale is constituted by Pulsed Laser Deposition (PLD).

We report the synthesis of Al-doped ZnO (AZO), a low-cost TCO, by PLD at room temperature with O_2 as a background gas. By controlling the O_2 deposition pressure, the material morphology and properties can be tailored: at low deposition pressure (< 10 Pa O_2) compact, nanocrystalline, TCO films are obtained with state-of-the –art optical and electrical properties, also on flexible polymer (Ethylene-TetraFluoroEthylene) substrates. Mean visible transparency is over 90% and minimum resistivity is of the order of 10^{-4} Ω cm, due to an effective interplay between extrinsic (Al) and intrinsic (oxygen vacancies) dopants. The optimal value is reached at 2 Pa O_2, where dopants contribute to carrier density in the conduction band ($7x10^{20}$ cm^{-3}), but their concentration is low enough to have a Hall mobility of 20 cm^2/Vs. At higher O_2 pressure (100 Pa and above), the material evolves towards a porous, hierarchical assembly of nanosized clusters resembling a nanotree forest. This mesoporous morphology maximizes visible light scattering (obtaining a haze, i.e. diffuse to total transmittance ratio, of 85% in the visible range, where optical transmittance is over 90%) but dramatically increases resistivity (up to 1 MΩ cm) due to low connectivity and saturation of O vacancies.

Two approaches have been devised to combine the high conductivity of compact films and the effective light management of porous films: the first employs mixed Ar:O_2 deposition atmospheres to achieve an independent control of morphology (Ar partial pressure) and stoichiometry (O_2 partial pressure) in order to induce oxygen vacancies in mesoporous structures. The second approach consists in the synthesis of graded materials, by decreasing the O_2 pressure during deposition to grow a compact AZO layer on top of a porous layer. By optimizing the deposition parameters, films with 1 mΩ cm resistivity, 80% transparency and 40% haze are obtained. Such properties, together with room temperature deposition, make this material appealing for employment in HOPV devices.

#414 - Photocatalytic properties of doped TiO$_2$ nanofibers

Luca Lozzi – Università de L'Aquila

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Titanium dioxide (TiO$_2$), thanks to its interesting properties as nontoxicity, low cost and high chemical stability, has been extensively investigated for several applications in which, following light absorption, the generated charges can be usefully applied, as for photovoltaic systems and photocatalytic devices. However, due to the wide intrinsic energy gap of TiO$_2$ (between 3.0 and 3.2 eV, depending on the crystalline structure), only a small fraction of the solar spectrum can be used to promote the electron-hole pair formation. In order to reduce the energy gap and, therefore, increase the fraction of the solar spectrum that can be absorbed, different approaches have been used, mainly by doping TiO$_2$ with metals or anions. In this work we will present our results on the deposition, by means of the electrospinning technique, of TiO$_2$ nanofibers doped with metals (iron, copper, tungsten). These nanofibers have been characterized by SEM, XPS and XRD for morphological, chemical and structural analyses, respectively. The effect of the metal concentration on the photocatalytic properties of these nanofibers have been investigated through the study of the degradation of a pollutant-model (Rhodamine 6G) by using visible lamp and sunlight as light source.

#415 - Nitro-catechol/ZnO(10-10): molecular dipole and energy level alignment in a model system for dye/ metal oxides interfaces

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Dye Sensitized Solar Cells (DSSCs) are one of the possible promising alternatives to conventional photovoltaic devices based on silicon technology. The electronic properties of the interface between the semiconductor metal oxide, the molecular dye and the electrolyte play a fundamental role in the DSSC functioning: The ability to tailor them is therefore crucial for the optimization of the device performances. Aiming at elucidating the basic mechanisms that determine the energy level alignment between the HOMO and LUMO states of the dye, the metal-oxide bands and the Fermi level, we have investigated a prototype system, i.e., nitrocathecol/ZnO(10-10), both experimentally and theoretically by means of electron spectroscopies and first-principles DFT-based calculations.

The energy position of the nitrocathecol occupied molecular levels relative to the zinc-oxide electronic bands is determined by UPS, while HREELS data provide information on the aligment of the empty states relative to the susbtrate bands. DFT calculations allow the understanding of electronic strucure modifications in terms of formation of new interface states with strong molecular character. Our combined approach also provide quantitative interpretation on the strong ionization potential variation induced by functionalization, that is exactly traced back to the formation of an interface dipole layer.

Moreover, we investigate the modification of the molecular adlayer induced by UV irradiation, observing the formation of aminocathecol moieties. Interestingly, this modification induces a significant variation of the energy level alignment, and in particular a ionization potential change of 0.7 eV. The influence of solvent co-adsorption on molecular level alignment is also discussed.

#416 - X-ray photoemission spectroscopy investigation of the bonding between 4-mercaptopyridine and the TiO_2 surface

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In the contest of the ongoing research on efficient and low-cost solar cells based on hybrid (organic-oxide) junctions, interface modifiers hold the premise of a better control over the process of charge collection at the interface with the oxide.

At variance with previous attempts with small molecules bonded to the TiO_2 surface through carboxyl anchoring groups [1], Canesi et al. [2] reported on a dramatic increase in device performances by the addition of 4-Mercaptopyridine (MPy) molecules as interface modifiers. According to their studies on P3HT infiltrated on a porous TiO_2 scaffold, the 4-MPy layer directly affects the adhesion of the conductive polymer to the oxide surface (i.e. the morphology of the interface).

As a part of the aforementioned device characterization, we present here a detailed X-ray photoemission spectroscopy (XPS) study on the bonding of 4-MPy molecules to the anatase TiO_2 surface.

The high surface sensitivity, element specificity, and the ability to discriminate between atomic species in different chemical environments make XPS particularly suited to the problem. In particular, we try to answer to the (not so obvious) question whether 4-Mpy bonding proceeds via the thiol group or the nitrogen atom (i), and to determine the nature of the bonding site on the oxide (ii). Implications on the nature of the 4-MPy action at the interface are discussed.

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#417 - Interface properties between $CuPc:C_{60}$ blend films and graphene

Roberta Totani – Università de L'Aquila

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Recently in the realization of organic-based photovoltaic cells graphene is being used as transparent and metallic contact. In this work we will report the spectroscopic results on the interface electronic states between organic blend films and a monolyer graphene sheet deposited on SiO_2. Very thin $CuPc:C_{60}$ blend films have been deposited onto graphene by ultra high vacuum evaporation. The interface properties have been followed by means of ultraviolet and X-ray photoemission spectroscopies. The valence band structures, in particular the HOMO molecular states, shows a shift depending on the film thickness. The shifts are different for CuPc and C_{60} HOMO states. These data have been used to determine the effects of the blend-substrate interface on the film ionization energy. The core levels also present a shift depending on the film thickness, while their line shapes do not depend on the thickness.

#418 - Visualization of electrons dynamics in real time

Luca Perfetti (I) - Ecole Polytechnique Fédérale, Lausanne

We will present recent advances of time resolved photoelectron spectroscopy in materials with strong electron-phonon interaction and large spin-orbit coupling. The structure of electronic excitation in such compounds strongly depends on the entanglement of different degrees of freedom. In particularly the spin-orbit interaction generates spin and orbital polarizations, while the electron-phonon coupling results in to insulating phases with speudogapped spectral density. Time resolved photoelectron spectroscopy offers new means to investigate the physics of such complex systems by monitoring the dynamics of excited electronic states out-of-equilibrium conditions. We will treat several problems of high scientific interest as selective coupling of coherent phonons to Bloch states, the giant anisotropy of spin-orbit coupling and the photoinduced quenching of an electronic gap.

#419 - Generation of high-field multi-THz transients and their application for nonlinear spectroscopy of semiconductors

Daniele Brida (I) - University of Konstanz

High-field effects in semiconductors are a subject of particular interest both for fundamental science as well as modern high-speed electronics. Recent advances in high-field THz technology have opened up exciting new perspectives for scaling up the applied electric fields by many orders of magnitude without irreversible breakdown of a sample. Latest experiments performed with THz peak fields up to 1 MV/cm have demonstrated a high potential of this approach.
Recently we have developed a hybrid laser source based on difference frequency mixing of two near-infrared pulses which enables generation and field-resolved detection of multi-THz transients with peak fields above 100 MV/cm. Further optimization of phase-matching conditions results in broadband single-cycle multi-THz transients with amplitudes above 10 MV/cm. Such ultrashort high-field pulses are perfectly suitable for nonlinear THz spectroscopy experiments on semiconductors and other condensed matter systems.
In order to study ultrafast optical response under the influence of an oscillating THz bias field we have developed an experimental setup which allows to detect simultaneously the inherently phase-locked THz field of the bias pulse and the field-induced changes in near-infrared absorption. The sub-10 fs short probe and gating pulses generated using the Er:fiber laser system ensure a sub-cycle time resolution of the experiment.
The sample under study is a 230 nm thick epitaxially grown InP layer deposited on a 0.3 mm thick diamond substrate by a lift-off process. Since the spectral components of the probe pulse are located below the energy of the interband resonance in InP the measured signal is dominated by the field-induced absorption below the band gap energy and reaches its maximum at the peak of the THz field (zero delay time). Interestingly, the transmission change shows a coherent modulation at exactly twice the carrier frequency of the driving transient. This behavior is expected for the Franz-Keldysh effect where the photon-assistant interband tunneling depends only on the absolute value of the electric field.

#420 - Development of active gratings for ultrashort pulses in the extreme-ultraviolet

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We present the design and characterization of active deformable gratings to be used for the realization of monochromators for extreme-ultraviolet ultrashort pulses. The device consists of a diffractive layer realized by UV lithography that is deposited on the top of a bimorph deformable mirror, whose curvature radius can be varied changing the voltage applied to an underlying piezo-actuator. The samples that have been tested have high optical quality, since the grating profile has been ruled on an ultrasmooth silicon wafer, are compatible with any coating deposition and have only vacuum-compatible materials. We present the characterization of the prototypes in the vacuum ultraviolet and in the visible, showing that the active grating can optimize the beam focusing through its rotation and deformation.
Two active gratings have been mounted in a compensated configuration to realize a grazing-incidence time-delay compensated monochromator for high-order laser harmonics, which is capable to select one of the harmonics within the comb and to preserve its duration in the few-femtoseconds time scale. The wavelength selection is performed through the grating rotation, the intermediate slit carries out the spectral selection of a single harmonic and the spectral focusing is maintained by adjusting the grating radii. The instrument has been initially tested in air with a Ti:Sa laser operated at 800 nm. We have been able to demonstrate that the double-grating configuration with active gratings compensates for the pulse front-tilt. The front-tilt given by the first grating is ~1 ps and is reduced to ~100 fs after the second stage. The final value is limited by the group delay dispersion of the monochromator within the 10-nm bandwidth of the laser centered around 800 nm.
Active gratings may be considered as a cheaper and more flexible alternative to standard gratings for the realization of extreme-ultraviolet ultrafast monochromators.

#421 - Recovering propagation delay of an optical pulse to achieve a "true" c-velocity

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In recent years, research in controlling propagation dynamics of optical pulses has been able to achieving extremely low group velocities ("slow-light"- regime) or superluminal or negative group velocities ("fast-light"-regime). In the fast-light case, the pulse peak is in advance in propagation respect to vacuum-case, in a way consistently with special relativity and causality. Although many experimental schemes proposed in literature exploit coherent effects, like electromagnetic-induced transparency, we showed theoretically [1] and experimentally that is possible to achieve an incoherent optical control of propagation dynamics of an optical pulse both in slow-light case [2], with induced delay up to 15 ns, and in fast-light case [3], with advances up to 1 ns, for a pulse of 3 ns of time duration.

The idea about a combination of these two effects in a same experimental set-up led to explore possibility of recovering a delay, induced by slow-light interaction, with a subsequent fast-light propagation stage. The experimental set-up consists in two cells filled with hot sodium vapor at low pressure and two pump pulses, resonant with different atomic transitions, in order to produce a passive medium in the first cell and an active medium in the second one. In a subsequent time, a probe pulse, with central wavelength tuned near resonance with an atomic transition, experiments an extra-delay in the first cell, because of normal dispersion properties probed in the passive medium, and an advance in the second one, because of anomalous dispersion zone in the active medium. Results showed a "saturation" in propagation advance, because the second fast-light stage is not only able to completely recover the previously induced delay (up to 1 ns order), but also produces an advance, respect vacuum propagation, equals to the case of the first slow-light stage switched off. Such effect suggests a "true propagation at c-speed" for an optical pulse envelope previously delayed, with the final fast-light stage that may be used in order to cancel previous history in propagation dynamics, acting as a kind of a "temporal invisibility cloaking" device. Such experimental work may open interesting scenarios in optical signal processing.

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#422 - Ultrafast non-thermal electron dynamics in single layer graphene

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The impulsive optical excitation of carriers in graphene creates an out-of equilibrium distribution, which thermalizes on an ultrafast timescale[1-3]. The hot Fermi-Dirac (FD) distribution subsequently cools via phonon emission within few hundreds of femtoseconds. While the relaxation mechanisms mediated by phonons have been extensively investigated, the initial stages, ruled by fundamental electron-electron (e-e) interactions still pose a challenge.

The equilibration processes change the transient absorption spectrum over a wide range of energies and on ultrafast timescale. Their time-domain observation calls therefore for the combination of very short pulsewidths and broad spectral tunability. Here we perform pump-probe spectroscopy on graphene using two-color few-optical-cycle pulses. We impulsively excite optical transitions with an ultra-broadband 7-fs pulse at 2.25 eV (2-2.5 eV bandwidth) and probe with a red-shifted 13 fs pulse covering the 1.45-1.2 eV range and a 9 fs pulse at 1.2-0.7 eV. Temporal resolution of our apparatus is less then 15 fs [3].

Pump-probe experiments are carried out on single-layer graphene films grown by chemical vapor deposition and transferred onto a 100-μm-thick fused silica substrate. In our experiments we observe a prompt rise of the photobleaching signal in the near-IR, that already points out to an ultrafast e-e relaxation, taking place over a timescale comparable to our temporal resolution (see Fig. 1.a). By shifting the probe pulse even to longer wavelenght we can observe a clear delay of ~50 fs in the formation in the bleaching signal (see figure 1.b). If we compare the two-color pump-probe experimental data with different models, that solve the quantum Boltzmann equation by implementing three different screening methods (see fig 1c), we can visualize the importance of Auger recombination processes, such as carrier multiplication, in the ultrafast relaxation of the electronic distribution in graphene.
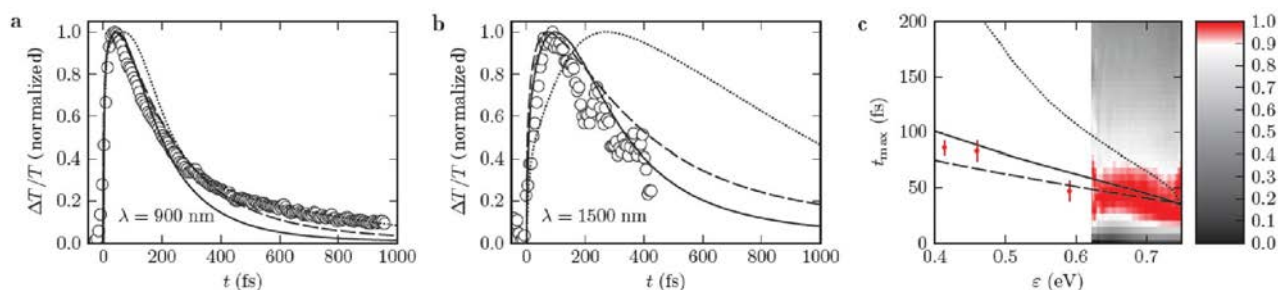
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#423 - Longitudinal acoustic phonons in 3-dimensional cobalt supracrystals detected by broadband picosecond acoustics

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Ultrashort light pulses allow to launch and observe coherent phonons in the time domain, providing a powerful alternative to inelastic light scattering techniques. A commonly use method is interferometric picosecond acoustics, a pump-probe technique in which an ultrashort optical pump pulse is partially absorbed by a thin metallic transducing layer deposited onto the surface of the sample, and launches by "instantaneous" thermal expansion a longitudinal acoustic wave-packet with a characteristic spectrum extending in the 40-400 GHz region. The acoustic pulse then travels inside the sample and its motion is monitored by a delayed optical probe pulse. We recently developed a novel setup for broadband picosecond acoustics using a white-light continuum probe coupled to an optical multichannel analyzer [1]. The system allows one to access, in a single measurement, acoustic parameters such as sound velocity and attenuation all over the whole bandwidth of the acoustic wave-packet launched by the pump pulse.
We will present the application of this setup to the study of solids and nanostructured materials. In particular we will report on the detection of longitudinal acoustic phonons with few-GHz frequency in three-dimensional supracrystals (with face-center cubic lattice) of 7-nm cobalt nanocrystal spheres. In analogy with usual atomic crystals, where longitudinal acoustic phonons propagate with the speed of sound through coherent movements of atoms of the lattice out of their equilibrium positions, in these supracrystals atoms are replaced by (uncompressible) nanocrystals and atomic bonds by coating agents (alkyl chains) which act like stiff mechanical springs holding together the nanocrystals. We could extract the speed of sound inside the supracrystal, which is 1100 ± 100 m/s at room temperature. Very interestingly, the speed of sound is found to be strongly dependent on the sample temperature: its value increases from 760 m/s at 410K to 3140 m/s at 110K, with a change in speed/temperature slope at approximately 250K. Such change can be associated to a temperature transition and is attributed to a change in the alkyl chain configuration from ordered to disordered.

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#424 - Time-resolved cluster dynamics driven by 1.5 micron laser pulses

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The ultrafast microscopic dynamics of atomic clusters exposed to intense femtosecond laser pulses has been extensively studied in the past [1]. However a common aspect to most studies was the exploitation of 800 nm driving pulses. In this work, by exploiting an ultrafast optical parametric amplifier [2], we extend these studies to mid-infrared (MIR) driving pulses in pump-probe configuration.
20 fs, 1.1 mJ MIR laser pulses at 1.5 µm (driver) were collinearly combined by a dichroic mirror with 100 fs, 450 µJ pulse at 800 nm (heater); afterwards the pulses were focused by a spherical mirror (R = -250 mm) in a jet of Kr clusters (estimated average size N $\cong$ 5000) produced by an Even-Lavie valve. The XUV radiation emerging from the interaction region was detected by a flat-field spectrometer operating in the 13-50 nm range as a function of the nominal delay τ between the two pulses. For large and negative delays negligible XUV emission was observed. Very strong emission from several ionized stages of Kr could be detected for positive delays; according to tabulated data [3] contributions coming from Kr^{3+} up to Kr^{9+} could be observed along with emission from N3+ and O^{3+} ions. The temporal evolution of the Kr XUV emission shows that the signal forms in about 300 fs and decays completely in about 1.5 ps. Moreover, emission from different ionized species show slightly different temporal dynamics.
In accordance to the cluster explosion mechanism, our outcomes can be interpreted as follows: the MIR driver photo-ionizes the clusters and accelerates electrons to large ponderomotive Up energies, thanks to the favourable scaling of Up with the driving wavelength; these electrons initiate impact ionization of atoms and ions. Then the clusters start to expand and their electron density change accordingly. If the heater comes before or slightly after the driver, modest effects are seen in the XUV emission since the heater is not efficiently absorbed by the clusters. However, in a range of suitable delays, the plasma density reaches a value which allows a resonant and efficient absorption of the heater. Impact ionization and excitation predominates at these delays, thus leading to strong radiation emission. For larger delays the plasma density drops owing to expansion and the heating mechanisms is inhibited again.
These results show that MIR sources can be efficiently exploited in the investigation of laser-cluster interaction, allowing to understand the role of photoelectron acceleration to large ponderomotive energies in the early stages of the process.

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#425 - Attosecond control of electron dynamics in highly-excited nitrogen molecules

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The ultrafast dynamics induced by photo-ionization in atoms and molecules plays an important role in a number of fundamental physical and chemical phenomena [1]. Understanding the coupling of electronic and nuclear degrees of freedom as well as the electron correlations immediately following, or accompanying, optical excitation is particularly important and requires the use of ultrafast methods [2,3].

In this work we photo-ionized N_2 molecules with attosecond pulses and we probed the ultrafast dynamics using 800 nm, 5 fs pulses. Attosecond, extreme-ultraviolet (XUV) pulses were produced by high-order harmonic generation in gas. A velocity-map imaging spectrometer was used to record the kinetic energy and momentum angular distribution of the N^+ ions resulting from the dissociative ionization induced by the attosecond pulses. The evolution of the kinetic energy release of N^+ ions vs. the delay between XUV and IR pulses shows two different processes. The first one, in the energy range between 2.3 eV and 3.7 eV, is characterized by a temporal evolution with a time constant of about 100 fs. We have demonstrated that this process is related to autoionization of highly excited states of N_{2+} [4]. In particular, the pump-probe data offer a clear evidence of a crossing between the potential energy curves of the highly excited N_2^+ ion and of the N_{22}^+ ion. It is found that the autoionization becomes energetically allowed when the two nuclei are still very close (about 3 Å) and that it can be coherently manipulated by a strong femtosecond infrared pulse. The second relaxation process, at ion energies below 2.5 eV, exhibits a faster temporal evolution, which can be explained in terms of a two-color dissociation mechanism. At short time delays (< 30 fs), the IR pulse induces the formation of an additional band between 1.3 and 2.5 eV, which subsequently disappears with a time constant < 20 fs. The formation of this band is delayed (delay about 7 fs) with respect to the formation of the high-energy band discussed above. The dynamics of the second process displays clear sub-cycle oscillations, resulting from coupling between different electronic states of the molecule.

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#426 - Active mode-locking of THz quantum cascade lasers

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Quantum cascade lasers are today very attractive powerful semiconductor light sources in a vast frequency range, spanning from the THz region up to 3 μm wavelength in the mid-infrared. In the past few years we have investigated the possibility of merging QC lasers with very well established technologies such as μ-waves and telecommunications in order to speed up their commercial exploitation [1]. We believe that by applying concepts and techniques that are imported from microwave technology, it will possible to spark new ideas for system applications and motivate physical investigations of carrier dynamics of QC lasers.

In this presentation, I will focus on the phase-locking and active mode-locking of THz quantum cascade lasers (QCLs). I will show experimental results on direct current modulation of mid and THz QC lasers [2,3] and demonstrate that when the frequency modulation matches the cavity resonance frequency – the roundtrip frequency – the QC lasers is injection-locked. In this situation the THz QC lasers enter in a regime of active mode-locking, generating ~10 ps wide pulses at a repetition rate of ~13 GHz [4]. Finally I will illustrate a coherent detection technique which allows the direct measurement of electric field of the mode-locked QC lasers. This coherent technique is enabled by the phase-locking of the of THz QC lasers to a harmonic of the repetition rate of an erbium-doped fs-fiber laser [5].

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#427 - Nonlinear microresonators: towards integrated ultrafast optical clocks

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Moving toward next generation time-domain multiplexed optical networks, a potential solution for the demand of pulsed laser with hundreds of GHz repetition rates and beyond is represented by passive mode locked lasers, free of the bandwidth bottleneck imposed by electronics. Among the many different methods to integrate such type of sources, some of them relies on very short semiconductor amplifying cavities where a very high repetition rate is achieved by simply reducing the pulse round-trip time, at the expense of the laser lines quality [1,2,3]. Very recent alternative approaches rely on external amplifying elements or pump lasers, like laser-pumped coherent optical parametric oscillator in silicon platforms [4,5] or our recent remonstration of a fully mode-locked ps and sub-ps source based on an integrated nonlinear resonator closed in an amplifying external loop [6,7]. These solutions are based on the development in the fabrication nonlinear micro resonators with Q factors exceeding 1 million and free-spectral-range above 100GHz that recently achieved the compatibility with the technologies of the electronic CMOS fabrication. An overview of the field with our investigations on the topic will be presented in details.

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#428 - Measurement of the subband electronic and lattice temperatures in scattering-assisted terahertz quantum cascade devices

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The terahertz quantum cascade laser (THz QCL) is one of the most promising sources for the generation of terahertz radiation. However, their operation is still limited to cryogenic temperature. The most used THz QCL share an active region scheme based on a resonant tunneling injection directly in the upper laser state. These devices appear to be limited to a maximum operating heat sink temperature $T_H < \hbar\omega/K_B$ (K_B is the Boltzmann constant). Recently a new active region scheme has been proposed, named scattering-assisted (SA) injection scheme, providing the possibility to circumvent the above limit. In this scheme, the energy difference between the injection level and the upper laser level is kept resonant to that of a longitudinal-optical (LO) phonon, so an efficient depopulation via electron-LO-phonon scattering is assured. A critical understanding of the actual lattice temperature (T_L) and the individual j-th subband electronic temperatures (T_e^j) is crucial to refine the design of THz QCL active regions with improved thermal

performance.

In this work we compare experimental results on the subband electronic and lattice temperatures for three GaAs/Al$_{0.25}$Ga$_{0.75}$As QCL active region structures based on the SA injection and resonant-phonon depopulation scheme. The investigated devices mainly differ for the energies of the phonon-assisted transitions as compared with the LO phonon energy. The experimental technique is based on micro-probe band-to-band photoluminescence experiments that allows the investigation of the device front facet down to a spatial resolution of ~ 2 µm. The electronic temperature is extracted by the lineshape analysis of the high energy slope of the photoluminescence bands. T_L is extracted by comparing the photoluminescence peak energy shift induced by heating with a calibration curve obtained by probing the device at zero-current while varying the heat sink temperature. A non-equilibrium hot electron distribution has been found above the band alignment for lasing. Differently from resonant phonon scheme where electrons are directly injected into the upper laser level, causing a large extra heating with respect to the lattice, in the investigated phonon-SA injection and extraction scheme both laser levels remain much colder and share the same electronic temperature of the extractor level while the injector level is the hottest one. At the largest value of the dissipated electrical power (~ 6 W) the extra-heating of the injector level respect to lattice is ~ 36 K while the extra-heating of the upper laser level respect to the lattice is ~ 26 K. The observed T_e increases are much smaller than what previously observed in THz QCLs (T_e - T_L ~ 100 K for 3 W of dissipated power in devices based on resonant-phonon active region scheme).

#429 - Ultra high figure of merit hydrogenated amorphous silicon waveguides for all optical signal processing

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Hydrogenated amorphous silicon (a-Si:H) is emerging as a promising new platform for silicon photonics. Low temperature required for its deposition provides an excellent compatibility with CMOS processes. Besides, recent works have pointed out that a-Si:H exhibits an enhanced nonlinear efficiency that, combined with low linear losses, makes this material as an ideal candidate for the development of all - optical signal processing silicon devices.

In this paper we present the results of an extensive characterization of a-Si:H waveguides fabricated by CEA-Leti.

The a-Si:H film was deposited by plasma enhanced chemical vapor deposition (PECVD) at 350 °C on 1.7 µm oxide layer deposited on a bulk wafer. After deposition of a silica hard mask, grating couplers were fabricated through two steps of 193 nm DUV lithography and HBr silicon etching. Several straight and serpentine waveguides (500×220 nm cross-section) were obtained with lengths varying from 0.2 cm to 8 cm. Finally, a 500nm oxide upper cladding was deposited on top of the waveguides.

The nonlinear Figure of Merit, defined as FOM = $(1/4\pi)(Re\{\gamma\}/Im\{\gamma\})$, was measured, carrying out both Continuous Wave (CW) and pulsed sources experiments.

The nonlinear efficiency was tested by means of a Four Wave Mixing (FWM) experiment using an intense CW pump and a weaker signal, tunable in the range 1530-1560 nm. In order to measure the real part of the nonlinear parameter γ, pump and probe signals wavelengths were initially set close each other (~0.4 nm), as to make negligible the role of the phase-mismatch. The power values were kept below the saturation threshold associated with the insurgence of Two Photon Absorption (TPA) and Free Carrier Absorption (FCA). The conversion efficiency, evaluated as the ratio between the power of converted beam and signal beam at waveguide output, for an input pump power of Pp = 6 dBm, is -29.4 dB. The analysis of the results obtained for several values of the input Pp and tested on a large number of different samples provides a reliable value of the real part of the nonlinear parameter Re{γ}= 790 ± 50 (Wm)$^{-1}$ which is in good agreement with some of the reported results for similar waveguides.

The imaginary part the nonlinear coefficient was also evaluated by means of an ultrashort pulse (120 fs @ FWHM, 82 MHz) transmission experiment, carried out at different power level. By evaluating the average transmitted power as a function of the average input power, we obtained the imaginary part of γ, which is Im{ γ}=20±1 (Wm)$^{-1}$.

By combining the measured real part and imaginary part of γ, a FOM=3.06 is obtained, which is ten times higher than the values measured for Crystalline Si strip waveguides with the same cross section.

#430 - High quality factor 1-D Er^{3+} activated dielectric microcavity fabricated by RF sputtering

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In the last decade a remarkable increase in the experimental efforts to control and enhance emission properties of emitters by tailoring the dielectric surrounding of the source has been performed [1, 2]. With this aim, several approaches, using nanocomposite materials or specific geometries, such as planar interfaces, photonic crystals, solid state planar microcavities, dielectric nanospheres, and spherical microresonators, have been proposed. Among these systems, planar microcavity resonators, also called one-dimensional (1-D) photonic crystals, are the simplest photonic band-gap (PBG) device exploitable to manage the spectroscopic properties of luminescent species such as rare earth ions, and quantum dots [1]. Oxide-based dielectric materials are particularly suitable for fabricating PBG structures because they have wide transparency from the ultraviolet to the near infrared and have good resistance to temperature, corrosion and radiation as well [1]. We have demonstrated as the rf sputtering is an extremely appropriate candidate to fabricate high quality and homogeneous 1-D photonic crystals [1, 3]. In this article, we report on a reproducible fabrication protocol based on rf-sputtering technique and on optical, spectroscopic and morphological characterization of the realized

high quality Er^{3+}-activated dielectric microcavity consisting of alternating silica and titania films. The cavity is constituted by an Er^{3+}-doped SiO_2 active layer inserted between two Bragg reflectors consisting of ten pairs of SiO_2/TiO_2 layers. Scanning electron microscopy is employed to put in evidence the quality of the sample, the homogeneities of the layers thickness and the good adhesion among them. Near infrared transmittance and variable angle reflectance spectra confirm the presence of a stop band from 1500 nm to 2000 nm with a cavity resonance centered at 1749 nm at 0° and a quality factor of 890. The influence of the cavity on the $^4I_{13/2} \rightarrow$ $^4I_{15/2}$ emission band of Er^{3+} ion is also demonstrated [1].

Acknowledgments: This research activity was performed in the framework of the ITPAR Phase III project.

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#431 - Effect of ultrasmall Au-Ag aggregates in Er-implanted silica on the 1.54 micron Er^{3+} luminescence

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An efficient way to increase the light emission from rare-earth ions in silica-based glasses, critical for photonic applications, is to embed ultra-small (i.e. subnanometer) metallic aggregates in the rare-earth doped glass: these clusters absorb light in a broad band and transfer part of the absorbed energy to rare-earths, that then de-excite radiatively. This process leads to an increase of the rare-earth excitation cross section up to three orders of magnitude. A very efficient energy transfer from small clusters to rare earths has been experimentally demonstrated for Au, Ag and Cu clusters. Metal ion implantation, followed by annealing at defined temperature and in selected atmosphere, is an elective tool to obtain a homogeneous distribution of small metallic aggregates in a dielectric thin film and to control the metal nucleation. In this work we focus on the use of bimetallic subnanometer Au-Ag structures to further improve the efficiency of the energy transfer process towards Er^{3+} ions in silica. Silica slides are first implanted with Er, and then annealed to activate the Er photoluminescence. Er-doped slides are then sequentially implanted with Au+Ag, to form subnanometer bimetallic aggregates. The role of separate Au and Ag clusters or of Au-Ag alloy structures on the Er^{3+} luminescence is experimentally investigated by x-ray absorption spectroscopy and by photoluminescence experiments.

#432 - Photorefractive response in the visible range of Mg- and Zr- doped lithium niobate crystals

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Lithium Niobate (LN) plays a key role in integrated optical devices for electro-optic (EO) signal modulation and frequency conversion. Unfortunately the use on LN for nonlinear optical devices is limited by the presence of photorefractivity in such crystals. Usually, photorefractivity can be strongly reduced keeping LN devices at high temperature (e.g. >100 °C), or using a doped-LN substrate, such as MgO-doped LN, to realize the components. Even if both these strategies are currently used they are not completely satisfactory: keeping the device at high temperature may reduce components reliability, and using 6 mol% MgO-doped LN requires to completely modify several fabrication processes, such as crystal poling and waveguide fabrication, as the Mg presence drastically affects substrate properties. It is known from the literature that photorefractive-resistant LN samples can be also obtained using a small amount (<3 %) of a tetravalent dopant, such as Zr. Zr-doped LN shows interesting aspects with respect to other doped substrate, in fact a lower dopant concentration eases the growth of large homogenous crystals, and also reduces the influence of the dopant ion on waveguide realization and crystal poling.
We will show a comparison of the photorefractive response of Mg-doped and Zr-doped crystals as a function of the wavelength in the visible. We measured the photorefractivity-induced beam-distortion on 4 mm thick samples (so as to obtain a high sensitivity to photorefractive effect), recording the beam shape in far field, both the time evolution, using high fps camera, and the final image once the effect has reached its steady-state. Three different laser sources (emitting a CW beam at 488, 532 and 775 nm) and four different intensity levels (in the range 1 - 100kW/cm^2) were considered, so as to relate the photorefractive response of the material to both the beam intensity and wavelength. The measurements were conducted on a series of samples with different Zr content and on a commercial Mg-doped sample. The analysis of the beam-distortion time-evolution shows a clear dependence of the photorefractive response on beam wavelength and intensity, as well as on Zr content. The obtained results show similar performances between Mg-doped and Zr-doped samples, even if some small differences in the wavelength dependence of photorefractivity appear, thus suggesting a different distribution of defects levels in the band-gap. This result, combined with the fact that Zr-doping allows easier waveguide realization and periodic poling (still unpublished results, manuscripts are under preparation), pushes for the development of industrial-quality large Zr-doped LN wafers, that could replace the current standards given by Mg-doped and pure congruent LN.

#433 - Backscattering differential ghost imaging in turbid media

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Ghost Imaging (GI) is a technique for the recovery of images by means of the spatial intensity correlation function of two light beams at the output of a beam splitter. In particular, the correlation is performed between a bucket detection of the light which has passed through an object and the two dimensional reference intensity distribution measured by a spatial-resolving detector.

Beyond a first academic approach to this technique, which includes a long-term debate on the classical or quantum-like nature of the correlations, GI begun to be employed in physical situations of more practical interest, such as compressive sensing and imaging in noisy environments. Improvements of the technique, such as differential ghost imaging [1], opened the way to the GI of weakly absorbing objects with a high signal-to-noise ratio.

In our work [2], we show that GI can be profitably used in a backscattering configuration for the imaging of small absorbing objects immersed in a turbid medium, in proximity of its surface. We present a study based on a detailed and quantitative comparison between GI and standard noncorrelated imaging techniques. In particular, we show that (*i*) GI recovers images with a contrast much better than noncorrelated *direct imaging*, which is the technique commonly used in biomedical imaging of superficial tissues and, (*ii*) it performs almost identically to an innovative method that we proposed for the first time in this work and called *diffusive imaging*, where the object is trans-illuminated by the light diffused by the turbid medium.

Within this picture of different optical imaging schemes, we describe a simple but efficient theoretical model capable of providing a correct interpretation of the experimental results.

A second seminal work on the GI of phase objects is presented. In order to measure the phase gradient of the object, we perform the difference of two GI images obtained by filtering the Fourier plane of the object image in two different parts, similarly to the Schlieren method. Theoretical and numerical analysis are presented, together with the first promising experimental measurements.

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#434 - Effect of functionalized gold nanoparticles on floating lipid bilayers

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The development of novel nano-engineered materials poses important questions on how these new materials will interact with living systems. On the one hand, possible adverse effects must be assessed in order to prevent risks for health and environment [1]. On the other hand, the understanding of how these materials interact with biological systems might result in the creation of novel biomedical applications [2]. We present a study on the interaction of model lipid membranes with gold nanoparticles (NP) of different surface modifications. Neutron reflectometry experiments on zwitterionic DSPC and two-component negatively charged DSPC/DSPG double bilayers were performed in the presence of gold nanoparticles (NP) functionalized with cationic and anionic head groups. Structural information was obtained that provided insight into the fate of the NPs with regard to the integrity of the model cell membranes. The NPs functionalized with the cationic head groups penetrate into the hydrophobic moiety of the lipid bilayers and cause membrane disruption at higher concentration. In contrast, the NPs functionalized with the anionic head groups do not enter, but rather stabilize the lipid bilayer at alkaline pH [3]. The information obtained might influence the strategy for a better nanoparticle risk assessment based on a surface charge evaluation and contribute to nano-safety considerations already during their design.

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#435 - A Time-of-flight chopper spectrometer for poly-chromatic investigations @ESS

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Within the ESS Design Update Phase Programme funded by the German Federal Ministry of Education and Research, we investigate the performance of a suit of time-of-flight spectrometers at the future ESS long pulse source. The instrument set promises the applicability to a wide manifold of scientific research activities: strongly correlated electron materials, disordered systems, functional materials, magnetism, soft-matter and biophysics.
Here we present the current state-of-the-art in the study of a wide wavelength band spectrometer concept and describe the main aspects of the conceptual design. The instrument is supposed to accept neutrons generated both at the cold moderator and the thermal pre-moderator, by making use of a super-mirror extraction system. The chopper system is specifically designed to make an efficient use of the flux provided by the source, by means of a combination of the poly-chromatic operation methods: Repetition Rate Multiplication (RRM) and Wavelength Frame Multiplication. It is integrated with a specially developed pulse suppression chopper that enables variable acquisition time frames, by means of selective pulse suppression of the sub-pulses generated by the resolution defining choppers.
As the secondary spectrometer is characterized by a 3 m detector covering a wide angular range, the instrument allows to carry out poly-chromatic measurements in a dynamic range that is estimated in 1-200 meV and 0.05-10Å^{-1}, thus leading to exploration of the reciprocal space in a wide range. The energy and wave-vector resolution can be adapted by quantized variation of the commensurate chopper frequencies. Simulations performed by means of ray-tracing methods, showed that the elastic energy resolution varies in the range from 1.2 % to 3 % at 5meV and from 5 % to 15 % at 82 meV, providing flexible trading of resolution for flux.
The instrument is specifically designed to allow the use of polarized neutrons and exploit the XYZ polarization analysis, by means of the so-called MAGIC Pastis coil layout. A prototype is under construction for the TOPAS spectrometer at the FMR-II, which uses a wide-angle banana shaped 3He Neutron Spin Filter cell to cover a large range of scattering angle, both in horizontal and vertical direction.

#436 - Kinetics of lipid exchange in model bilayer systems

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The phospholipid bilayer is the basic structural motif of most biological membranes. Many biological processes occur within or in the proximity of the membrane, and therefore, there has been considerable interest in the study of the properties and behavior of organized lipid layers. Lipid translocation in membranes is a crucial process in biological science still far from being understood and characterized. In nature the lipid distribution across the inner and outer leaflet of cell membranes is asymmetric [1] and this asymmetry plays a prominent role during cell fusion, activation of the coagulation processes, recognition and removal of apoptotic cell corpses by macrophages [2].
In literature big discrepancy between the typical timescale and the occurrence of lipid flip-flop in model bilayer systems are present [3,4] but these results were based on indirect observation of the process.
By neutron reflectometry it is possible to detect directly a compositional asymmetry in a lipid bilayer. We have recently shown [5] that an asymmetric reconstituted system, where traps and enzymes were not present, spontaneously relaxed towards the symmetric structure if the lipids were in the fluid phase i.e. in biological relevant conditions. Moreover, by joint neutron reflectometry and small

angle scattering experiments, it was possible to model the temperature dependence of lipid translocation and exchange processes between the reference bilayer and a "bulk" reservoir of lipids providing then a clearer interpretation of the process.

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#437 - What can the European Spallation Source do for fusion?

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A large effort is being put into understanding how to best exploit the capabilities of the European Spallation Source (ESS). An area that has so far received limited attention is fast neutron applications. Yet the intense (up to 10^{15} n/cm^2/s) fast neutrons fluxes expected at ESS could be used for valuable applications other than the neutron scattering studies using low-energy neutrons, for which the facility is designed.

The use of fast neutron ports for irradiation of materials is already within the scope of ESS. Materials will be irradiated for the investigation of radiation effects on, e.g., structural components in use at ESS. Further applications can be considered taking into account earlier studies on the use of fast neutron fluxes at spallation sources (especially, SNS and earlier ESS concepts). Foreseeable applications include

• testing of fusion reactor materials
• testing of fast fission reactor materials
• radionuclide production for nuclear medicine,
• electronic chip irradiation.

Applications to fusion reactor materials are especially intriguing. On one hand, the need for dedicated neutron sources (i.e. IFMIF, MTS) has been clearly advocated in the recent past and there is no reason to believe that ESS could provide a replacement. On the other hand, the early availability of an intense source would allow for testing of fusion materials in parallel with the early ITER operation. Results of neutron transport simulations of the latest ESS target and moderator assembly will be reported that suggest that the ESS can, in principle, offer an attractive range of values for the key parameters (i.e. dpa, He and H production) for fusion-related studies.

Further applications of the ESS of relevance for fusion research are based on the use of thermal/cold neutrons. Plasma-facing and structural materials pose questions on their mechanical strength, but also on wall erosion and consequent deposition; the crystal structure of the deposits can be investigated by neutron diffraction, especially in the case of low-Z materials. Residual stresses induced in metals and alloys are investigated by Neutron Diffraction (ND) in diffusion or transmission geometry, and by Energy-selective neutron transmission imaging. Finally gas retention in plasma-facing materials is studied by Small Angle Neutron Scattering (SANS). All these neutron-based techniques are available at present-day neutron facilities but can be further optimised by dedicated developments on ESS.

#438 - Speckle sensing microscopy for fast detection of malaria

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Malaria is an infectious disease caused by the bite of a female anopheles mosquito infected by Plasmodium. Every year, 243 million new cases are reported by the World Health Organization (WHO) with almost a million deaths, mostly of African children. Diagnosis of malaria must be rapid, accurate, simple to use, portable and low cost, as suggested by the WHO [1]. Despite recent efforts, the gold standard remains the light microscopy of a stained blood film. This method can detect low parasitemia and identify different species of Plasmodium but it has some inconvenient. The time to diagnosis is about 8-10 hours in African medical centers [2]. The cost of equipment and training is considerable, even if the apparent cost for an individual sample examination is relatively low. Moreover, the equipment cannot be easily transported and installed. An improvement of diagnostic tools is in this context highly demanded. New innovative technologies could be used to enhance the accuracy while reducing time, complexity and cost of actual diagnosis.

In this work we propose a new technique called "secondary speckle sensing microscopy" (S3M) to implement fast and accurate detection of malaria [3]. The approach involves illuminating the red blood cells (RBCs) with a tilted laser beam and capture the time varied speckle patterns generated due to the thermal vibration of the RBCs for one second. The patterns are analyzed via a correlation based algorithm that extracts the change in the position and in the value of the correlation peak. Then, the statistics related to the position and value of the correlation peak is analyzed using two automated approaches: fuzzy logic based ruling and principle component analysis (PCA). We present the compact portable system, the detection processing and preliminary experimental results demonstrating the potential for automatic detection of malaria. Preliminary experimental results show high capability of detection of infected cells (100% probability using PCA analysis). The combination between the fuzzy logic and the PCA analysis can provide also good results in detection of healthy cells (both techniques produce errors for different samples).

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#439 - Time-resolved fluorescence resonance energy transfer as a diagnostic tool for population screening of susceptibility to diabetes

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The highly polymorphic DQB1 human gene is used as a marker for the assessment of compatibility in organ transplantation. Moreover, it is known that manifestation of certain DQB1 allelic variants is associated with the susceptibility to insulin-dependent diabetes mellitus (IDDM).

Distinguishing the subjects with IDDM susceptible genomes before the onset of the disease discloses important opportunities of risk-factor evaluation and early diagnosis. The ambition of introducing wide-scale preventive screening protocols calls for the development of rapid high-throughput DQB1 typing technologies. Although sequencing is the election technique for characterizing genes polymorphism at the academic level, its cost makes any wide-range application impractically expensive. Nevertheless, as the possible allelic variants of DQB1 have been previously determined, it is feasible to assess which of them are manifested in one given genome without recurring to sequencing. Techniques allowing this kind of assessments are called molecular typing techniques. Quantitative assessment of the fluorescence resonance energy transfer (FRET) efficiency between chromophores labeling the opposite ends of gene-specific oligonucleotide probes is a powerful tool to type DNA polymorphisms with single-nucleotide resolution. The FRET efficiency can be most conveniently quantified by applying a time-resolved fluorescence analysis methodology, time-correlated single-photon counting. Recently, we showed that by this method it is possible to pursue the recognition of pathogenic genomes by working on non-amplified DNA samples contained in untreated cell extracts. Namely, we focused on the homozygous DQB1-0201 genotype, which is over-represented in subjects affected by IDDM in north-eastern Italy. To this aim, a single oligonucleotide probe complementary to the sequence displayed by the DQB1-0201 variant in a highly polymorphic trait of DQB1 was made to hybridize to any of the eight possible allelic variants. As a tag of each allele, the fluorescence lifetime of the donor fluorophore labeling the probe was measured with 30 ps resolution. Unambiguous identification of subjects bearing the homozygous DQB1-0201 genotype was obtained by exploiting the subtle, yet statistically significant, structural differences between the duplex formed by the probe with DQB1-0201 on the one end and duplexes formed with any of the other alleles, on the other end. Here we report on additional in-vitro experiments aimed at characterizing the duplexes obtained by annealing of the DQB1 allelic variants with a second oligonucleotide probe, with the final goal to achieve full genotyping of DQB1 on raw DNA samples by means of cross-combination of the FRET responses of both probes.

#440 - A combined fluorescence-Raman optical probe for tissue diagnostics applications

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The recent introduction of optical and spectroscopic techniques in the clinical settings is contributing to the achievement of a more accurate tissue diagnostics. The majority of these techniques is based on tissue auto-fluorescence or on spontaneous Raman scattering. Tissue auto-fluorescence takes advantage of the signal generated by endogenous molecules and has been already demonstrated as a possible method for diagnosing tissues in various conditions. Raman spectroscopy takes advantage of the inelastic scattering process in which non-resonant photons excite vibrational molecular modes. The measurement of the energy lost in the process allows measuring a vibrational spectrum, characteristic of the molecule involved in the process. With the technical improvements in optical fibre technology, new flexible fluorescence and Raman probes, employing optical fibre bundles, have been developed.

In this work, we designed and developed two different optical fibre probes for combined Raman and fluorescence measurements on human tissues. The devices were successfully used for diagnosing melanocytic lesions in a good agreement with common routine histology, and further tested on both colon and brain tissues. The diagnostic capabilities of the method in discriminating between various skin lesions were evaluated by means of a scoring algorithm, finding a 89% sensitivity, 100% specificity for discriminating melanocytic nevus from malignant melanoma. Additional measurements were performed on colon tissue including healthy colon mucosa, adenomatous polyp and adenocarcinoma, as well as on brain tissue affected by glioma and dysplasia.

In conclusion, we demonstrated the capability to discriminate among melanocytic lesions in a good agreement with "gold-standard" histology. The combination of fluorescence and Raman spectroscopy provided also a more detailed classification of colon and brain lesions. Our system can potentially contribute to improve clinical diagnostic capabilities on a broad range of tissues.

#441 - Extension of time-domain diffuse spectroscopy beyond 1100 nm

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Time-resolved diffuse spectroscopy permits to recover the absorption and scattering spectra of a diffusive material from the temporal broadening of a laser pulse travelling through the medium, with applications to non-invasive medical diagnostics, like detection of breast cancer or functional imaging of brain activation. Up to now, most of time-resolved studies have been performed in the 600-1100 nm range, while there are no broad-band in-vivo works beyond 1100 nm. The main problem is the difficult combination of continuously tunable sources and detectors with sensitivity down to the single-photon level, together with high absorption and low scattering properties of the probed medium, which can distress both the detection system and the analysis tools.

In this work we present a unique system for broadband diffuse optical spectroscopy working in the time-domain and operated beyond 1100 nm up to 1700 nm. The system is composed of a supercontinuum source coupled to a prism-based optical stage for continuous and PC-controlled slicing of gaussian-like spectral pulses. Detection is achieved using a properly designed free-space coupled time-gated InGaAs/InP Single-Photon Avalanche Diode (SPAD), while pulse timing is performed by a Time-Correlated Single-Photon Counting board.

The system was thoroughly tested on calibrated tissue phantoms, demonstrating a record linearity range extending in absorption up to 3.4 cm^{-1} thanks to a tight optimization of the measurement system and the adoption of a Monte-Carlo based iterative fit for the recovery of the optical properties.

The uniqueness of the proposed system permitted to achieve the first time-domain spectral measurements of biological tissues and key tissue absorbers beyond 1100 nm. Namely, the absorption spectrum of collagen powder is derived in the whole 900-1700 nm range, exhibiting important peaks around 1200 nm and 1500 nm. Further, in-vivo absorption and scattering spectroscopy of the arm and the breast of healthy volunteers were collected in the spectral range 960-1360 nm. From the absorption spectra we can recognize a major peak around 1200 nm mostly due to lipids and a steep increase for longer wavelengths mainly caused by water.

These results demonstrate the feasibility of time-domain diffuse optical spectroscopy beyond 1100 nm, in a spectral range still largely unexplored that could be valuable to identify important constituents (e.g. collagen, glucose, elastin) whose detection in the <1100 nm range is quite challenging.

#442 - A method for discriminating systemic and cortical hemodynamic changes by time domain fNIRS

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Functional near-infrared spectroscopy (fNIRS) is an optical technique to non-invasively measure hemodynamic response in the human brain cortex. Differently from continuous wave fNIRS, the time domain (TD) approach to fNIRS intrinsically has the potentiality to infer depth information from the time-of-flight of collected photons, and thus to discriminate superficial (systemic) from deeper (cortical) hemodynamic changes. However the depth selectivity is still an open issue, especially for what concerns absolute quantification of cortical hemodynamic changes: key point is in fact the correct quantification of the time-dependent photon pathlength, that is the time spent by photons in the perturbed (e.g. cortical) area. In this work a novel method in TD fNIRS, based on a precise computation of the mean photon pathlengths within a multilayered medium, is proposed. The new method has been

validated by means of numerical simulations and its range of applicability assessed. The influence of various parameters has been tested and this can be exploited to choose the optimal configuration of device and experimental setup. Preliminary analyses on in vivo TD fNIRS measurements have been performed, confirming the applicability of the new method on real data and its good ability to reject superficial contribution from cortical hemodynamic changes.

#443 - Small-scale laser based electron accelerators for biology and medicine: a comparative study of the biological effectiveness

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Electron accelerators relying on the Laser WakeField Acceleration mechanism in plasmas are now entering a mature phase, allowing them to be considered as reliable alternatives to the RF LINACs used in medical practice such as, for instance, radiotherapy. As a matter of fact, electron accelerators based upon ultrashort and ultraintense table-top lasers exhibit a wealth of advantages when compared to conventional accelerators in terms, for instance, of radioprotection requirements, operation reliability and flexibility and so on. Furthermore, due to the intrinsic accelerating fields being much larger than those achievable with RF LINACs, electron bunches with energies up to a few tens or even hundreds of MeV would be easily achievable, thus representing a new option in radiotherapy and other medical practices.

As of today, the figures of the electron bunches delivered by small-scale laser based accelerators are comparable to the ones produced by conventional LINACs as for electron energy, total charge, average current and delivered dose, etc. However, due to the ultrashort bunch duration (of the order of a few up to a few tens of femtoseconds), the peak current is much higher (typically, up to six orders of magnitude) than in conventional LINACs. From one side, this opens up a wealth of potential new studies and applications, involving possible unexplored biological responses to such high electron currents. On the other hand, this demands accurate studies at a pre-clinical stage before even considering laser- driven accelerators for an actual medical use. The group operating at the Intense Laser Irradiation Laboratory of the CNR in Pisa is currently pursuing a 3-year project aimed at sudying the biological response to electrons from laser-driven accelerators. The project gathers together people with multidisciplinary expertises (namely, physics, medicine and biology). As a starting point, different human cells (namely, human lymphocytes and fibroblasts) have been irradiated using laser-accelerated electrons at low energy (up to a few MeV) and the induced biological effects in terms of cell alteration and survival have been studied by means of well-established biological techniques (MN assay, scoring of gamma-H2AX, etc.). The delivered dose was studied by combining experimental measurements and Monte Carlo (GEANT4 based) simulations. The biological response was compared to the one induced with electrons produced by a conventional LINACs used for Intra-Operatory Radiotherapy and/or to previous results obtained with LINACs found in the literature. A discussion of the experimental issues and the obtained results will be given together with an overview of the planned activity for the next few years.

#444 - Azo functionalized iron oxide nanoparticles for sub-nanometer spatially resolved temperature mapping and drug release modulations

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Local heating can be produced by iron oxide nanoparticles (IONPs) when exposed to an alternating magnetic field (AMF). We developed a molecular temperature-probe based thermo-labile azo-ligands anchored to superparamagnetic nanoparticles via PEG spacers. We have demonstrated that these azo-probes can be utilized for: i) spatially resolved measurement of temperature surface profile on dilute solutions of iron oxide nanoparticles exposed to an AMF with sub-nanometer resolution and ii) as linker between the cytostatic drug doxorubicin and a PEGylated iron oxide nanoparticle for AMF triggered drug release. Upon excitation with an AMF, the local temperature around the nanoparticle decays exponentially with increasing distance. Significant local heating, with a temperature increase up to 45 K, was found at distances below 0.5 nm from the surface of the nanoparticle. We implemented these findings in AMF-triggered drug release system in which doxorubicin was covalently linked at different distances from the IONP surface bearing the same thermo-labile azo molecule. We demonstrated the AMF triggered distance dependent release of the drug in a cytotoxicity assay on KB cancer cells. This work not only gives access to a new type of temperature sensors at the nanoscale for measuring the surface temperature gradient of magnetic nanocrystals under AMF exposure, but will allow for remotely triggering of combinatorial drug delivery in which more than one drug can be released using different kinetics. This novel type of carrier shows the following promising features as smart drug delivery systems: i) the mass ratio between the delivery vehicle and the drug is significantly reduced; ii) hydrophobic as well as hydrophilic drugs can be bound; iii) the drug release rate can be adjusted based on molecular building blocks (i.e. the azo molecules); and iv) combinations of different drugs bound on the same nanoparticle at different distances would enable independent release of each of them.

#445 - Picophytoplankton dynamics in a real ecosystem in the presence of environmental noise

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The dynamics of picophytoplankton communities in marine environment is studied by a stochastic reaction-diffusion-taxis model. The model, valid for weakly mixed waters, is used to obtain the stationary spatial distributions, along a water column, of two groups of picophytoplankton, i.e. picoeukaryotes and Prochlorococcus, which accounts about for 60% of total *chlorophyll a* on average in Mediterranean Sea. The model is based on three stochastic differential equations, which describe the dynamics of diffusion of the picophytoplankton biomass and nutrient concentrations, in the presence of environmental noise and intraspecific competition for light and nutrient. Specifically, the random fluctuations of the environmental variables are considered by inserting terms of multiplicative white Gaussian noise into the differential equations. The spatio-temporal dynamics of the picophytoplankton biomass and nutrient concentrations along the water column is obtained by numerically solving the equations of the model. In particular, the equations are integrated over a time interval long enough to obtain the steady spatial distributions of the biomass concentrations, expressed in cell/m^3, of picoeukaryotes and Prochlorococcus. The total biomass concentration is converted into *chlorophyll a* concentration and compared with experimental data collected in two different sites of the Sicily Channel (southern Mediterranean Sea). The comparison indicates that real *chlorophyll a* distributions are better reproduced, respect to the deterministic case, by theoretical profiles obtained in the presence of noise. In particular, position, shape and magnitude of the theoretical deep chlorophyll maximum exhibit, for suitable values of the noise intensities, an improved agreement with the experimental values, as confirmed by goodness-of-fit statistical tests.

#446

Ursula Roethlisberger (I) – EPFL, Lausanne

#447 - Dominant reaction pathways for protein folding

Silvio A. Beccara - Fondazione Bruno Kessler, Trento

PIetro Faccioli (Università di Trento e INFN), Roberto Covino (Università di Trento), Tatjana Škrbić (INFN, Padova)

The Dominant Reaction Pathways (DRP) approach [1] is a framework which allows for a very efficient computation of the statistically most significant folding pathways connecting given denatured protein configurations to the native state, at an atomistic level of detail, with realistic force fields. In my talk I will outline the basic features of the method and give accounts of our most recent results, including the folding of the FIP35 WW domain [2] and of a natively knotted protein [3]. Preliminary results about the conformational transitions of a serpin between folded and misfolded states will be given.

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#448 - Knotted proteins: folding pathways and the role of non-native interactions

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Silvio Beccara (LISC, Fondazione Bruno Kessler, Trento), Roberto Covino (Dipartimento di Fisica, Università di Trento), Cristian Micheletti (SISSA, Trieste), Pietro Faccioli (Dipartimento di Fisica, Università di Trento)

Knotted proteins are the object of an increasing number of experimental and theoretical studies, because of their ability to fold reversibly in the same topologically entangled conformation. The topological constraint significantly affects their folding landscape, thus providing new challenges to the funnel folding theory [1]. Firstly, we study the propensity of the knot formation in the early stages of the folding of two homologous proteins, one of which dispalys the knot in its native state, by means of stochastic Monte Carlo simulations. Two coarse-grained protein models are employed: one promoting exclusively native interactions, and the other additionally including non-native quasi-chemical and electrostatic interactions. With the former model neither protein shows propensity to form knots. With the additional non-native interactions knotting propensity remains negligible for the natively-unknotted protein, while for the natively-knotted protein significantly increases. We argue that the mechanism by which the knot is formed is dominated by the tendency of the C-terminal alpha-helix of the natively-knotted protein to approach and eventually thread other protein regions [2]. Seconly, we report on the first atomistic simulation of the folding of a natively-knotted protein, MJ0366, based on a realistic force field. Employing so-called Dominant Reaction Pathways approach [3,4] we identify the threading mechanism, involving the passage of the C-terminal alpha-helix through the native loop closed by the native beta-sheet formed at an earlier stage, as the dominant knotting mechanism. The dominance of the knotting by threading mechanism is not observed in

MJ0366 folding simulations using simplified, native-centric models. This points to a previously underappreciated role of concerted amino-acid interactions, including non-native ones, in aiding the appropriate order of contact formation to achieve knotting [5].

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#449 - Flexibility and growth polarity in fungal prion amyloid fibrils

Antonio Trovato - Dipartimento di Fisica e Astronomia, Università di Padova

Stefano Zamuner, Flavio Seno (Università di Padova)

The prion-forming C-terminal domain of the fungal prion HET-s forms infectious amyloid fibrils at physiological pH. The conformational switch from the nonprion soluble form to the prion fibrillar form is believed to have a functional role, as HET-s in its prion form participates in a recognition process of different fungal strains. The high resolution structure of the prion forming domain HET-s(218-289) in its fibrillar form is known from solid state NMR, exhibiting a rigid core with a beta-solenoid topology decorated by highly flexible parts [1]. A different non infectious (non-prionic) HET-s fibrillar polymorph is stable at acidic pH, and is known tp be much more rigid than the prion form, as shown by the comparison of their NMR spectra [2]. This raises an intriguing question about the origin of the relationship between structural flexibility and prion infectivity, that may be of possible interest in the understanding of mammal prion infectious diseases. In order to properly assess the role of structural flexibility in the mechanisms underlying fibril formation, we employ the full information from all 20 available NMR conformers of the prion form to define a structure-based Go-like Hamiltonian for a simple coarse-grained model of HET-s prion fibril. Our approach emphasizes the general role of the topological properties of the fibrillar structure and, in particular, the importance of considering different alternatives for the higly flexible portions of HET-s prion fibril. Indeed, our analysis of NMR conformers shows that residue-residue contacts involving residues in the flexible portions of HET-s fibril are present with a probability that changes in a non symmetric way from one end to the other of the fibril. Moreover, those contacts nicely complements the solenoid topology maintained by the rigid portions involved in the beta-sheet structure. A numerical simulation of the fibril growth process within our approach highlights the existence of a crucial interplay between the asymmetric flexibility of HET-s chain termini at fibril ends and the occurrence of growth polarity in HET-s fibrils. The latter had been already suggested in [3] for HET-s fibrils with rigid ends, only on the basis of their topological properties.

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#450 - Temperature accelerated molecular dynamics simulations of rare events in biological molecules

Luca Maragliano - Istituto Italiano di Tecnologia, Genova

I will present a method designed to explore the free energy landscape of a system associated with a large set of collective variables. An extended system is introduced where the collective variables and the physical ones are evolved concurrently in effective adiabatic separation. This allows to explore directly the free energy space of the collective variables, and the sampling is accelerated via an artificially high temperature acting on them. I will discuss the technique and its implementation, and illustrate its potential via applications to ligand diffusion and conformational changes in proteins and RNA molecules.

#451 - Unwinding dynamics of polymers

Marco Baiesi - Università di Padova

G. T. Barkema (Institute for Theoretical Physics, Universiteit Utrecht and Instituut-Lorentz, Universiteit Leiden), E. Carlon (Institute for Theoretical Physics, KU Leuven), D. Panja (Institute for Theoretical Physics, Universiteit Utrecht), J.-C. Walter (Laboratory Charles Coulomb, Department of Theoretical Physics, Université de Montpellier)

We study numerically and analytically polymers relaxing from configurations wound helically around other objects. The motivation is both in understanding the basis of unwinding dynamics, and from a more practical problem of understanding better DNA denaturation. The latter is modeled by two lattice polymers, initially wound around each other in a double-helical conformation, which evolve through Rouse dynamics [1]. If no attraction between them is present, as it would be in a DNA quickly brought at high temperature, the strands separate to form an entropically favored unbound state. The strands unwind by rotating around each other until they separate. The process proceeds naturally from the ends inward; intermediate conformations can be characterized by a tightly wound inner part, from which loose strands are sticking out. The total time needed for the two strands to unwind scales as a power law of the chain length. In order to shed some light on such scaling form, a simpler system is also analyzed [2]: the relaxation dynamics of a single polymer wound helically around a fixed bar. Analyzing a Langevin equation, we can predict a relaxation time scaling as a power of the polymer length times a logarithmic correction related to the equilibrium fluctuations of the winding angle. Numerical data support this result and show that at short times the winding angle decreases as a power law. The Langevin equation is

also consistent with such scaling, provided that a winding-dependent friction is used in that regime. Hence, such reduced description of the system captures the basic features of the problem.

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#452 - Localized longitudinal nonlinear excitations in DNA

Angelo di Garbo - CNR - Istituto di Biofisica, Pisa

In this contribution a model of DNA molecule is proposed in which the bases are subject to small displacements along the molecular axis. The effect of such additional degree of freedom on the DNA dynamics is studied analytically and numerically. The model is an extension of a well known model and describes the double helix as two chains of pendula (each pendulum representing a base). Each base (or pendulum) can rotate and translate along the helix axis. In the continuum limit the system is described by the perturbed sine-Gordon equation describing the twist of the bases and by a nonlinear partial differential equation (PDE) describing the longitudinal displacements of the bases. This coupled system of PDEs was studied analytically using different approaches and the corresponding results were tested through numerical simulations. It was found that if the coupling parameters satisfy a well defined relationship, then there exist bounded travelling wave solutions.

#453 - Exploring the interplay among morphology, strain and electronic structure in SiGe nano-systems by spectro-microscopy techniques

Giovanni Maria Vanacore (I) - California Institute of Technology

Physical, chemical and optical properties of the matter exhibit important changes as a result of size shrinking and morphology modifications down to the nanometer length scale. Improving the optical and electronic properties as compared to bulk systems, while preserving a wide compatibility with the existing technology, is a fundamental issue for advancements in micro, opto and nano-electronics applications. Among the materials that show promising features for future design of new-generation devices, SiGe heterostructures are one of the most investigated systems. This interest comes from the possibility of opening new degrees of freedom via electronic structure warping induced by strain engineering.

In this contribution, several approaches for tuning the strain field within SiGe nanostructures are explored, and the relationship between morphology, elemental composition, strain state and electronic structure is critically addressed by means of several spectro-microscopy techniques. The interplay between elastic relaxation, plastic lattice deformation and SiGe intermixing is investigated in self-assembled islands obtained in a bottom-up approach. Lithographic patterning of thin Ge layers is used to unravel the mechanism of strain state conversion during the downscaling from two-dimensional (2D) to one-dimensional (1D) structures. Finally, a new strategy, where SiGe structures are laterally confined by the Si substrate, is used to obtain high tensile strain. This is shown to be originated by an out-of-plane frustrated relaxation induced by the nano-constrained geometry, and to be responsible for a significant narrowing of the direct energy band gap.

#454 - Ge on C-covered Si(100) surface: from continuous surface diffusion to discrete islands nucleation

Maurizio Zani – CNISM e Dipartimento di Fisica, Politecnico di Milano

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We investigated the surface diffusion and island nucleation of Ge on a Si(100) surface in presence of a submonolayer coverage of carbon as surfactant by using scanning Auger microscopy and atomic force microscopy. The sample consists of Ge stripes (about 3-5 μm) obtained by a photolitographic patterning of pure Ge thin films (thickness about 50 nm) grown on a Si(100) substrate by low-energy plasma enhanced chemical vapor deposition (LEPECVD) [1].

The stripes have been used as sources for the surface diffusion of Ge in case of C-free Si surface promoted by annealing at several temperatures (from 600 °C to 700 °C). The temperature dependence of the diffusion coefficient has been determined by fitting the postannealing coverage profiles measured by Auger microscopy with a one-dimensional Arrhenius diffusion equation.

Then, the carbon coverage has been spatially modulated on a single sample, allowing the measurement of the diffusion coefficient as a function of the C thickness at 600 °C. We show that the reduction in the diffusion coefficient while increasing the surfactant coverage is described by a linear dependence of the diffusion activation energy on the C coverage. This dependence is discussed in terms of the chemical interactions among Si, C, and Ge, of the surface roughness and the local strain field induced by the C surfactant.

Finally, spontaneous nucleation of SiGe islands coexists with the continuous surface diffusion of Ge. The transition of the island nucleation as a function of the carbon coverage is observed to be continuous from the Stranski-Krastanov mode to the Volmer-Weber regime. We propose a consistent scenario correlating diffusion and nucleation parameters within a diffusion limited growth regime and show the existence of a threshold for C coverage below which no effect is observed [2].

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#455 - Solid-liquid interfaces studied by electrochemical scanning tunneling microscopy

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On-surface chemistry of organic molecules in ultra-high vacuum (UHV) has been extensively studied in the last decade with great success in terms of producing layers of interest for applications in molecular electronics [1]. UHV technology offers the advantage of studying systems with highly controlled parameters but it is expensive and exploits ideal conditions.

In this respect, the study of solid-liquid interfaces represents a new approach which uncovers the processes at the interface between organic molecules in solutions and suitable surfaces, also exploiting the fundamental role of the electrolyte.

In order to study on-surface reactions in solution traditional electrochemical spectroscopies can be used, taking the sample as the working electrode (WE) of the three-electrode electrochemical (EC) cell. A great improvement to the study of solid-liquid interfaces has been provided by the coupling of the electrochemical cell with scanning tunneling microscopy (STM). We use an electrochemical-STM (EC-STM) to image systems at a fixed potential of the substrate or during a measure of cyclic voltammetry, in order to study at atomic scale the reactions taking place at the solid-liquid interface.

Commercial EC-STM usually study systems in a small volume of solution and concentration changes can occur near the sample

surface; moreover electrolytes cannot be effectively degassed from oxygen. We employ an home-built EC-STM [2] to investigate samples dipped in EC cell containing a larger volume of solution (> 2 ml) gaining an higher control on experimental conditions. We focus on two main subjects of wide interest for applications in devices: the first one concerns surface polymerization, namely dipping a gold single crystal (catalyst metal) in a solution containing precursor molecules and activating them with different strategies in order to obtain 1D or 2D polymers [3]; the second subject deals with the I^-/I_3^- electrolyte-TiO2 single crystal interface, significant for photovoltaic devices based on the Grätzel cell [4].

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#456 - Crystallization of amorphous silicon by infrared laser irradiation

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Laser Thermal Annealing receives a great interest as heating sources and several options, depending on the emission wavelength, are well described in literature. In particular, crystallization of amorphous silicon using a continuous wave Infrared Semiconductor Diode Laser has emerged as an effective possibility for solar cell production.

We investigated the homogenous nucleation of crystalline grains in α-Si, obtained by ion implantation of c-Si, during high temperature pulse lasting few milliseconds IR laser irradiation. Significant crystallization occurs in non-steady regime because of the rapid temperature variation. The temperature rises 10^6 °C/s, faster than during a RTA process. Our model combines the time evolution of the crystal grain population with the consumption of the amorphous volume due to the growth of grains. Thanks to the experimental approach based on a laser source to heat α-Si and the theoretical model we extended the description of the homogeneous crystallization up to 1323 K, or 250 K above the temperature investigated by conventional annealing. Crystallization of amorphous Si in the presence of Arsenic has been investigated and modeled also. With respect to intrinsic Si, in Arsenic-doped Si nucleation is reduced of a factor 3 and grain growth is enhanced by up to 8 times. In millisecond laser annealing process this produces a grain size 10 times bigger than that observed in intrinsic Si. Arsenic is causing an increase of the grain growth velocity of twin–defective crystal clusters corresponding to the transition from the <111> to the <100>. This experiment may have an impact in the realization of thin doped layers on intrinsic Si like in photovoltaic cells.

After that, we explore the effect of IR Laser irradiation on amorphous silicon layers deposited by plasma enhanced chemical vapor deposition. Crystallization occurs via homogeneous nucleation at high temperature or by layer melting and solidification. Amorphous layers of thickness in the range 50 - 1000 nm have been crystallized up to 80 % of their volume. We observed a 2D growth when the thickness is 50 nm, whereas a 3D growth occurs for thicker layers with an average grain size of ~ 30 nm, weakly dependent on the thickness. We also found that hydrogen desorption occurs without layer degradation regardless of the layer thickness. The coalescence of hydrogen before out diffusion produces voids only for layers thicker than 200 nm.

#457 - Maskless implants of 20 keV Ga$^+$ in thin crystalline SOI and in si substrate

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A nano-size ion beam apparatus has been used as maskless lithography to implant 20 keV Ga+ ions into a 26 nm thick silicon crystalline film on insulator (SOI) and into a (001) silicon substrate. The ion beam, with about 5 nm standard deviation, delivered few hundred ions during a single shot. Circular areas with nominal diameter as large as 1 um and Single Pixel Lines, along the [100] and the [110] directions, were irradiated to a fluence of $5x10^{14}$/cm^2. In the SOI film the damaged regions extend across the film thickness, while, in the case of the Si substrate, an amorphous/crystalline interface was formed at a depth of about 30 nm.

The implanted regions are characterized by irregular contours and disordered filaments, as evidenced by Transmission Electron Microscopy. Fourier Transform analysis indicates that implantation causes the amorphization of a region which extends beyond the nominal extension. In situ annealing experiments demonstrated that the disordered filamentary regions disappear in the 250-450 °C temperature range and the interfaces with the surrounding crystalline regions sharpen. A temperature as high as 600 °C is required to fully re-crystallize the implanted areas. Regrowth arises by multi-orientation lateral solid phase epitaxy, limited by the crystallization kinetics of the slowest planes.

In the implanted SOI film, the breaking of (111) and (101) interfaces, due to the formation of twins, triggers a fast crystallization kinetics. Rapid thermal annealing (890 °C-10 s) in the same system, instead, completely crystallizes the amorphous regions without twin formation. Multi-orientation regrowth only produces small cluster of defects, matching the different a-c interfaces.

In the implanted Si substrate, in situ annealing demonstrated that regrowth is dominated by the fast (001) interface and no extended defect is observed in presence of this interface, while twins emerge in the thinnest region of the TEM sample, where the (001) amorphous/crystalline interface is etched.

Scanning capacitance measurements indicate that the implanted atoms, after crystallization, are electrically active. The implant method is then a viable processing step for the local doping of SOI and of bulk Silicon.

#458 - Tuning colloidal interactions by controlling the solvent properties: critical Casimir forces and beyond

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Nicoletta Gnan, Francesco Sciortino (Università Sapienza, Roma)

It is known that effective forces can deeply modify the phase diagram of colloidal particles. This happens, for instance, in the presence of depletion forces, i.e. effective forces that originate from the presence of a co-solute (polymers, surfactants) in the suspension.

Beside short-range depletion, also long-range effective interactions can be exploited for controlling the behaviour of a colloidal solution. The most famous example is that of the critical Casimir force [1], which arises when two colloids are immersed in a solvent close to its critical point. In such a case, the confinement of the density critical fluctuations between the colloids surfaces give rise to a long-range force [2], that can be controlled through a tiny variation of the temperature close to the critical point.

In this talk I will discuss the results of numerical studies of the effective potential V_{eff} between two hard-sphere colloids dispersed in an implicit solvent in the presence of interacting depletant particles approaching the depletant gas-liquid critical point. We find that V_{eff} decays exponentially at long distances, with a characteristic decay length compatible with the bulk critical correlation length. By investigating the stability of the particles interacting via V_{eff}, the locus of colloidal aggregation in the phase-diagram of the depletant is evaluated, assessing under which conditions critical Casimir forces can be used to manipulate colloidal aggregation [3,4]. In addition, the variation of colloid-solute interactions allows to tune the effective long-range potential from attractive to repulsive [5], in agreement with theoretical calculations and experimental results.

Finally, building on the analogy between critical phenomena and the percolation transition [6], I will also discuss a Casimir-like potential between colloidal particles dispersed in a solvent close to percolation. In this case, the range of the effective interaction is controlled by the connectivity length of the solvent and diverges at the percolation transition [7]. These results provide the geometric analogue of the critical Casimir force, opening the way for a fine tuning of colloidal interactions by controlling also the clustering properties of the solvent.

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#459 - Multiple arrested states in a charged colloidal system

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Dynamical arrest in colloidal and, more generally, in soft matter systems, has recently become the subject of intense research activity also because of its theoretical and technological implications. It is well known, in fact, that colloidal systems are very good models for understanding the general problem of dynamic arrest, showing a larger flexibility compared to atomic and molecular glasses. The fine tuning of the control parameters opens the possibility to tailor the macroscopic properties of the resulting nonergodic states. Several mechanisms of dynamical arrest have been identified. Few real systems are suitable for use as experimental counterparts for the vivid theoretical speculations on non-linear, complex and non-equilibrium systems. Among these colloidal clays have emerged as suitable candidates to investigate the formation of multiple arrested states.

In this presentation we show the results obtained on dilute suspensions of Laponite, an industrial synthetic clay. Once dispersed in water Laponite originates a charged colloidal system of nanometer-sized discotic platelets with inhomogeneous charge distribution and directional interactions. The presence of competing attractive and repulsive terms in the interactions, combined with the anisotropy of the face-rim charge interactions and with the discotic shape of Laponite, produce a very rich phase diagram including a nontrivial aging dynamics towards multiple arrested states. We focus here on two different disordered arrested states of gel and glass, obtained respectively for low (Cw < 2.0 %) and high (Cw ≥ 2.0 %) clay concentrations in salt free water conditions.

The arrested state at low concentration is governed by attractive interactions and experimental findings supported by numerical simulations have recently furnished the first experimental evidence of empty liquid and equilibrium gel, respectively found for (Cw < 1.0 %) and (1.0 % < Cw < 2.0 %) [1]. These new concepts were formulated for patchy colloids [2] of different shapes, patterns and functionalities, that are considered the novel building blocks of a bottom-up approach toward the realization of self-assembled bulk materials with pre-defined properties.

On the other side the comparison between Dynamic Light Scattering, Small Angle X-ray Scattering and dilution experiments with theoretical and numerical results have permitted to individuate a high concentration (Cw ≥ 2.0 %) Wigner glass [3] state, i.e. an arrested state formed by disconnected particles or clusters and stabilized by the electrostatic repulsion. Moreover very recent results show that the attractive interactions are playing a role also in this case and that even in the glassy state the local structures and the interactions among the colloidal particles are still evolving, originating an interesting dichotomic behaviour [4].

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#460 - Dichotomic aging behaviour in a colloidal glass

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The continuous interest in studying dynamics of colloidal systems has over the last decade led to a broadening of our knowledge on dynamical arrest and the glass transition. Many experiments performed on colloidal glasses and gels as well as theoretical and numerical simulation results aim at understanding the nature of the aging phenomena that are typical for systems with time evolving dynamics. Studying the time evolution of the dynamic structure factor allows to extract the characteristic times of the system (relaxation times τ_Q) as well as their distribution (β_Q exponent). The commonly accepted physical picture in a disordered, glass-like material, is that the motion of a particle is constrained by the cage of its neighbors resulting in the emergence of different relaxation times - e.g. motion inside the cage, rearrangements of cages, etc. In order to fit the decay of the intensity correlation functions over a wide time window, the Kohlrausch-Williams-Watts expression is generally used $f(Q,t) \sim \exp[-(t\backslash\tau_Q)^{\beta_Q}]$ where τ_Q is an "effective" relaxation time and β_Q measures the distribution of relaxation times. Most commonly, the different relaxation times present in glassy materials lead to a stretching of the correlation functions and an exponent $\beta_Q < 1$ (which is referred here as "stretched behavior"). On the contrary, the existence of anomalous dynamics with $\beta_Q > 1$ (compressed behavior) has been recently shown on a gel [1]. This unusual dynamics has been attributed to the relaxation of internal stresses and more recently it has been recognized as a salient feature of disordered arrested materials. Among these, colloidal clays, have recently emerged as complex fluid systems characterized by a peculiar aging dynamics and a very rich phase diagram encompassing fluid, gel, glassy states [2-4] as well as several ordered phases.

Here we show that an unexpected dichotomic aging behaviour is observed in a Laponite colloidal glass investigated through X-Ray Photon Correlation Spectroscopy and Dynamic Light Scattering. For spontaneously aged samples a stretched behavior ($\beta_Q < 1$) is always found. Surprisingly a compressed exponent ($\beta_Q > 1$) appears only when the system is rejuvenated by application of a shear field but in both cases the relaxation times scale as Q^{-1}. This observation sheds light on the origin of compressed exponential behavior and helps in classifying previous results in the literature on anomalous dynamics [5].

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#461 - Dynamical heterogeneities and morphology of a 2D gel network at the air/water interface

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The talk shall report a detailed characterization of the morphology and the dynamics in a bidimensional gel at the air water interface: the 2D geometry is peculiar in that it allows a continuous and controlled variation of the density of the system over a wide range. This study combines different microscopy techniques (SEM, AFM & optical techniques), together with interfacial micro-rheology and synchrotron-based X-ray Photon Correlation Spectroscopy (XPCS).

First, the evolution of the statistical properties of the structured network, as a function of the externally controlled density, is related to the corresponding evolution of the mechanical properties. Three steps can be identified in the gel formation: a first step occurs in the incubation time, in which the individual nm-sized gold nanoparticle aggregate to form quasi 1D structures of typical length of a few microns. The second step occurs in the first stages of the compression, with the growth of the branched structure, finally yielding to the onset of the infinite percolativo cluster, which is related to the building of the mechanical elastic modulus. The final step identifies with the homogenization and regularization of the distribution of holes sizes, which relates to the further increase of the elastic modulus upon compression [1].

The talk shall then focus on recent results obtained by interfacial rheological techniques [2] and by XPCS [3] on this system. Our results demonstrate that the dynamics is anisotropic, confined in the plane of the interface. The good quality of the XPCS data allows the characterization of dynamical heterogeneity by measuring- for the first time in an XPCS experiment- the 4th order correlation function g (4)(t,τ). A superdiffusive regime can be identified on the nano scale, and the relaxation parameters can be controlled over a wide range. The XPCS results are compared with those from Tracking Microscopic techniques, which access the same phenomena in the direct space.

We speculate that this study may guide the fine tuning of certain parameters of practical relevance, such as mechanical strength, or film porosity, aiming at the formulation of gels with desired characteristics, such as increased mechanical strength, or increased mobility.

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#462 - Structure, mechanical properties and dynamics of 2D DPPC based foam-like structures stabilized by silica nanoparticles

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The spreading and affirmation of nanotechnologies poses new safety issues, such as the effect of NPs on the respiratory system: classical pathologies like asthma,severely aggravated by air pollution, and silicosis raise increasing alarm. Silicon NPs have been widely used as a benchmarks to assess the effects of NPs on the respiratory system in general, and on the mechanical properties of phospholipidic pulmonary surfactants (PL) in particular. Detailed mechanical experiments conducted by interfacial rheological techniques have shown a modification in the relaxation mechanisms when NPs are added to the PL layers [1]. Moreover, the interaction of PL layers with NPs induces important modifications in the domain structure of the monolayer, with effects on the liquid-expanded / liquid-compressed phase transition: we evidenced the onset of a new 2D-foam like structure.
The mechanisms at the bases of the formation of this particular layer, driven by the modification of the complex balance between line tension of the domains and the dipolar moments of the molecules, have been analyzed and a wide characterization of these structures has been carried out both from the structural point of view and for the rheological properties [2]. The fluctuation dynamics of this intriguing new phase has been investigated very recently by X-ray Photon Correlation Spectroscopy (XPCS) in grazing incidence geometry. In this geometry, XPCS directly accesses the dynamical correlation functions of the monolayer on the microscopic scale, allowing to indicate -under certain conditions- a detailed model describing the spontaneous fluctuation dynamics of the lung surfactant in the presence of NPs[3].

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#463 - Optoelastic effects in nematic colloids

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We present here the main features of the optoelastic [1] interaction in dielectric microparticles dispersed in nematic liquid crystals denominated Nematic Colloids (NC). The interest in the study of their interaction has been driven by the observation of self-assembling phenomena which make these systems attractive to build artificial materials.
This interaction gives rise to optical trapping occurring when the conventional trapping conditions typical of optical tweezers are not fulfilled [2,3]. We have demonstrated trapping when the refractive index of the particle is lower with respect to the one of the surrounding medium and at the same time the numerical aperture of the focusing systems is lower than 0.1 , dropping in this way all the conditions for the conventional trapping induced by high gradient optical field.
In our case optical trapping of NC originates from the elastic interaction between the distorted area around the particle and the area reoriented by the laser light, denominated "ghost colloid" (GC). The picoNewton interaction force is characterized by a wide range, scaling as R-2, being R the distance between the particle and the focal waist. It has been shown that liquid crystal nonlocality plays a major role in this interaction [4].
The orientational properties of liquid crystals allow exploiting low frequency electric field to control the strength and the range of the interaction range. We have demonstrated that for a homeotropic sample with positive dielectric anisotropy the electric field is able to reduce the interaction between the NC and the GC up to a complete quenching of the trapping effect. An opposite effect is foreseen in negative dielectric anisotropy media where macroscopic (mm) interaction range should be possible [5].

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#464 - Solubility of oligo(3-alkylthiophenes) in molecular solvents by model potential molecular dynamics

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Conducting polymers such as poly(3-alkylthiophenes) are of particular interest for organic electronics applications. Polymer-based systems are often synthesized from solution: for example, by dissolving poly(3-hexylthiophene) together with ZnO nanoparticles into suitable solvents it is possible to obtain hybrid heterojunctions for photovoltaic applications [1]. Polymer-solvent interactions

affects the polymer molecules conformations and their adhesion on the nanoparticles. For example, the experimentally observed P3HT polymer wrapping on carbon nanotubes has been attributed to polymer-solvent interactions and predicted to be unlike to occur in vacuo [2-4], though a clear theoretical demonstration that includes explicitly the role of the solvent is still missing. Any reliable prediction depends on the precise modeling of the polymer-solvent interaction. In this work we study by model potential molecular dynamics the solubility of a set of oligo(3-alkylthiophenes) as a function of the alkyl chain length in toluene and tetrahydrofuran (THF) liquids. These solvents are among the most used in the synthesis of hybrid materials; furthermore, toluene has been recently used in applications for selective wrapping of carbon nanotubes by poly(3-alkylthiophenes) [5]. By using a modified Flory-Huggins theory, we study the solubility of the oligo(3-alkylthiophenes) in toluene and THF at ambient conditions and we extrapolate a trend for long chain polymers of the same type. Some potential parameters for the solvents have been also modified in order to obtain a better reproduction of the experimental properties of interest.

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#465 - All-optical radiation sources for applications

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The progress of high power lasers driven by the Chirped Pulse Amplification (CPA) concept [1] is leading to the realization of new large laser systems within the Extreme Light Infrastructure (ELI) that will start paving the way to the exploration of new physical domains, approaching the regime of electron-positron pair creation and the possibility to reach the critical field of quantum electrodynamics [2]. Meanwhile, laser-plasma acceleration [3] is being considered for the development of novel, all-optical radiation sources. Bremsstrahlung X-ray and γ-ray sources have already been explored [4] and successfully tested. More recently [5], self-injection sources are being considered to generate γ-rays via Thomson/Compton scattering.

In view of these promising developments, a collaboration is being established aimed at pursuing development of all-optical laser-plasma acceleration for secondary electron and radiation sources. The ILIL laser installation at INO-CNR (Pisa) is currently being used for a range of applications including electron microradiography and comparative dosimeter with standard electron sources at sub 10 MeV electron energy. The recently commissioned FLAME laser system at LNF-INFN (Frascati) is instead used to explore the higher electron energy range up to 1 GeV, in the so-called bubble regime and experimental runs [7] have already been performed recently in view of the development of a γ-ray source based upon Thomson back-scattering [8]. Along with the experimental programme at ILIL and FLAME, numerical simulations are being developed [9], starting from the optimization and control of the laser-plasma acceleration process using advanced 3D GPU particle in cell code.

Finally, we point out that the practical use of laser-driven electron and γ-ray sources will require the development of high-efficiency and high-repetition rate laser systems for pumping ultra short lasers currently based on Ti:Sa amplifiers. This problem can be solved by adopting the so-called Diode Pumping Solid State Laser (DPSSL) technology, instead of flash-lamps. Within the framework of the HiPER programme and the LASERLAB Joint Research Activity named EUROLITE, we are developing an optical cavity based on Yb for a high energy amplifier to be used to pump future high-rep rate Ti:Sa PW scale systems.

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#466 - State-of-art of transport understanding in toroidal plasmas: experimental results and model validation

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In the last decade, great progress has been achieved in the understanding of turbulent transport mechanisms in toroidal plasmas. Electron and ion energy transport, main particle and impurity transport, momentum transport have been intensively addressed by dedicated experiments with high quality diagnostics and theory development allowing model validation against experimental results. This collaborative effort between large and small size experiments and theory groups has produced a number of key results towards the long-standing aim of developing fully predictive capabilities for future machines. A selection of these results will be illustrated, amongst which the concepts of critical temperature gradient length and profile stiffness and their parametric dependencies, the turbulent particle convection, toroidal and poloidal momentum transport and intrinsic rotation, centrifugal effects and poloidal asymmetries in the spatial distribution of heavy impurities. The present status of understanding will be discussed in relation to its relevance for maximizing performance in next-step fusion devices and remaining open issues will be highlighted.

#467 - Cross scale phenomena in solar wind plasma

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Solar wind represents a space laboratory where fundamental problems in plasma physics can be studied. In particular space experiments devoted to analyze plasma turbulence over a scale range covering more than ten decades are currently being performed. While large scale MHD turbulence has been well characterized in the last years, the mechanisms which transfer the energy from the fluid, relatively ordered, scale to the kinetic, microscopic and disordered, scale are not yet fully understood.

Ion distribution functions, which display non-maxwellian features are commonly observed in solar wind. Moreover observations of the ultraviolet spectrometer UVCS onboard the SoHO spacecraft have shown that highly anisotropic ion distribution functions are found also in the solar corona. These distribution functions can give rise to strong wave-particle interactions, which could contribute in degrading the energy of large scale motions. The study of these processes, which occur on the kinetic scales is mainly based on the use of advanced numerical techniques as well as considerable computing facilities.

Using hybrid Vlasov–Maxwell simulations we have investigated the dynamics of the solar-wind plasma in the tail of the MHD nonlinear cascade, where the energy injected in large-scale slab-type Alfvenic fluctuations is transferred toward short spatial scale lengths, across the proton skin depth. In particular we have shown that a significant level of electrostatic activity can be generated at wavelengths smaller than the proton inertial scale and propagating in the longitudinal direction with respect to the ambient magnetic field. A careful study of the generation process of these electrostatic fluctuations in terms of the electron-to-proton temperature ratio T_e/T_p has allowed to furnish a clear evidence that even in the case of cold electrons, i. e. T_e of the order of T_p (an appropriate condition for solar-wind plasmas), the resonant interaction of protons with large-scale left-hand polarized ion-cyclotron waves is responsible for the excitation of short-scale electrostatic fluctuations with an acoustic dispersion relation. Through our numerical results we also suggest a physical mechanism to explain the observation of beams of accelerated particles along the direction of the ambient magnetic field for both protons and alpha particles. This mechanism is found to be more efficient for protons than for alpha particles, in agreement with recent solar-wind data analyses.

#468 - Radioactive dust re-suspension problems inside a tokamak in case of L.O.V.A: STARDUST facility

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The macroscopic erosion of hazardous materials (radioactive, toxic or explosive) and consequent accumulation of dust represents a risk for workers and population especially if these dust are mobilized during a Loss Of Vacuum Accident (L.O.V.A) inside a nuclear fusion plant like ITER. The objective of this paper is to show a comparison between experimental and numerical modeling of a L.O.V.A and evaluate the consequent dust mobilization in several thermal and fluid-dynamics conditions. The specific approach includes an experimental facility, STARDUST, in order to investigate mobilization and dust behavior during accidents. Experimental and numerical results obtained in these years by the Quantum Electronics and Plasma Physics Research Group will be presented together with a validation and benchmarking of the analysis codes.

#469 - Superdiffusive transport in space and laboratory plasmas

Gaetano Zimbardo – Università della Calabria

In the last few years it has been shown that the transport of plasma particles in the presence of electric and magnetic turbulence can be superdiffusive rather than normal diffusive (Gaussian). The term 'superdiffusive' refers to the mean square displacement of particle positions growing superlinearly with time, as compared to the normal linear growth. The so-called anomalous transport, which in general is comprising both subdiffusion and superdiffusion, has gained growing attention during the last two decades in many fields including laboratory plasma physics and space physics. The control of particle transport is perhaps the biggest physics problem to solve for attaining fusion in magnetically confined plasmas. Both anomalous regimes, i.e. sub- and superdiffusion, are found in such plasmas by a number of techniques. In parallel, it has been found, both by data analysis and by numerical simulations, that the transport of energetic particles in the presence of solar wind magnetic turbulence can be superdiffusive.
The theoretical description of anomalous transport in the cases of both sub- and superdiffusion involves the use of a variety of tools like non-Gaussian statistics, Levy flights and walks, stochastic differential equations, long-range correlations, Hurst exponents, and fractional derivatives. In this presentation we will discuss the most common theoretical approaches to superdiffusion, that is the one based on fractional transport equations, and the one based on a non Guassian jump probability corresponding to Levy walks. The two approaches are compared, since they lead to slightly different predictions for the anomalous diffusion exponents, and we try to identify which tool is most appropriate to each plasmas system. Examples of anomalous transport for laboratory plasmas and astrophysical plasmas will be given.

#470

Keith Wilson (I) – University of York

#471

Bauke Dijkstra (I) – ESRF, Grenoble

#472 - Rheology at high pressure and high temperature using large volume press and synchrotron radiation

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At the beginning of the 2000's, coupling synchrotron radiation to a new large-volume apparatus for high-pressure controlled deformation, the Deformation-Dia, represented a breakthrough in studies of rheological properties under extreme conditions of pressure and temperature. Flow properties and interactions with dynamic processes (e.g. phase transformations) can be studied in-real time under typically up to 20 GPa and 2000 K. Deformation mechanisms (e.g. dislocation slip systems) can be identified and quantified on polycrystals and single crystals, by measuring in-situ bulk sample strains, lattice preferred orientations, and stresses, from grain scale to sample scale, using x-ray diffraction and radiography. Only three such setups in the world are installed on synchrotron beamlines and running. One is located in Spring-8, Japan, and two others in the USA, at the Advanced Photon Source (APS) and at the National Synchrotron Light Source (NSLS). Recently, developments using acoustic emissions measurements at the APS have significantly widened the range of problematics that can be addressed with these experiments, including the study of phase transformations at high pressure and associated mechanical instabilities.

These techniques can be used to investigate plasticity of materials relevant to subduction zones, where a tectonic plate slides and bends under another one. Materials there undergo large and heterogeneous deformations and stresses, which are released occasionally and suddenly through seismicity. The rheology of minerals is therefore a critical parameter for understanding the stress balance in subduction zones. Minerals also undergo phase transformations with increasing pressure and temperature, some of which are believed to be related to deep seismicity through unclear mechanisms.

We will illustrate with a "classical" deformation study on a hexagonal dense hydrous phase called phase A ($Mg_7Si_2O_8(OH)_6$). Phase A can form in deep shear zones after destabilization of serpentine, an abundant phyllosilicate within subducting slabs. We will also present in situ data on dehydrating serpentine under stress, coupled with acoustic emission monitoring (a proxy for unstable mechanical behavior and potential generation of seismic waves). This dehydration reaction has been invoked to explain intermediate-depth seismicity in subduction zones (50 -250 km depth), but remains a controversial explanation.

#473 - New structures of carbonates in the lowermost earth's mantle determined by single crystal techniques

Marco Merlini - Università degli Studi di Milano

Calcite, and dolomite, two of the most common minerals on the Earth's surface, undergo phase transitions at high pressure. Their structures have be identified by single-crystal diffraction experiments under extreme conditions. Dolomite-III, in particular, was found to be triclinic with 80 atoms in the unit cell and has unexpected structural complexity. It is thermodynamically stable at the high pressures and temperatures found in the Earth's interior, and may constitute a significant carbon repository in the lower mantle. These results clearly reveal the actual capability of synchrotron single crystal microdiffraction technique in solving crystal structure at the most extreme conditions, such as the pressures and temperature existing at the Earth's core/mantle interface. Further, the results indicate that the view of a phase transformation of materials into mixture of simple oxides at high pressure, is not fully correct, since low symmetry and complex phases are easily found experimentally.

#474 - High pressure-induced supermolecular organization of water and ethanol in an all-silica hydrophobic zeolite

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Simona Quartieri (Dipartimento di Fisica e di Scienze della Terra, Università di Messina), Giovanna Vezzalini (Dipartimento di Scienze Chimiche e Geologiche, Università di Modena e Reggio Emilia, Modena)

The behavior of water and other small molecules confined to spaces of nanoscopic dimensions is an important issue in many areas of science and technology. The special situations in which the confining substrates are hydrophobic have attracted great interest in the past decade. The confinement of molecules inside the cavities of high silica zeolites can be obtained under pressure using solution containing water and the molecules as pressure transmitting medium.

The high-pressure (HP) studies performed on zeolites using pore penetrating aqueous solutions, as P-transmitting media, demonstrated the so called Pressure-Induced Hydration effect (PIH), an interesting phenomenon in which the water content inside the zeolite cavities increases ("over-hydration") in response to the applied pressure, through selective sorption of H_2O molecules from the P-medium. Recently, a number of studies on water intrusion/extrusion on all-silica hydrophobic zeolites showed that these phases can be hydrated by the application of even moderate pressure (~ 0.1 GPa). However a structural characterization of the water-loaded systems is still lacking.

In this paper the HP-induced confinement of water and ethanol in an all-silica ferrierite [s.g Pnnm, a=14.0690(8) Å, b= 7.4177(3) Å, c= 18.708(1) Å V = 1952.3(2) Å3] compressed with two different aqueous media [(methanol, ethanol and water (16:3:1; mew); ethanol and water (1:3; ew)], is presented and the structural features of the HP-induced phase is discussed. The HP SR-XRPD experiments were performed at the BM01 beam line (European Synchrotron Radiation Facilities, Grenoble, France) with a fixed wavelength of 0.697 Å and an image plate detector, using modified Merril-Bassett DACs. Structural refinements were performed by Rietveld profile fitting up to 1 GPa in e.w. and up to at 0.2 GPa in m.e.w. (the data quality of the higher pressure patterns being too low for refinement). The structural results indicated the penetration of extraframework species even at the lowest investigated pressure in both experiments.

In ferrierite compressed in ew, a chain of water (w.) and ethanol molecules (e.) running along the central axis of the channels was localized even at 0.2 GPa, accounting for a total of 5 w. and 3.6 e. The HP-induced increase of the occupancy factors of the localized sites leaded a total load of 10 w. and 4 e. at 1 GPa. The refinement at 0.2 GPa of ferrierite compressed in mew indicated the penetration of only water (15.6 molecules) organized in similar chains. The interactions among the extraframework species and the framework oxygen atoms are very weak, due to the hydrophobicity of the framework.

#475 - Inside the lipid main transition by SAXS in an ultra-stable temperature scan: what gel and fluid phase co-existence?

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Elena Del Favero, Valeria Rondelli, Simona Motta, Laura Cantù (Università di Milano)

Small and wide angle X-ray scattering SAXS and WAXS are applied to investigate the multibilayer system of pure DMPC in the maximum swelling condition, undergoing the main phase transition, L_α- $P_{\beta'}$, along the cooling path. The anomalous swelling course, from 30°C to 24 °C, ends at 23.9 where a 0.7 degree interval of co-existence of gel and fluids domains occurs whose ratio is T dependent. This is the T-interval of the gelling transition. In particular we observe a 0.2 °C interval (from 23.8 a 23.6) where nearly undetectable amount of gel chains in the WAXS S(q) peak are detected, at the same time as the rising of the in-plane Bragg line of the Λ ripple phase, by SAXS S(q). This small T-interval is followed by a larger interval of 0.4 °C in which gel-ordered chains get stepwise more prevalence, corresponding to the rising of the Λ/2 ripple of the $P_{\beta'}$ phase.

Our finding partially disagree with findings by other authors applying neutron inelastic scattering on oriented membrane multistacks of DMPC[1], AFM microscopy on supported DMPC bilayer [2] and neutron diffraction on DPPC multilayer system [3]. In those studies a gel and fluid coexistence is evinced throughout a wide temperature interval even deep in the L_α phase. In particular, although our X-ray S(q) agrees with the S(q) by neutron scattering [1], the inelastic S(q,ω) by neutrons suggested the presence of two, gel and fluid, contributions even far above the transition temperature in the L_α phase. It was argue that those domains should have been smaller than the coherence length of neutrons (hundred A) otherwise a gel/ fluid coexistence would have lead to a peak splitting of the chain S(q) peak. Of course, in our case, the coherence length of the X radiation cannot affect the S(q).

We suggest the explanation of those discrepancies by analyzing the role of hydration water in lipid confined lamellar systems, with respect to their thermotropic behaviour. During the last decade, this point had given rise to what was known as the 'vapour pressure paradox' [4]. We show SANS and WANS from low hydrated multistack supported systems to corroborate our interpretation [5].

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#476 - How multipurpose in-house XRD systems can contribute to an efficient use of synchrotron beamlines: from SAXS to PDF

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Modern in-house X-ray diffraction systems are becoming more and more multipurpose analysis platforms, meaning that the same system can allow the user to perform many different types of measurements with easy reconfiguration of the instruments. Such possibilities are reducing the gap concerning what is possible at a diffraction beamline in a synchrotron facility, or at least to prepare and properly test the materials before synchrotron experiments.

In this presentation we will give an overview of the wide range of applications which are possible on a multipurpose in-house XRD system, in particular focusing on those techniques which are typically performed at dedicated synchrotron beamlines, such as small angle X-ray scattering for the study of weakly scattering nanomaterials, total scattering for the investigation of the local structure [1,2], and in-situ diffraction in many non-ambient conditions like high temperature and high pressure of reactive gases [3].

Case studies of the mentioned applications will be described and a comparative study on the same sample showing total scattering

experiments performed on an Empyrean multipurpose diffractometer and at two different synchrotron beamlines will be shown in detail.

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#477 - The degradation process of lead chromate yellows in paintings by Vincent Van Gogh

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Chrome yellows are a class of pigments commonly employed by painters of the late 19t[h] - early 20th century, such as Vincent Van Gogh [1] . These compounds are characterized by different chemical composition [$PbCrO_4$, $PbCr_{1-x}S_xO_4$, $0.1 \leq x \leq 0.75$] and crystalline structure (monoclinic and/or orthorhombic). Their shades range from the yellow-orange to the paler yellow hues with increasing sulfate amount. Since the alteration of the original chrome yellows is thought to be one of the causes that has led to changes in the original scheme colors of several paintings by Van Gogh, the comprehension of the photochemistry of this familiy of pigments is relevant in the paintings conservation field. We demonstrated that the degradation process of chrome yellows, is ascribable to a photochemical reduction of the Cr(VI) to Cr(III) and that the darkening behavior of these compounds is critically influenced by their chemical composition and crystalline structure [2,3]. Synchrotron radiation-based μ-XRF and μ-XANES investigations were performed on photochemical aged model paints [2,3] and two paint microsamples taken from the following Van Gogh paintings conserved at the Van Gogh Museum in Amsterdam: *Bank of the Seine* and *Field with flowers near Arles*.[4] The results revealed the presence of several Cr(III)-based compounds, such as $Cr_2O_3 2H_2O$ and either $Cr_2(SO_4)_3 H_2O/KCr(SO_4)_2 12H_2O$ or Cr(III)-acetate/Cr(III)-acetylacetonate. Among the paint models prepared by using historical and in-house lead chromate-based pigments, only those composed of a sulfate-rich orthorhombic $PbCr_{1-x}S_xO_4$ featured a significant darkening after the aging, revealing the formation of up to 60% of Cr(III) at the exposed surface [2,3]. We also demonstrated that different chrome yellow types can be distinguished by means of X-ray diffraction, FTIR and Raman spectroscopy (with bench-top and portable instrumentation) [5]. Various chrome yellow forms were identified on 17 embedded paint microsamples taken from paintings by Van Gogh and some of his contemporaries.

In situ analysis, by employing non-invasive portable instrumentations allowed a $PbCr_{1-x}S_xO_4$ chrome yellow type to be revealed on the Van Gogh paintings *Portrait of Gauguin* (Van Gogh Museum) and *Falling leaves (Les Alyscamps)* (Kröller-Müller Museum, Otterlo), while different forms of the chrome yellow pigment [alone or mixed with each other] were detected on the painting *Sunflowers* (Van Gogh Museum). A detailed description of the aforementioned results and recent developments of this research will be presented.

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#478 - Structural insights into inhibitor of apoptosis proteins recognition by pro-apoptotic compounds

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Inhibitor of Apoptosis Proteins (IAPs) are negative regulators of apoptosis and their overexpression is observed in many cancer cells. IAPs inhibitory function is exploited by the BIR domains, which were firstly identified in baculovirus. Among the IAP family, XIAP (X chromosome-linked IAP) directly inhibits caspases preventing proteolytic cleavage through its BIR2 and BIR3 domains; furthermore, XIAP-BIR1 in a dimeric form recognizes TAB1, a kinase activator, regulating pro-survival pathways. In the last years, cIAPs have become crucial players of the extrinsic pathway; in fact, through the recognition of TRAFs (TNF Receptor Associated Factors) by the cIAP2-BIR1 domain, they are recruited to the TNF- Receptor Signaling Complex and act as E3 ubiquitin ligases. One of the most promising approaches that have been proposed to inhibit these proteins is represented by the structure-based design of small molecules, named Smac-mimetics, that mimic Smac/DIABLO (Second mitochondria-derived activator of caspases/Direct IAp Binding protein with Low pI), an endogenous antagonist of IAPs. Initially designed in 2001 against the BIR3 domain of XIAP, Smac-mimetics have shown to prevent the inhibitory action of XIAP on initiator and executioner caspases, but also to bind to the BIR3 of cIAPs, inducing their autoubiquitylation and degradation. This work focuses on the cloning, expression and purification of the IAPs constructs of interest and their biochemical and biophysical characterization alone and in the presence of some of the Smac-mimetics from our library. The X-ray technique on crystals and protein solutions allowed a structural study of the protein-ligand complexes at atomic level. Furthermore, the screening of libraries of pharmacologically active compounds through in silico docking searches on new targets, such as XIAP- and cIAP2-BIR1, resulted in the discovery of potential new pro-apoptotic leads, whose clinical properties are known. Since in the last months new macromolecular protein complexes have been identified as involved in apoptosis and pro-survival pathways, novel protocols for the expression and purification of cIAP1 and TRAFs full length constructs have been optimized to obtain pure and homogeneous samples ready for the structural characterization.

#479 - Carbon nanotube/silicon hybrid solar cell devices

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Conventional Si solar cells have p-n junctions inside for an efficient extraction of light-generated charge carriers. However, the p-n junction is normally formed through very expensive processes requiring very high temperature (ca. 1000 °C). Moreover, Si itself is very costly. Therefore, there is a significant interest in forming heterojunctions at low temperatures (LT) and in reducing the total amount of Si. To achieve these goals, several systems are currently under study. Among them, carbon nanotube (CNT)/Si hybrid solar cells are very promising. In these cells, the p-type Si layer is replaced by a semitransparent CNT film deposited at room temperature on the n-doped Si wafer, thus giving rise to an overall reduction of the total Si thickness and to the fabrication of a device with inexpensive methods at LT. In particular, the CNT film functions as a charge carrier collecting conductive electrode and establishes a built-in voltage for separating photocarriers. Moreover, due to the CNT film optical semitransparency, most of the incoming light is absorbed in Si; thus the efficiency of the hybrid CNT/Si solar cell may in principle be comparable to a conventional Si p-n junction solar cell. However, under particular conditions, also CNTs are an efficient photon absorber which extends the conventional Si cell spectral range towards the near ultraviolet and the near infrared regions. In this scenario, it is important to take into account several parameters in order not only to improve the current power conversion efficiency of these CNT/Si hybrid solar cells, but also to extend the conventional Si cell spectral range. In the present talk a review of our last results will be given. Furthermore, our recent results on CNT/amorphous Si hybrid solar cells will be also discussed. In fact, it is well known that a good alternative to crystalline Si is amorphous Si that is much cheaper and can be used in very thin layers. In this case one of the open problems is the research for semitransparent electrodes less rigid and brittle than ZnO or Indium-Tin-Oxide. In this regard, we found that CNTs give encouraging results that suggest they can act mainly as semitransparent electrode and, at a lower extent, as photocurrent generator. The external quantum efficiency (EQE) response of the CNT/a-Si:H or the CNT/n-Si devices varies as a function of the CNT network thickness. Actually, photocurrent generation picks up quickly with the CNT film thickness, then attains its maximum and finally declines after an optimum thickness has been reached. Moreover, EQE spectral shape changes dramatically as the CNT network thickens up to resemble the typical spectrum of the same a-Si:H device covered by an Au film or that of a crystalline silicon solar cell, respectively. All our results are promising and work is in progress in order to improve their power conversion efficiency.

#480 - Ultrafast hot exciton dissociation at organic interfaces

Margherita Maiuri - Politecnico di Milano

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Interface physics is at the heart of photovoltaics, one of the most important challenges of this century. At the interface photons get absorbed and charge separation takes place. The accepted photophysical scenario in efficient organic solar cells based on low band gap copolymers, suggests that at the interface both bound interfacial charge transfer states (CTS) and free polarons are generated in the first hundred of fs. However, there is no experimental evidence on the charge generation mechanism on such a short timescale. Here, we monitor for the first time the exciton dissociation process in a low-band gap polymer: fullerene (PCPDTBT:PCBM) blend combining ultrafast transient absorption spectroscopy with sub-15 fs time resolution and high level quantum chemical calculations. We find that exciton dissociation leads to both bound interfacial CTS and free polarons within a time scale of 20-50 fs, with a branching ratio that depends on the excess energy.

In particular, upon pumping the first excited singlet state, the resonant lower-energy CT1 state and free polarons are populated. However, in the first 500 fs, the CT1 does not evolve, indicating that it does not contribute to the early-time charge dissociation yield. On the other hand, by exciting the more energetic singlet states, a fast conversion to the hot CTS manifold opens up a new channel for effective charge dissociation that we find to occur with a time constant of 22 fs. Such hot CTS undergo further separation into free polarons within 150 fs while partially thermalizing within the CT manifold, but before complete relaxation in the CT1 state. We relate this higher efficiency to the nature of the hot CTS involved in the process, since they are more delocalized and preferentially dissociate into free polarons. Thanks to stronger coupling between high energy singlet states and hot CTS, we demonstrate the opening of additional paths for charge generation that would otherwise be quenched by internal conversion to the lowest lying states. These results demonstrate that providing a large amount of excess energy, the higher lying polymer singlet states dissociate before internal conversion, ultimately leading to a higher fraction of polarons. Our results provide a new framework to understand charge generation in organic systems, suggesting that hot injection is a strategic option to enhance the photovoltaic conversion.

#481 - ZnO nanostructured metal/oxide systems for solar energy conversion

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The exploitation of sustainable energy sources is one of the most challenging topics in latest research, due to the increasing energy requirements and rising prices of fossil-based fuels, so far as the environmental impact. Dye-Sensitized Solar Cells (DSSC), which

realize optical absorption and charge separation by association of an organic dye with a wide band gap semiconductor oxide, have shown to be a promising device, but studies are required to improve efficiency [1].

ZnO is a wide band gap semiconductor (Eg ~ 3.37 eV at 300 K), with large exciton binding energy and high mobility, it is a good thermal conductor and a very stable material [2]. Thanks to its properties, reduced cost and wide variety of available nanostructures ZnO has proved to be a promising material for many applications from microelectronics to catalysis and photovoltaics (DSSC in particular).

With this purpose in mind this study focuses on ZnO metal/oxide model systems in order to deepen the comprehension of the physical mechanisms at the atomic level of oxide surfaces and interfaces. Nanostructured ZnO films have been grown on metal substrate by reactive deposition of Zn in oxygen partial pressure in UHV. The influence of parameters, like oxygen pressure, deposition rate and temperature treatments on surface morphology and stoichiometry have been determined by using Scanning Tunneling Microscopy (STM) and X-Ray Photoemission Spectroscopy (XPS).

Additionally Ag nanoparticles have been thermally evaporated on ZnO(10-10) surface. Since plasmon resonances in metal nanoparticles enhance light absorption and photocurrent generation, they are expected to significantly improve efficiency in thin film inorganic solar cells and possibly also in DSSC [3]. Self-assembly and size distribution of the metal nanoparticles have been investigated with STM and have been correlated to the electronic properties and the optical response of the system by using XPS and Electron Energy Loss Spectroscopy (EELS).

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#482 - Record polymeric solar cells synthesized at low temperature

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Organic solar cells can be processed from solution at room temperature and have been considered as an alternative photovoltaic technology, thus having been receiving considerable interest in the field of optoelectronics. Nevertheless Bulk Heterojunction (BHJ) devices grown by means of spin-coating techniques and starting from polymers (P3HT) and fullerene (C70) are extremely sensitive to ambient contamination and need proper passivating packaging, while research prototypes are synthesized and measured in controlled ambient.

Furthermore a strong annealing is necessary to reduce substantially the series resistance and to increase the shunt resistance of the device. For instance world record P3HT/PCBM BHJ with efficiency of about 8 %, [1] has been reached by an annealing processes at 180 C. We present an original method developed in Camerino [2] to grow high efficiency cells by using low temperatures annealing below 140C, particularly useful in case the substrates cannot be heated over such temperatures. Under this conditions the efficiency is larger than that of spin coated ones [3]. Furthermore, due to limited equipment of our lab such devices have been moved in air and transferred under glove box after 1-2 week time period for metallization and measure in another lab, while the spin-coated devices we use in the comparison have been fully under controlled atmosphere. Finally the specific growth mode used by separating solvent and solute by electric spray is particularly useful to obtain sophisticate z-axis heterostructures by choosing successive acceptor, and donor layers, able to optimize the photovoltaic efficiency by another 25 % [2], with respect to simple BHJ.

We believe that guaranteeing similar ambient conditions control we shall increase even more the efficiency gain in favor of the electro-spray case.

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#483 - Hyperbranched quasi-1D hierarchical mesostructures for dye sensitized solar cells and hydrogen generation

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The assembly of nanoscale building blocks in engineered mesostructures is one of the fundamental goals of nanotechnology. In this communication, we report on a novel fabrication method exploiting self-assembly from the gas-phase: Scattered Ballistic Deposition (SBD). SBD is a general physical phenomenon that arises from the interaction of a supersonic molecular beam with an ambient gas and enables the growth of quasi-1D hierarchical mesostructures (HM). Overall, they resemble a forest composed of individual, high aspect-ratio, tree-like structures, assembled from crystalline nanoparticles. The hierarchical quasi-1D nature of each tree represents an innovative compromise between nanorods/nanotubes (better electron transport) and the conventional isotropic nanoparticle photoanode (high surface area). We demonstrate the successful application of the novel quasi-1D hierarchical TiO_2 mesostructures deposited by Pulsed Laser Deposition assisted SBD onto FTO coated glass for two different solar energy conversion and storage technologies: Dye Sensitized Solar Cells and Photoelectrochemical hydrogen generation. The so-fabricated Hierarchical Mesoporous Photoanodes (HMP) exhibit tunable properties controlled by deposition conditions and thermal treatments: high surface area (from

50 to 350 m^{2}g^{-1}); roughness factors up to 100; porosity and pore size distribution (5-20 nm); grain size (10-30 nm); refractive index (1.5-1.9); amorphous or anatase phase. In contrast to typical nanoparticle based mesoporous photoanodes (NMP), they are characterized by vertical channels through the entire thickness that assure execellent diffusional path for liquid electrolytes and easy infiltration for solid hole transporting materials. Optimized photoanodes show enhanced light trapping capabilities with high broadband scattering efficiency. Hence, upon sensitization of the transparent TiO$_2$ HMP with visible light sensitive species, like dyes or Quantum Dots, they show increased optical density and broader absorption features with respect to standard NMP. These characteristics make the novel HMP ideal for solar capture and conversion technologies employing liquid or solid electrolytes. As an example, Solid State Dye Sensitized Solar Cells (SSDSC) fabricated with the novel hierarchical TiO$_2$ photoanode show higher short circuit current, Jsc, in accordance to the higher optical density measured, and higher power conversion efficiency than conventional NMPs. A similar effect is obtained when the HMPs are used for hydrogen generation, upon sensitization with CdS QDs by the successive ionic layer adsorption and reaction (SILAR) technique. The as synthesized CdS/ TiO$_2$ electrodes showed close to ideal photocurrent density and Internal Quantum Efficiency close to unity.

#484 - Characterization of hybrid solar cells by positron annihilation spectroscopy

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We report on the characterization of polymer-based hybrid solar cells namely poly(3-hexylthiophene) (P3HT) finely infiltrated with different molecular weights in a porous TiO$_2$ skeleton. A step-change improvement in the device performance is enabled by engineering the hybrid interface by the insertion of a proper molecular interlayer namely 4-mercaptopyridine (4-MP). The working mechanisms of excitonic solar cells are strongly dominated by interface processes, which thus influence the final device efficiency. Positron annihilation spectroscopy was used to monitor the effect of 4-MP on the penetration of P3HT in the pores of the oxide substrate (TiO$_2$) as a function of the chain lengths. In order to obtain depth-resolved data, positrons were implanted in the sample using a variable-energy positron beam. The characteristics of the partially filled nanoporous structures were evaluated in terms of the depth profile of the positronium yield and the S-parameter. A quantitative evaluation of the pore filling in the deep region is given from the analysis of Coincidence Doppler Broadening (CDB) taken at fixed implantation energy. We note a remarkable difference in terms of the positronium (Ps) fraction when the 4-MP interlayer is introduced. In fact, the Ps depth profile drops when TiO$_2$ is infiltrated with P3HT in presence of 4-MP. On the other hand, only a limited difference was observed in terms of the CDB information, which indicates that the presence of 4-MP does not affect sizably the polymer infiltration. We conclude that the reduction of Ps fraction is due to a reduction of free TiO$_2$ surface, that induce Ps inhibition and ortho-Ps quenching, which means a better contact between the oxide and P3HT phases and a closer polymer packing at the interface in agree with atomistic simulations. The results also suggest that the pores filling by itself is not the limiting factor controlling the device performances. The cells that contain the more shorter polymer chains result more efficient. The presented information, inaccessible by optical and electron microscopy techniques previously used, is in agreement with an improvement of charge generation and device photocurrent.

#485 - Plasmon-enhanced secondary electron emission from copper phtalocyanine deposited on Al(111)

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Aluminum \copper phthalocyanine (CuPC) interface is relevant in applications such as organic solar cells consisting of Al\CuPC\Ag thin layers that have shown enhancement of photoelectron conversion efficiency by surface plasmon excitation [1]. Furthermore, STM induced light emission from metal phthalocianine films on metal surfaces have been observed to enhance via plasmon excitation in the metal substrate [2]. In this paper coupling of the metal substrate plasmon excitation with the CuPC ionization is studied through observation of the secondary electron yield. Early experiments on Al(100) [3,4] propose that secondary electrons are emitted via a mechanism similar to photoemission with plasmon decay playing the role of photon absorption. The system studied is a 4Å thick CuPC film deposited in vacuum on Al(111) surface. The Al bulk plasmon is excited by electron impact in specular reflection geometry and the secondary electron spectrum is acquired in coincidence. The secondary electron spectrum coincident with the bulk plasmon excitation is fully interpreted in terms of photoemission events from CuPC initiated by photons with energy equal to the bulk plasmon electron energy loss. These findings suggest that the plasmon de-excitation generates an intense electromagnetic field at the interface that is responsible for the molecular photoionization.

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#486 - Reduce thickness and trap sunlight: how thin-film solar cells can be more efficient than bulk ones

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A central focus of solar cells research is to conceive and realize devices that approach the maximum efficiency limits, while being cost-competitive with present technologies. Bulk crystalline silicon (c-Si) solar cells with a thickness of few hundreds microns have a leading role in solar market, consolidated after decades of technological advances. However their efficiency are still lower than ultimate limits, and their cost is relatively high, a big fraction of it being determined by the large usage of active material. For these reasons thin-film c-Si solar cells are emerging as alternative to thick wafers, yet their efficiency is still much lower than the bulk case due to the incomplete absorption of sunlight in the thin layer. Here we show that c-Si solar cells with (isotropic) Lambertian light trapping and thickness down to a few microns can outperform the bulk ones. We develop a new electro-optical model which is capable of quantifying the effects of radiative and non-radiative (Auger, Shockley-Read-Hall in bulk and at surfaces) recombination mechanisms in the devices. We validate our model against numerical solution of the drift-diffusion equation obtained with the Silvaco-ATLAS software package, and obtain good agreement in a wide range of bulk and surface qualities. A crucial concern for conversion efficiency is the role of surface recombination, which becomes more important in thin cells due to the larger surface-to-volume ration. The scenario is further complicated for the case of light trapping, where surfaces may be textured with resulting increased surface area. We find that thin-film solar cells with light trapping remain more efficient than bulk ones provided that (effective) surface recombination velocities are below about 100 cm/s. This is the surface quality requirement in order to fully exploit the benefits of increased absorption (witch leads to higher photocurrent) and reduced thickness (which leads to higher voltage). Although rather stringent compared to bulk cells requirements, this value is compatible with present surface passivation techniques, which provide recombination velocities down to 1-10 cm/s, and with nanostructuring methods, which increase the surface area up to a factor of about 2.5. These results prove that c-Si solar cells with thickness down to a few microns can reach high efficiency and outperform the bulk ones by adding Lambertian light trapping. The analysis proves that present-day standard material quality and surfaces passivation techniques are adequate to ensure this results.

#487 - Vibrational dynamics in amorphous materials revealed by broadband photo-acoustics

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The behavior of high-frequency acoustic excitations in disordered materials is one of the most provocative and less understood aspects of glass science. The frequency dependence of sound velocity and damping, in particular, is the result of the interplay of several physical mechanisms related to anharmonicity and topological disorder. In an effort to address an emerging, highly debated scenario, we recently developed Broadband Picosecond Acoustics (BPA), a novel time domain technique for interferometric photoacoustics. BPA allows accessing -in a single measurement with unprecedented sampling efficiency- wave-packet acoustic frequency regions bridging the gap existing between frequency domain techniques such as Brillouin light and X-ray scattering [1].

I will discuss here a few examples elucidating the interplay between acoustic attenuation and anomalous density of states (Boson Peak) in strong glasses and the connections between ultrastability against crystallization and mechanical properties in amorphous pharmaceuticals. An acoustic pulse is launched at time zero by a thin (10-20 nm) absorbing transducer layer deposited onto the surface of the sample, irradiated by an 800 nm, 50 fs pump pulse obtained by a regeneratively amplified 1-kHz Ti:sapphire laser source. The acoustic pulse then travels through the sample first and then enters the substrate. The wavepacket motion is monitored by a delayed white-light continuum probe pulse generated by the Ti:Sa fundamental focused onto a rotating CaF_2 plate, with a spectrum extending in the 350-1100 nm range [2]. Two dimensional transient reflectivity maps as a function of probe delay and wavelength are recorded: each optical frequency in the broadband probe phase-matches a single acoustic frequency of the travelling acoustic wavepacket, following the momentum conservation law of stimulated Brillouin scattering.
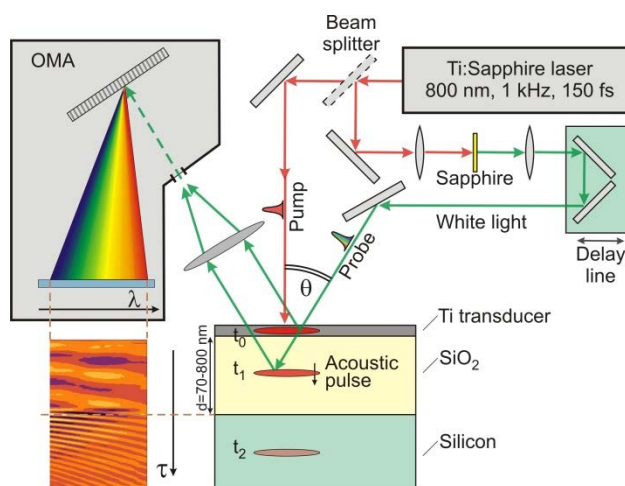
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#488 - Ultrafast nano-optics: Using strong laser fields to control the motion of electrons in and around metallic nanostructures

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Sharp metallic nanotapers irradiated with few-cycle laser pulses are emerging as a source of highly confined coherent electron wavepackets with attosecond duration and strong directivity [1-6]. The possibility to steer, control or switch such electron wavepackets by light is expected to pave the way towards direct visualization of nanoplasmonic field dynamics and real-time probing of electron motion in solid state nanostructures. Such pulses can be generated by strong-field induced tunneling and acceleration of electrons in the near-field of sharp gold tapers within one half-cycle of the driving laser field. Here, we study for the first time the effect of the carrier envelope phase of few cycle laser pulses on the motion of electrons emitted from metallic nanostructures by strong-field tunneling.

We illuminate very sharp, single-crystalling gold tips with CEP-stable few-cycle near-infrared pulses at 1.5 µm and record angle-resolved kinetic energy spectra of the photoemitted electrons. Our experiments give first evidence for the effect of absolute phase of the laser pulses on the emission direction and kinetic energy distribution of the photoemitted electrons. We observe pronounced modifications of the photoelectron spectra when varying the CEP phase, paving the way towards a light-driven control of motion of electrons in the near field of metallic nanostructures on sub-femtosecond time scales and nanometer length scales. In my talk, I will give an introduction into this emerging field, discuss our own recent experimental observations and their interpretation within simple theoretical models and will give an outlook, illustrating possible applications of such electron sources.

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#489 - Ultrafast charge photogeneration in semiconducting carbon nanotubes

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Single-walled carbon nanotubes (SWNTs) show distinctive physical and optical properties that are particularly promising for the development of a new generation of advanced devices with enhanced mechanical, electronic, and optical capabilities. A comprehensive picture for their photoexcitation scenario is however necessary for further developments in photonics and optoelectronics applications. It has been demonstrated that after photo-excitation other excited species can coexist with neutral singlet excitons. Examples are bi-excitons [1], charge carriers [2] and trions [3]. Recently, Crochet et al. [4] reported on free carrier photo-generation in aggregated SWNTs following high energy excitation, at the π-π^* transition associated with the M saddle point of the graphene lattice. Inter tube interactions may play a role in many SWNT samples because colloidal suspensions are generally metastable and have the tendency to aggregate with time, leading to efficient inter tube energy transfer [5] and possibly charge separation.

In this work we apply ultrafast pump-probe spectroscopy, with tunable pump photon energy and broadband coverage, on a sample of highly enriched (6,5) SWNTs. We demonstrate that the transient absorption signal, following the initial ultrafast relaxation, is dominated by a long lived spectral feature that is extended on a broad probe energy window. The long lived signal is well described by the derivative of the ground state absorption spectrum and is independent of the pump photon energy. The signal is consistent with an energy red shift of ground state absorption that we ascribe to the Stark effect induced by photo-generated and trapped charge carriers. Our results suggest that about 1-2% of the absorbed photons generate long lived charges.

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#490 - Ultrafast optical mapping of nonlinear plasmon dynamics in Cu$_{2x}$Se nanocrystals

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Plasmon-polaritons in metals have opened unprecedented avenues for nanoscale manipulation of light. Most of research have dealt with the linear optical properties of plasmonic systems, but during the very last years the nonlinear response of plasmonic nanostructures have received an increasing attention in view of the giant optical nonlinearity exhibited by metallic media [1]. Strong efforts are now being carried on in different directions to improve the efficiency of the nonlinear processes in plasmonic structures. One research line is aimed to optimizing the linear part of the phenomenon, that is plasmonic resonances, by seeking the best nanostructure geometry capable of full exploitation of the nonlinearity in noble metals. A different approach has been recently started by working on the intimate physics underlying material nonlinearity, thus opening a material route to nonlinear plasmonics.

Beside gold and silver, a novel class of synthetic plasmonic media based on heavily-doped semiconductors has been recently reported. These materials exhibit a metallic behaviour with a free-carrier density that can be chemically controlled, allowing the plasmonic resonance to be tuned in a broad wavelength range. Most importantly, since the nonlinearity exhibited by metallic systems is governed by the dynamics of the free carriers optically excited, these materials offer the unique capability to enhance the nonlinear response of the plasmonic resonance by controlling the free carriers density.

Cu$_{2-x}$Se is one of these novel plasmonic materials [2], where the free carriers are the holes in the valence band generated by copper vacancies (so-called self-doping mechanism) responsible to the sub-stoichiometry of the compound, with x ranging between 0.1 and 0.3.

We report on a detailed experimental investigation of the ultra-fast nonlinear response exhibited by Cu$_{2-x}$Se nanocrystals in the visible and near-infrared under excitation with fs laser beams.

The onset of the plasmon dynamics is spectrally resolved by fs pump-probe spectroscopy with broad-band probe pulses. We also provide a consistent theoretical model mimicking the one exploited for noble-metal plasmonic systems, and in particular we considered here an extended version of the two-temperature model (ETTM) that is reminiscent of the one originally proposed for gold by Sun and coworkers3. The combination of broad-band pump-probe measurements and the ETTM allowed us to access the

temporal dynamics of non-thermalized carries taking place on the sub-ps time scale, and dominating the peak of the nonlinear optical response.

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#491 - Time-resolved charge carriers dynamics in carbon nanotube / n-silicon heterojunctions for photovoltaic applications

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In these last years, carbon nanotubes (CNTs) have emerged as new building blocks for constructing light-energy harvesting and charge transport assemblies in photovoltaic devices [1,2,3]. The intriguing photoexcited carriers behaviour in CNT aggregates, that significantly affects the device performances, has been proved to be strongly dependent on multiple factors, such as CNT types, bundling and growth architectures [4,5].

Recently, among the hybrid systems based on carbon nanotubes, CNT/n-doped Silicon (CNT/Si-n) interface has revealed as a suitable configuration for making solar cells [6,7] showing an overall efficiency larger than 10% [8].

However, an understanding of the role of carbon nanotube in CNT/Si-n heterojunction is missing, even if it is mandatory for the improvement of the solar cell efficiency.

In this framework, performing time resolved optical spectroscopy, we try to shed light on the steps immediately following the arrival of the light on CNT/Si-n solar cell.

Tuning the pump photon energy across the Silicon absorption edge, we are able to unambiguously track the photoexcited carrier relaxation in the CNT layer and to reveal the hole injection from Si to CNT driven by the drift current at the heterojunction interface.

The results here reported show that transient optical spectroscopy could be a powerful technique for measuring the processes occurring immediately after the photogeneration of electron-hole pairs in an heterojunction solar cell.

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#492 - Charge and spin dynamics information from magneto optical signal

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Over the last two decades the physical origin of laser induced magneto-optical response and its interpretation have been at the center of community debates mainly in the hundreds of femtoseconds time domain.

By measuring both Kerr ellipticity and rotation in appropriate conditions, one can disclose the genuine magnetic dynamics. We employed this technique capable to disentangle spin and charge effects in the MOKE signal, to investigate the magnetic dynamics of diverse ferromagnets.

We observed a significant charge contribution in correlated oxide transition metals e.g. CrO_2 and $La_{1-x}Sr_xMnO_3$. The results demonstrate that in order to obtain reliable information on the spin dynamics, one should not restrict to the analysis of Kerr rotation or ellipticity alone.

Furthermore to achieve a more comprehensive understanding of the optically-induced effects on spin or charge we probed transient reflectivity and MOKE in a wide spectral regime (400-700 nm). As anticipated, the outcomes revealed remarkable information about electron and spin dynamics in the time scales ranging from tens of fs to tens of ps.

#493 - Attosecond electronic wave packets in molecular nitrogen

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In this work we will present experimental and theoretical results regarding two experiments performed in helium and nitrogen using the attosecond transient absorptions spectroscopy technique. Tunable isolated attosecond pulses were generated using the polarization gating technique in combination with different metallic filters (indium, tin and aluminum) for the selection of different portions of the broadband extreme ultraviolet (XUV) supercontinuum. These pulses were used to excite complex electronic wave packets composed by states below and above the ionization threshold in helium (Ip = 24.6 eV) and nitrogen (Ip = 15.58 eV). The XUV radiation transmitted through the atomic and molecular samples was analyzed using flat-field XUV spectrometer composed by a toroidal mirror, a concave grating and an MCP coupled to a phosphor screen and a CCD camera. The characteristics of the transmitted XUV spectra were modified using a carrier-envelope-phase (CEP) stable synchronized few-cycle infrared (IR) pulse co-propagating with the attosecond pulse. The modifications of the transmitted XUV spectrum were characterized as function of the delay between the two XUV and IR pulses and for different intensities and polarization directions of the IR beam.

In nitrogen the XUV spectrum allowed to populate the manifold of excited states converging to the ground and first excited state of the molecular ion, as well as the series of autoionizing resonances around 17 eV. The CEP-stabilized few-cycle pulses coupled the levels below and above the ionization threshold by a two-photon mechanism. Changing the delay between the IR and XUV pulses clear sub-cycle oscillations in the absorption of the XUV light were observed. We will present the results of different theoretical models based on a resonant and a non-resonant coupling between the two groups of states.

In helium the XUV spectrum allowed to efficiently populate the single excited states 1snp. In the presence of the strong IR field, additional absorption features characterized the transmitted spectrum corresponding to absorption of XUV light by atomic excited states dressed by the IR field. These absorption features oscillated as function of the relative delay between the two pulses. We will show how the absorption of these dressed states can be controlled by changing the polarization direction of the IR field.

#494 - Tailoring diffractive properties of photonic crystals for out-of plane operation

Thomas Krauss (I) - Department of Physics, University of York

Planar Photonic Crystals have added value and functionality to many areas of photonics due to their ability to confine light strongly in the plane. More recently, it has become apparent that they also offer interesting properties for out-of plane operation. We discuss two examples for such out-of-plane operation; a) Diffractive optics for solar cells. We have shown that photonic crystal principles allow us to design diffractive structures that enable almost complete trapping of light for silicon solar cell applications. These structures are multiperiodic, and appear almost random, yet they use k-space engineering familiar from other planar photonic crystal devices; b) High contrast mirrors (HCGs). Photonic crystals can also act as very high reflectivity mirrors for out-of-plane operation, where they are often referred to as "high contrast gratings". We show how such high reflectivity is achieved, and more importantly, how the reflected phase can be tailored to achieve focussing mirrors and confocal Fabry-Perot cavities.

#495 - Imaging and tuning of photonic nanocavities

Massimo Gurioli (I) - Dipartimento di Fisica e Astronomia, Università di Firenze

Photonic crystals microcavities (PCMCs) design allow to realize optical modes with large quality factor which have been already successfully exploited for the realization of low-threshold lasers, single photon sources, add-drop filters, and for the implementation of cavity quantum electrodynamics experiments.
In this talk I will review recent results obtained in Florence on three crucial issues in the progress of photonic crystal microcavities (PCMCs).
1) Imaging the optical local density of states (LDOS) of PCMCs [1] by using the tip-induced modifications of the PCMC modes by scanning near-field optical microscopy (SNOM). Mapping of the magnetic field has also been achieved by using a metallic coated tip [2].
2) Tuning the optical resonances in PCMCs. Three different approaches to the local and reversible tuning have been realized. i) Water micro-infiltration, at the level of the PC single pore [3]. ii) local evaporation of the infiltrated water [3] iii) Laser induced nano-oxidation [4].
3) Coupling the optical modes of adjacent PCMCs via evanescent waves. The photonic coupling of two closely spaced PC-MCs have been demonstrated and by means of near field imaging [4]. Control of the cavity detuning is obtained by locally tuning a single cavity mode [5]. Mode hybridization [6] and antibonding ground state [7-8] are found and discussed.

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#496 - Optimizing silicon-on-oxide polarization diversity 2D-grating couplers for integrated Si-photonic circuits

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We report the optimization of a partially etched 2D-grating coupler in the 220 nm silicon-on-insulator (SOI) platform for telecom applications, using fully 3D finite difference time domain (3D-FDTD) calculations. A campaign of 3D-FDTD simulations is used to test the practical parameter space of the photonic crystal array (PCA) etched in to the 220 nm SOI platform that makes up the active region of the polarization diversity 2D-grating coupler. The aim of this campaign is to identify that unique combination of etch-depth (E), hole-radius (R), and grating-pitch (P) that gives the highest coupling efficiency between the input fibre mode and the pair of Si waveguides exiting the coupler into the SOI platform at 1550 nm. Fig 1(a) illustrates a subset of coupling spectra generated by these 3D-FDTD calculations for the case of an etch-depth of 70 nm. There are many different combinations of hole-radius and grating-pitch that tune the 70 nm-etch design to 1550 nm. However, as shown in Fig 1(b), there is always a unique radius-pitch pair that gives the highest coupling efficiency for a given etch-depth. When all possible etch-depths are tested in this way, the optimum combination of etch-depth, hole-radius and grating pitch can be identified, and delivers a coupling efficiency of 48% (-3.2 dB), which is the highest value reported to date for 2D-grating couplers in the SOI platform. While 3D-FDTD is a powerful tool for optimizing the coupler design, it is computationally intensive. Extending the parameter space of 3D-FDTD optimization to include the SOI layer thickness, angle of incidence for the input fibre mode, etc., is not currently practical. Calculations of the photonic mode dispersion, made by means of guided-mode expansion (GME), indicate that the high coupling efficiency of the 2D-grating coupler originates from an optically active resonant guided mode in its PCA. Furthermore, the resonance wavelengths predicted by the GME calculations correspond very closely to the coupling spectra peaks of the 3D-FDTD calculations, despite treating the $11\mu m \times 11\mu m$ PCA of the 2D-grating coupler as an infinite array. Even when etch-depth and hole-radius are swept over large ranges, the agreement between computationally light GME and computationally intensive 3D-FDTD remains within the full-width half-maximum of the spectra line-width. This close correspondence points towards a combined optimization approach in which fast GME calculations

generate initial values that are then fine-tuned by 3D-FDTD calculations. With this scheme, it may be practical to globally optimize the 2D-grating coupler in terms not only of etch-depth, hole-radius, and grating-pitch, but also the SOI layer thickness, angle-of-incidence, etc., in order to offer even higher coupling efficiencies.
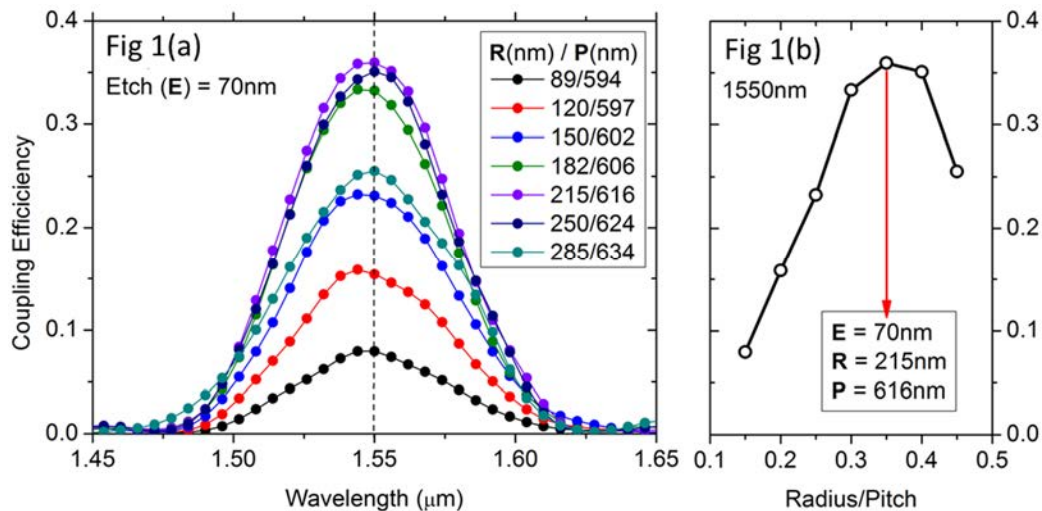
#497 - Fractional Bloch oscillations in photonic lattices

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Bloch oscillations, the oscillatory motion of a quantum particle in a periodic potential, are one of the most fascinating effects of coherent quantum transport. This phenomenon was first studied in the context of electrons in crystals and it is a consequence of the wave nature of matter. Actually, decoherence and dephasing effects prevent Bloch oscillations to be experimentally observed in natural crystals. On the contrary, they have been successfully visualized in semiconductor superlattices and ultracold atoms, as well as in photonic model systems.

Bloch oscillations were originally originally studied at the single-particle level. However, interesting novel dynamics may arise in case several interacting particles are considered: in fact, they can form bound states and co-tunnel through the lattice. In particular, for few strongly interacting particles, Bloch oscillations of the bound states have been predicted, happening at a frequency twice (or multiple) that of single-particle. This intriguing phenomenon has never been observed, up to now, not even in model systems.

Here we report on the first experimental observation of fractional Bloch oscillations in a photonic model system. A waveguide lattice is fabricated by femtosecond laser direct writing technique and is used to simulate two-particle extended Bose-Hubbard Hamiltonian. In detail, the dynamics of two correlated particles hopping on a one-dimensional lattice is mimicked by light transport in a square waveguide lattice with bent axis. Engineered defects in the lattice allows to simulate the attractive interaction potential of the two particles.

#498 - Colloidal Systems: suitable tools for photonic applications

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The control of light transport is crucial to design and tailor new photonic devices with increased optical performance in the same manner as controlling electron transport is at the basis of semiconductor and electronic technology.

In recent years different type of structures have been realized with the goal of controlling light propagation through interference phenomena; in particular several attention has been dedicated to the fabrication and the study of colloidal systems that permit to create easily ordered (photonic crystals) and disordered (photonic glasses) systems.

In this communication we want to highlight the optical properties of different colloidal confined systems such as:

(i) polymeric composite systems, based on polystyrene colloidal nanoparticles assembled and embedded in an elastomeric matrix (polymer colloidal crystal, PCC), designed in order to display a visible opalescence and able to change their properties under an external stimulus.

(ii) heterostructures colloidal crystals, constituted by multistack layers of colloidal photonic crystals, where the superposition of the properties of each single colloidal crystal, permit to develop systems that present multi-frequency stop bands.

(iii) metallic dielectric structures, where the infiltration of colloidal crystals with metallic nanoparticles permits to modify the optical properties of the common opal systems with the potentiality to develop optical switching devices.

(iv) disordered structures, based on monosize nanoparticles with no spatial correlation, that exhibit a band-gap-like- effect called also

"Mie Resonance"; these structures can be used to study fundamental phenomena in random media and can be employed as starting platform for the realization of Random Laser systems.

#499 - Thin porous structure containing liquid crystal: key technology for low voltage tuning capability of photonics devices

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Thin photonics structures base their operating principle on the interaction material-electromagnetic wave on a length scale comparable to the wavelength of light. Photonic structures made by porous materials infiltrated with liquid crystal give a great potential for tunable photonic devices due to ease of fabrication, the possibility of obtaining compact and switchable optoelectronic devices and the flexibility in wavelength design. In these novel devices, it is easy to obtain very high refractive index modulation (Δn) only by alternating two or more suitable materials. An interesting consequence is the capability to achieve high photonic band gap efficiency with a thickness of just few micrometers.

In this study we present the fabrication and the optical characterization of a very thin photonic crystal made by porous materials (as metal oxide nanoparticle-based film), infiltrated with the nematic liquid crystal realized by drop casting with a simple and fast procedure. Two methods of the photonics band gap tunability have been proposed. In the first one, the real time analysis of the photonic band-gap during the E7 liquid crystal infiltration shows a red shift (60 nm) due to the increase of an effective refractive index of the multilayer. Tunability with electric field - by aligning the liquid crystal director - has been observed at very low applied voltage, with a blue shift of the photonic band gap of 8 nm at only 8 Vrms [1]. This result is one order of magnitude smaller with respect to previously reported liquid crystal infiltrated photonic crystals, corresponding to the ratio between electric field and wavelength shift of about 0.5 V/(μm nm). In the second one, we put forward the possibility of tuning the photonic band gap of the porous multilayer just by infiltration with different and selected liquid crystals, in accordance with results carried out by a custom software [2]. In order to increase the range of wavelength tunability, fixed the thickness of the device a new combination of Bragg and Snell law has been proposed taking advantage from a particular wafer device. The obtained performances - improvement through the choice of the most suitable liquid crystals for lower voltage operation - could be very interesting for realization of low cost and portable devices for high density integrated optics.

[1] L. Criante, F. Scotognella, Mol. Cryst. Liq. Cryst., 572, 31-39 (2013).
[2] L. Criante, F. Scotognella, J. Phys. Chem. C, 116, 21572-21576 (2012).

#500 - Hybrid plasmonic - photonic nanostructures: gold nanocrescent over opals

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In this work we demonstrate that it is possible to decorate the surface of an artificial Opal Photonic Crystal (PhC) with an ordered hexagonal array of isolated noble metal nanostructures shaped as half-moon crescents. This has been achieved by evaporating gold at grazing angles on the top close-packed layer of microspheres; in this way atom deposition is forced only on the portion of the microspheres, which is illuminated by the atom beam. The asymmetric shape of the nanocrescents is reflected in their anisotropic optical response, under linearly polarised illumination, due to the excitation of localised plasmon resonances (LSPRs). By changing the size of the microspheres, we are able to modify both the period of the close-packed microsphere lattice and the size of the metal nanocrescents, thus affecting at the same time the stop-band of the photonic crystal and the spectral position of the LSPRs along the main symmetry directions. The optimisation of the morphological parameters of the microsphere/nanocrescent array and of the incidence scattering conditions of light allows tailoring the spectral positions of the plasmonic and photonic bands finding the favourable parameters for which the two excitations overlap in energy and momentum. Under these conditions a dramatic change of the properties of both excitations is observed, as revealed by the modification of the dispersion relation, which evidences the creation of a new hybrid excitation whose spectral position and dispersion properties are a combination of those of localised bare plasmons and photonic modes [1]. The possibility to increase field localisation in the hybrid photonic-plasmonic modes observed in the 3D opal structures might be used in order to obtain field amplification in novel sensors and photonic applications.

[1] V. Robbiano, M. Giordano, C. Martella, F. Di Stasio, D. Chiappe, F. Buatier de Mongeot, D. Comoretto Advanced Optical Materials in press (2013).

#501 - Diamond technology for multielectrodes electrochemical biochips

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Electrochemical biochips fabricated using thin-films of synthetic boron-doped diamond (BDD) grown on insulating substrates, can deliver unmatched performances thanks to the extreme mechanical, thermal, chemical, electrical and optical properties uniquely possessed by diamond.

BDD-devices are typically fabricated on non-transparent silicon wafers. Envisioning simultaneous electrochemical and fluorescence detections of biological events, we developed a new diamond-on-sapphire technology, which made use of a thin silicon interlayer of ~50 nm, to provide a convenient interface for diamond growth onto the sapphire surface. In this way a variety of Microelectrode Arrays (MEA), with layouts ranging between 4 and 16 independent electrodes has been successfully fabricated.

Being Diamond a distinctive type-0 electrode material, those chips were primarily employed for amperometric detection of secretory events, showing excellent sensitivity, very low noise, fast response and long-term reliability. Besides that, the device characterization conducted by means of classical electrochemical methods like impedance spectroscopy and Mott-Schottky plots, made us clear that our BDD-MEAs were also suitable for potentiometric detection, provided tailored read-out electronics is available. This approach conducted to successful recordings of action and field potentials and even transient pH-variations, as reported elsewhere in this conference.

On the side of optical transparency major improvements were demanded. In fact the silicon interlayer caused a significant absorption in the blue-violet region of the transmissivity spectrum, thus limiting the potential use of fluorescent detection to the red-green range only, where at least 50 % transparency was available.

Our last developments were focused on better transparency and layouts with higher complexity. New technological processes have been optimized, to grow highly-doped BDD-layers onto transparent substrates, without silicon interlayer. Remarkable improvements of the transmissivity in the whole visible spectrum have been obtained.

BDD-film thickness of ~ 200 nm in combination with electron-beam lithography allows now the fabrication of MEAs with 12 electrodes in a round sensing area of 20 µm in diameter for subcellular spatial resolution. Also new BDD-MEAs with 64-channel arranged on a grid with 200 µm spacing, for cell populations and tissue samples are presented.

#502 - Boron-doped diamond MEAs for revealing amperometric and potentiometric signals in living cells

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Sara Gosso, Andrea Marcantoni (Dipartimento di Scienza e Tecnologia del Farmaco, Università di Torino e CNISM), Suaad Alsawafi, Elisabetta Colombo, Ziyao Gao, Alberto Pasquarelli (Institute of Electron Devices and Circuit, University of Ulm, 89069 Ulm, Germany), Emilio Carbone (Dipartimento di Scienza e Tecnologia del Farmaco, Università di Torino e CNISM)

We developed different prototypes of boron-doped nanocrystalline diamond arrays (NCD-MEAs) with the aim of monitoring either quantal secretory events of released oxidizable neurotransmitters (amperometric mode) or voltage signals in excitable cells (potentiometric mode). All multisite recording arrays were fabricated in diamond thin-film technology as described in the preceding presentation by Pasquarelli et al.

Detection of released catecholamines from chromaffin cells can be performed in the amperometric-recording mode of NCD-MEAs. Transient current signals of ~ 100 ms duration and 50 - 200 pA spike amplitude (caused by the oxidation of catecholamines with a + 800 mV polarized NCD-MEA), can be easily detected to obtain direct information about the kinetics and amplitude of quantal secretory events. Catecholamine release can be simultaneously measured from 4-16 cells, previously positioned onto the NCD-MEAs. Alternatively, the diamond array prototype can be patterned with a higher density of microelectrodes that match the size of bovine chromaffin cells. In this case, the high-density and the narrow areas of the microelectrodes can provide an accurate spatial mapping of release sites within a single cell (see Gosso et al. for more details).

NCD-MEAs are suitable as well for performing high-resolution potentiometric recordings, to monitor the extracellular electrical activity of excitable tissues. We tested this recording mode using intact mouse sino-atrial tissues and measured synchronized action potential (AP) signals by all the 16 electrodes on the array (150 ms duration, 3 Hz frequency, 360 microV amplitude). Detected APs were comparable in size and shape with those recorded using commercially available TiN MEAs. Thus, the proposed NCD-MEAs can be successfully used as multi-task biosensors for in vitro recordings and drug-screening tools.

#503 - A diamond-based biosensor for exocytosis detection from chromaffin cells realized with ion beam lithography

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Sara Gosso, Ettore Vittone (Università di Torino), Alberto Pasquarelli (Ulm University), Emilio Carbone, Paolo Olivero, Valentina Carabelli Università di Torino)

Buried graphitic channels fabricated in monocrystalline diamond by selective damage induced by focused MeV ions, can be considered an effective alternative to the commonly used carbon-fibers to detect the catecholamine release from cells as individual secretory granules discharge their contents during the process of quantal exocytosis.

It is shown a biosensor fabricated by using a focused 1.6 MeV He ion beam scanned over monocrystalline diamond sample (3x3x0,5 mm^3) to define micrometric highly damaged region few micrometers below the surface. After the irradiation, the sample was annealed at high temperature (900 °C) to promote the conversion to the graphitic phase of amorphized region.

This process provided buried highly conductive graphitic channels embedded in a highly electrically insulating and chemically inert diamond matrix; and with end points (with dimension below 10 micrometer) emerging to the surface and available to be used as electrodes.

Quantal secretory responses have been measured from stimulated chromaffin cells, which were positioned on the graphitic microelectrode, polarized to + 800 mV. Sequences of amperometric spikes started after cell stimulation with the KCl solution, with amplitudes well above the background noise within the range of 8-180 pA and comparable with signals obtained by conventional carbon fiber electrodes (CFE). These results demonstrate the potential of the ion beam micromachining technique to fabricate micrometer sized arrays of microelectrodes in monocrystalline diamond with an electrochemical sensitivity suitable for high-resolution measurement of quantal exocytosis

#504 - Organic ultra-thin film transistorfor extracellular stimulation and recording of stem cell derived neuronal networks

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Electronic transducers of neuronal cellular activity are important devices in neuroscience and neurology. Organic field-effect transistors (OFETs) offer tailored surface chemistry, mechanical flexibility, and high sensitivity to electrostatic potential changes at device interfaces. These properties make them attractive for interfacing electronics to neural cells and performing extracellular recordings and stimulation of neuronal network activity. In this work we operate pentacene ultra-thin film (9 nm thick) transistors with a liquid gate both as transducer and electrical stimulator of neuronal network activity. These devices are highly sensitive to small potential changes in cell medium and exhibit sufficient stability in standard cell culture conditions for nine days. We show that murine neural stem cells can be adhered on top of functional devices with no need of an additional layer of cell-adhesive molecules, and then differentiated into neuronal networks. OFET response is monitored during the different phases of the neuronal differentiation process up to nine days. Only when stem cells are differentiated into neurons, it was possible to measure electrical signals in the OFET current following the stimulation. Due to the large sensing area of our device, which accommodates from hundreds to thousands interconnected neurons, the OFET electrical signals arise from the collective electrophysiological response of the neuronal population. The maximum extracellular potential change in the cleft region adjacent to the transistor surface amounts to 350 micro volts. This demonstrates that pentacene ultra-thin film OFETs enable good cellular adhesion and efficient coupling of the ionic currents at the biological-organic semiconductor interface with the OFET current.This work is supported by EU NMP Project I-ONE Grant Agreement n. 280772.

#505 - Three-dimensional MEA to record long-term plasticity in brain slices

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Extracellular field potentials were recorded from acute cerebellar slices with three-dimensional Multi-Electrode Array (MEA).The conventional MEA system consisted of a chip (a silicon substrate supporting thin film platinum wires leading to the electrodes and insulated with a 5mm-thick SU-8 epoxy layer) connected to amplifiers via printed circuit boards. MEAs contained 60 conic electrodes covered with a thin platinum film arranged in an 8X8 matrix (without corner electrodes) and spaced by 100 mm. The electrodes had a base diameter of 40 mm and height of 30 mm, with an effective recording area of 1600 mm 2. Here we present the results obtained by employing MEAs recordings to investigate the spatial organization of long-term synaptic plasticity [long-term potentiation (LTP) and long-term depression (LTD)] which is supposed to play a critical role for distributed signal processing in neuronal networks, but its nature remains undetermined in most central circuits. We have reconstructed activation maps of the granular layer in cerebellar slices. Furthermore by combining MEAs to stimulate in multiple sites and Voltage Sensitive Dye Imaging to detect circuit responses, we have investigated complex network functions which favored the emergence of combinatorial operations.

#506 - Spatial detection of amperometric spikes in microareas of chromaffin cells using high-density diamond MEAs

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Carbon fiber microelectrodes (CFEs) are the most used commercially available electrochemical sensors for detecting neurotransmitter molecules. The technique has some major restriction, mainly related to a low spatial resolution and lack of optical transparency. To partially overcome these limitations, a new 9 channels nanocrystalline diamond ultra-microelectrode array (NCD-UMEA) has been developed and tested. The prototype is fabricated in nanocrystalline diamond on sapphire technology and the layout is achieved by standard microfabrication techniques like photolithography, lift-off, dry etching and PECVD. Calibration of the 9 channels NCD-UMEA was performed by cyclic voltammetry with different adrenaline concentrations. The device consists of 9

boron-doped diamond microelectrodes emerging in a central sensing area of 20 μm diameter, where the chromaffin cell is positioned. Each electrode is able to detect quantal exocytotic release of catecholamines by means of amperometric recordings. Taking advantage of the small areas of the diamond ultra-microelectrodes (of 12 to 27 μm^2), we developed a MatLab routine that localizes the distribution of release sites of in vitro bovine chromaffin cells. The routine allows to show the 9 channels on a grid overlap with a colorimeter scale that indicates the amount of exocytic events recorded by each channels. We found that the 9 channels NCD-UMEA can resolve amperometric spikes with the same sensitivity and temporal resolution of CFEs. The microchip prototype was used to map membrane areas and revealed the existence of a marked heterogeneous distribution of exocytotic events in bovine chromaffin cells.

#507 - Recording of neuronal activity from cellular subdomains by Ca^{2+} imaging: an innovative analytical approach

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Davide Lovisolo (Dipartimento di Scienze della Vita e Biologia dei Sistemi, Università di Torino), Mario Ferraro (Dipartimento di Fisica Sperimentale, Università di Torino), Alessandra Gilardino (Dipartimento di Scienze della Vita e Biologia dei Sistemi, Università di Torino)

Cytosolic calcium signals control a large set of cellular functions. In nerve cells, activation of calcium channels both by voltage, during firing activity, and by neurotransmitters and other signaling molecules generates changes in cytosolic calcium concentration, $[Ca^{2+}]_i$. These signals, that can be recorded by means of fluorescent calcium indicators, have often complex time courses and information they convey can be coded both in amplitude and frequency. For this reason their quantitative analysis is not easily accomplished and, in particular, it may be difficult to evidence subtle differences in their temporal patterns. In general, spectral analysis is mandatory, but it provides a mean of analysis solely in the space of frequencies. To overcome this limitation we developed new tools based on wavelet analysis in order to extract information on the structure of $[Ca^{2+}]_i$ oscillations. In particular we have derived a set of indices by which different $[Ca^{2+}]_i$ oscillatory patterns and their change in time can be extracted and quantitatively evaluated. This approach has been applied to a particularly complex set of calcium signals, those generated by the neurotrophic factor FGF-2 at the growth cone, the leading edge of an extending neurite, that are involved in its control of growth and correct orientation. By this approach, it has been also possible to detect the effects of blockers of specific classes of calcium channels, that could not be straightforwardly evidenced with a qualitative approach. Another crucial feature of neuronal calcium signals is their spatial compartmentalization (e.g. dendritic subcompartments, presynaptic terminal, the growth cone itself). To analyze this aspect, high resolution fluorescence imaging has been combined with a further development of the wavelet approach by including the spatial variable, in order to compare $[Ca^{2+}]_i$ oscillations in distinct cellular subdomains (in our case growth cone, neurite and soma). By this way it has been possible to show that the differences in oscillatory activity between the different regions are not simply due to geometrical/morphological parameters, such as the surface to volume ratio, but also to differences in the spatial distributions of the molecular entities involved in calcium influx/efflux (channels and/or transporters).

#508 - Magnetic nanoparticles in biomedicine

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In the last two decades, a lot of attention was devoted to novel multifunctional nanostructures based on magnetic nanoparticles (MNP) useful as agents for Magnetic Resonance Imaging, Optical Imaging and Magnetic Fluid Hyperthermia, as carriers for drugs and molecular targeting vectors. Most of the systems reported by different research groups, have been shown to be useful as MRI contrast agents, fluorescent systems and magnetic fluid hyperthermia mediators, displaying high nuclear relaxivity and Specific Absorption Rate (SAR). For these compounds, the possibility to collect images of the regions where the MNP are delivered through MRI and Optical Imaging, is joint to the use of radio-frequency fields that heat locally the tumour cells, possibly inducing their death; a theranostic agent is thus obtained. In the field of drug delivery and molecular targeting, few examples of reproducible experiments using superparamagnetic nanoparticles are actually present in literature. All the above cases will be introduced and briefly discussed.

#509 - Controlled synthesis of noble metal nanoparticle arrays and their behaviour as SERS substrates

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The interest in the production and control of nanoparticles (NPs) and cluster-assembled nanometer-sized films is steadily increasing. Nanosecond (ns) pulsed laser deposition is a suitable technique to achieve these objectives. Atomic, or molecular, particles grow during the propagation through an ambient gas of the plasma plume generated upon target irradiation. Deposition parameters including laser wavelength and energy density, target to substrate distance, nature and pressure of the ambient gas affect plasma expansion and thus NP size and kinetic energy, together with the related distributions. The size of the NPs at landing, their energy and their mobility on the substrate determine film growth and morphology, resulting in broad ranges of values of the physico-chemical properties of the deposited films. Controlling the onset of different stages of film growth is vital to obtain films with ad hoc tailored properties. We report on a method for the growth of films consisting of self-assembled NPs, with specific attention to Ag and Au. Nanostructured films were obtained by ns pulsed laser ablation of metallic targets in presence of a controlled Ar atmosphere. The morphology of the films ranged from isolated NPs to island structures (Fig. 1), as observed by SEM and TEM. It sensitively depends on gas pressure (10-100 Pa) and on laser pulse number (500-30000), keeping other deposition parameters such as target to substrate distance, incidence angle, laser wavelength, laser fluence constant [1-4]. Fast imaging respect to the arrival of the laser pulse, allows revealing the plasma propagation regime and deducing plasma initial velocity. This data along with the measured average ablated mass per pulse were taken as input parameters in a phenomenological model of the growth of NPs nucleated in the plume. The average asymptotic cluster size is deduced and compared with NP sizes measured from TEM pictures. Results indicate narrow gradients of NP sizes. Hence strict control of growth parameters favors fine tuning of NP size, vital to applications, including SERS active substrates. SERS spectra obtained with increasingly lower concentrations of the reference dye rhodamine 6G (Rh6G) [3] (Fig.2), the medical drug apomorphine, lysozime, naphthalenethiol, are discussed.
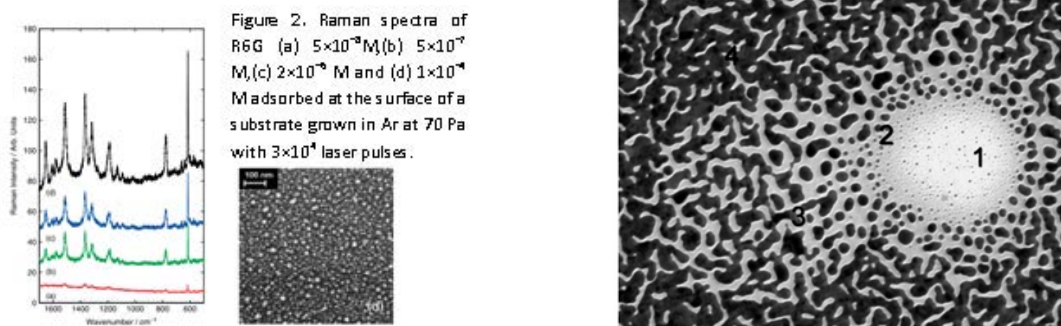

Figure 1. TEM image of a Ag sample grown at 10 Pa of Ar. Different morphologies are evident, corresponding to different stages of film growth. (1) small, isolated NPs sized 1-3 nm; (2) larger, still isolated particles; (3) onset of coalescence; (4) fully percolated Ag network.

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#510 - Neutral-cluster implantation in polymers by computer experiments

Claudio Melis – Dipartimento di Fisica, Università di Cagliari

Claudio Melis, Roberto Cardia , Luciano Colombo (Dipartimento di Fisica, Università di Cagliari)

Our theoretical activity is included within a project named 'ELDABI' (Elettronica Deformabile per Applicazioni Biomedicali) funded by the regional governaments of Lombardia and Sardegna. The final goal is the production of a novel type of biocompatible and flexible electrodes, to be implanted into the human brain with the aim of treating several neurological diseases. These electrodes are prepared by the implantation of metallic nanoclusters on a biocompatible polymeric PDMS matrix using the "Supersonic Beam Implantation" (SCBI) technique in order to create metallic tracks inside a polymeric matrix. While the effectiveness of this technique has been already demonstrated, the physicochemical phenomena underlying SCBI at the microscopic scale remain to be fully understood. In this perspective, computer simulations represent a key tool.

In this seminar, we will present the latest results on the characterization through large-scale atomistic simulations of the main physical processes underlying SCBI. All the simulations have ben performed on realistic substrate models containing up to 4.6 millions of atoms having depths up to 90 nm and lateral dimensions up to 25 nm. We consider both entangled-melt and cross-linked Polydimethylsiloxane amorphous structures. We show that even a single cluster impact on the Polydimethylsiloxane substrate remarkably changes the polymer local temperature and pressure. Moreover we observe the presence of craters created on the polymer surface having lateral dimensions comparable to the cluster radius and depths strongly dependent on the implantation energy. Present simulations suggest that the substrate morphology is largely affected by the cluster impact and that most-likely such modifications favor the the penetration of the next impinging clusters. The results show that the cluster penetration depth inside the polymer matrix strongly depends on the implantation energy, the cluster diameter and the polymer microscopic structure. We also characterize the heat and pressure waves generated on the polymer substrate upon the cluster implantation. Finally, we will show that the surface roughness strongly increases upon the cluster implantation and depends on the implantation energy.

#511 - Contact X-ray microscopy on lithium fluoride using laser-plasma soft X-ray sources

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The research toward a cheap table-top X-ray microscope available for biologists is still a challenge. Among the different techniques of soft X-ray microscopy, the contact method offers not only a high compactness, but also the possibility to image living biological samples without any chemical treatment and without any freezing process, since the exposure time can be at the nanosecond scale. The key point of this technique is the availability of very high-resolution and wide-dynamic-range X-ray imaging detectors, such as the innovative solid state detectors based on the generation of photoluminescent color centers in lithium fluoride (LiF) crystals and films. After a brief description of the laser-plasma soft X-ray sources developed at the ENEA Frascati Laboratories and at the Tor Vergata University of Rome, based on UV and IR (respectively) high-power pulsed lasers, experimental results of soft X-ray contact microscopy of different biological samples imaged on LiF crystals and films will be presented and discussed. The results confirm the high spatial resolution of these detectors and the relevance of their high dynamic range (comparable to that of a 16-bits CCD camera) for X-ray imaging.

#512 - Blood fluxes studies in zebrafish embryos by cross-correlation spectroscopy

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Important issues in vasculogenesis and cardiogenesis of small animal models can be addresses by correlative methods which provide quantitative characterization of fluxes in blood vessels in vivo. In this work, we study the vascular system of Zebrafish embryos by means of multispot Fluorescence Correlation spectroscopy and compare the results obtained with Image Correlation Spectroscopy experiments.

We developed a two-spots two-photon setup in which the spots are spaced at adjustable micron-size distances (1-40 µm) along the selected vessel and the fluorescence signal is acquired by means of an EM-CCD and cross-correlated. Accurate calibrations measurements have been performed with fast diffusors (Rhodamine 6G) and slow diffusors (gold nanorods) in order to test the setup.

In vivo measurements are shown on Zebrafish, chosen as a model system since the transparency of its embryos facilitates morphological observation of internal organs in-vivo, both by exploiting the endogenous (autofluorescence) or the exogenous (dsRed transgenic erythrocytes) signal in the vessels, detecting the velocity of red cells and of small plasma proteins. These data are compared to those obtained by image correlations on Zebrafish vessels obtained with a confocal setup. The two

methods allow to characterize the motion of plasma fluids and erythrocytes in healthy Zebrafish embryos to be compared in the future to pathogenic ones.

#513 - NMR study of the fundamental polarization and relaxation processes in biological molecules hyperpolarized by DNP

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In this work a Nuclear Magnetic Resonance (NMR) investigation of Dynamic Nuclear Polarization (DNP) of biological molecules is presented, at the aim to unravel the physical parameters affecting the DNP efficiency in biomedical applications.

DNP is one of the most effective ways to attain a giant nuclear hyperpolarization through the polarization transfer from the electron to the nuclear spins, under microwave irradiation close to the electron Larmor frequency. Accordingly, DNP allows to perform NMR and Magnetic Resonance Imaging (MRI) of low sensitivity nuclei with a dramatic enhancement of the signal to noise ratio. In preclinical research the recent development of dissolution-DNP has boosted advances in the metabolic imaging of 13C enriched endogenous molecules, injected in animal models after previous hyperpolarization and dissolution [1]. However, for decades many crucial aspects of the complex DNP phenomenon have remained unexplained by the available theoretical models [2]. The aim of this study is thus to clarify how some microscopic parameters involved in DNP vary with temperature (T), the concentration of 13C nuclei and with the concentration of paramagnetic radicals.

A detailed characterization of the DNP and NMR properties of [1-13C] pyruvic acid (PA) added with the trityl radicals has been performed at 3.46 Tesla and below 5 K. PA is a compound of major interest, since it is involved in a metabolic reaction assisted by lactate dehydrogenase, an important biomarker of tumoral activity. The DNP phenomenon has been studied by measuring both the13C nuclear polarization (P) and the polarization time (Tpol). Below 5 K DNP takes place in the thermal mixing (TM) regime where the electron linewidth is larger than the nuclear Larmor Frequency. Thus, we present an interpretation of these data in the light of a recent dynamical model of TM developed by Colombo Serra et al. [3].

Moreover, we present a study of the nuclear spin-lattice relaxation time T1 in low concentration PA solutions, at room T and low field (1–104 Gauss). Notably, this experiment is relevant to understand the main hurdles to the use of DNP in the clinical routine, since it mimics the conditions probed by the hyperpolarized molecules during the route to the MRI spectrometer.

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#514 - Non-invasive optical assessment of breast density and identification of subjects at high-risk for developing breast cancer

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Breast density (i.e. the relative amount of fibroglandular tissue) is a strong and independent risk factor for developing breast cancer. At present, it is assessed through mammography, thus implying the use of ionizing radiation. The ability to non-invasively identify high-risk women would allow the design of earlier personalized screening paths and preventive interventions.

Optical techniques can provide functional and structural information on biological tissue in absolutely non-invasive way. We exploited the potential of diffuse optical spectroscopy operating in the time domain to assess both tissue composition in terms of key constituents and scattering parameters that are related to the microscopic structure of tissue and specifically to breast density.

Time domain multi-wavelength (635-1060 nm) optical mammography was performed on 147 subjects, and average breast tissue composition (water, lipid, collagen, oxy- and deoxyhemoglobin) and scattering parameters (amplitude a and slope b) were estimated using the diffusion approximation to the radiative transfer theory to model photon propagation in tissue. Mammographic density was classified through BI-RADS categories 1 to 4, where the highest cancer risk is associated with category 4.

An increase in BI-RADS category corresponds to increasing average amounts of optically estimated water and collagen content, while the lipid content decreases. A gradual increase is also observed in both scattering amplitude a and slope b. Such observations are consistent with expected differences in composition and microscopic structure between fatty and fibroglandular (dense) tissue. To develop a procedure for the identification of high-risk women, the mammographic density was dichotomized, comparing subjects in BI-RADS categories 1 to 3 to subjects in category 4, and regression logistic analysis was applied to optically derived parameters. The best model for the risk probability resulted to depend on collagen content and scattering parameters. It provides a total misclassification error of 12.3%, corresponding to a simple kappa of 0.84, which compares favorably with the reproducibility of BI-RADS measures among radiologists and even intra-radiologist.

Work is on-going to determine further information that can be derived non-invasively from optical data on breast density and cancer risk.

#515 - Investigation of spatial distributions of free radicals irradiated samples by means of cw- and pulsed EPR techniques

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The radiation therapy carried out by means of heavy charged particles (such as carbon ions) and neutrons is rapidly becoming widespread worldwide. The success of these radiation therapies relies on the high density of energy released by these particles or by secondary particles produced after primary interaction with matter. The biological damages produced by ionizing radiations in tissues and cells depends more properly on the energy released per unit path length which is the linear energy transfer (LET), which determines the radiation quality.

In order to improve the therapy effectiveness it is necessary to grasp the mechanisms of free radical production and distribution after irradiation with these particles as compared to the photon beams.

In this work the spatial distributions of the free radicals produced after exposure of organic compound to various radiation beams (^{60}Co γ-photons, protons, thermal neutrons) was analyzed. The choice of organic compounds is due to their suitable properties, such as high efficiency of radiation-matter energy transfer, tissue equivalence [1- 3].

Electron spin resonance analyses were carried out by the quantitative continuous-wave EPR method (cw-EPR) and by the Electron Spin Echo (ESE) technique, which allow the determination of total and local spin concentrations, respectively. While ESE is measuring the Instantaneous Diffusion, a more detailed survey on the distribution of free radicals inside the samples was carried out by the Double Electron-Electron Resonance (DEER) technique which is able to measure distances (range 1.5-8 nm) among pairs of radicals in solids. The distributions of radical pairs depend on the type of the radiation impinging on the sample. Simulation on the basis of the AT crystal structure and of the track structure theory describing the spatial distribution of the energy released by ionizing particles are also discussed.

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#516 - From Eu^{3+} incorporation in sol-gel silica to real time monitoring of therapy beams by Eu^{3+} doped scintillating fibers

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Significant improvements have continuously been made in radiation therapy technologies, and therefore innovative detectors must also be developed to ensure the beam quality of these new irradiation systems and to allow in vivo dosimetry measurements. Optical fiber based radioluminescence (RL) dosimeters are a promising option for these purposes. They can enable real time dose measurement and their small size can be exploited in small radiation field dosimetry. A major difficulty involved in marketing these systems is the spurious luminescence, generally known as stem effect, that is intrinsically present in this type of detector. The possible mechanisms causing the stem effect during irradiation are fluorescence phenomena and especially Cerenkov light, produced in the undoped fiber portion.

In this study we have faced the problem by making use of a spectral discrimination method exploiting the sharp 5D0-7F2 line emission of Eu^{3+} [1].

First, the incorporation of Eu^{3+} ions in sol-gel silica was investigated as a function of dopant concentration and synthesis parameters. Preliminary structural (TEM), vibrational (Raman, FTIR) and optical absorption studies [2, 3] have allowed to find the most suitable rare-earth (RE) concentrations and synthesis conditions for optimizing both RL efficiency and RE dispersion, avoiding the formation of aggregates. Indeed, clusters of few tens of nanometers were observed already for SiO_2:3 mol% Eu^{3+}. The 10 mol% doped sample contains also aggregates of much larger dimensions, whose diffraction patterns are in agreement with the presence of rare earth crystalline oxide silicates.

Eu^{3+}-doped fibers were realized by drawing cluster-free silica with 600 ppm doping level. The spectral emission of composite fibers made of a small portion (1 cm) of doped silica fiber coupled to a long (15 m) undoped fiber for remote signal transport has then been investigated under irradiation with photons and electrons of different energies, field sizes and orientations, in order to discover the origin of the stem effect and to evaluate its influence on the RL spectral shape. The possibility of an efficient discrimination between the RL dosimetric signal and the spurious one is proved and discussed.

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