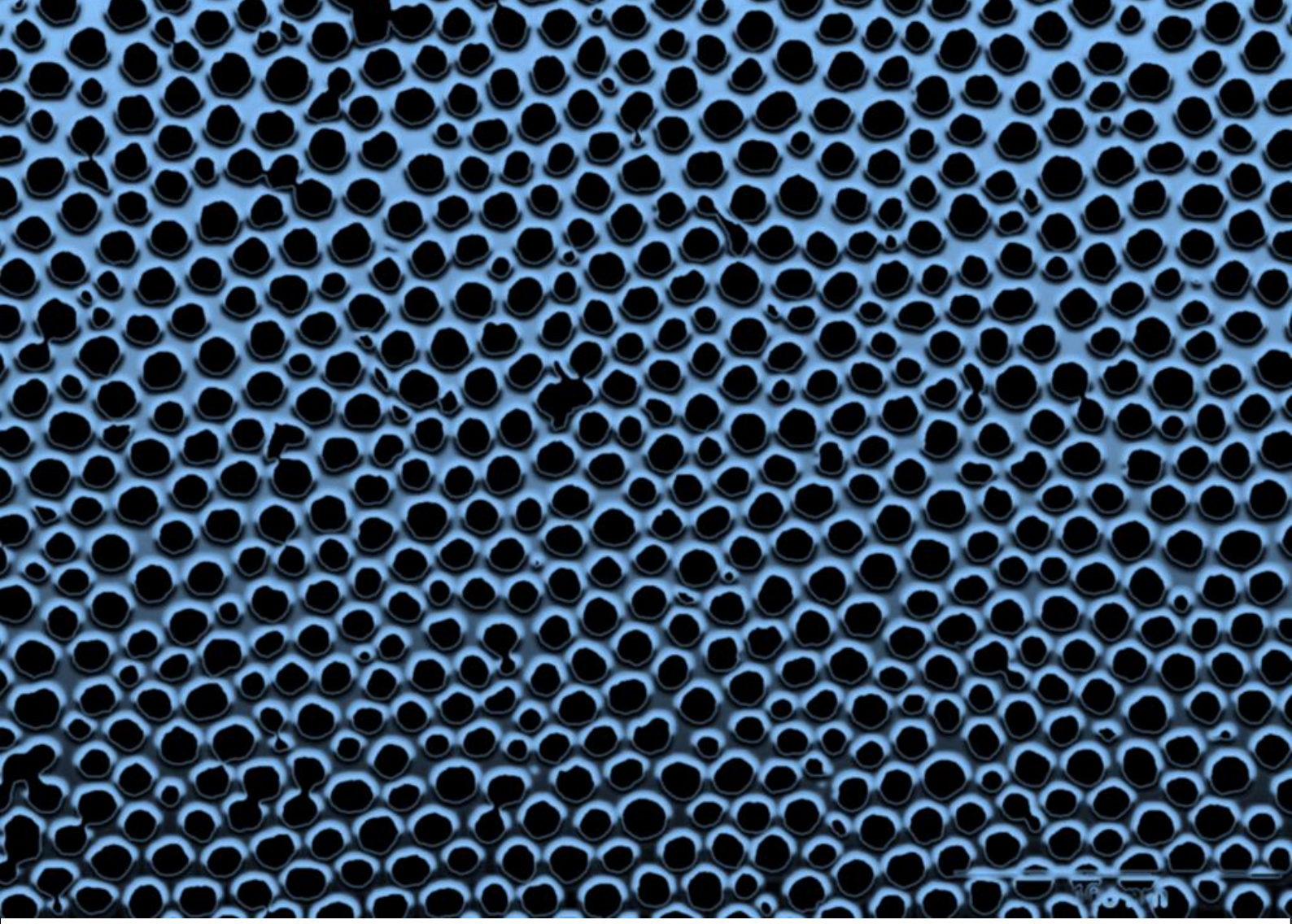


Nanoscience Institute
2nd Workshop

CNRNANO

ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE

2ND MEETING OF THE NANOSCIENCE INSTITUTE | CNRNANO

JUNE 10-11 | 2013
MODENA | ITALY

INDEX

PRESENTATION

This booklet includes the program of the Workshop of the Nanoscience Institute of the National Research Council (CnrNano) that takes place in Modena on June 10th and 11th 2013. It also lists the participants to the workshop, the abstracts of both oral and poster presentations and offers a list of Cnr authors.

The Nanoscience Institute was established in February 2010 from the merging of three former INFM (National Institute of Matter Physics) centers: NEST in Pisa, NNL in Lecce, and S3 in Modena. Prominent in this Institute is the presence of young researchers and students. In fact, the Institute has 62 permanent and 19 fixed-term staff members, and about 50 young researchers among PhD students and post doctoral fellows. Furthermore, 130 affiliated researchers (50 of which with a permanent position) participate in the research activities of the Institute. A strength of our research comes from convergent contributions of scientists with background in different disciplines, and from combining advanced experiments and simulations. A further peculiar characteristic of the Institute is the strong interaction with the Universities. Besides Scuola Normale Superiore of Pisa, University of Salento of Lecce, and University of Modena and Reggio Emilia, which host the Institute centers, we share common projects with several Italian and foreign research institutions and companies.

The program of the workshop includes a selected number of oral presentations and a large number of posters that will offer the participants an opportunity to discuss their recent results.

Pisa, 14th May 2013

Lucia Sorba
Director of the Nanoscience Institute -CNR

PROGRAM - MONDAY JUNE 10, 2013

10:00	Registration and Coffee	
10:45	Welcome and introduction *(Lucia Sorba)*	
	I session | **Light & matter** *chair M. De Giorgi*	
11:00	*CA Rozzi* | Light harvesting from first principles in the time-domain	
11:25	D. *Sanvitto* | Shock waves and solitons in a pond of exciton polaritons condensate	
11:50	*A. Tredicucci* | Shaping light-matter interaction in four dimensions	
12:15	*V. Grillo* | Vortex electron beams and spin polarization	
12:40	*MS Vitiello* | Nanowire and Graphene Terahertz Photodetectors	
13:05	***LUNCH***	
	II session | **Frontier nanodevices and spectroscopies** *chair M. Rontani*	
14:00	*F. Giazotto* | Coherent caloritronics with Josephson nanocircuits	
14:25	*V. Corradini* | Magnetic cooling at single molecule level: a spectroscopic investigation on isolated molecules on surface	
14:50	*S. Roddaro* | Field-effect manipulation of single-electron systems based on InAs/InP nanowires: high-temperature Coulomb blockade and electrostatically-driven spin transit	
15:15	***COFFEE BREAK***	
	III session | **Bio & Nano** *chair M. Cecchini, S. Corni*	IV session | **Photovoltaics, nanocrystals** *chair A. Calzolari*
15:40	*GM Ratto* | Visualizing brain plasticity	*M. Mazzeo* | High Efficiency ITO-free flexible white organic LEDs based on multi-cavity technology
16:05	*A. Alessandrini* | Nanomechanical properties of lipid bilayers and their relevance for membrane proteins activity	*I. Marri* | Carrier multiplication in isolated and interacting silicon nanocrystals for photovoltaic applications
16:30	*C. Cecconi* | Single-molecule folding mechanism of an EF-hand neuronal calcium sensor	*S. Colella* | Hybrid and Organic Photovoltaics
16:55	*G. Maruccio* | Lab-on-chip devices for cancer diagnostics	*L. Persano* | Nanofiber-based devices for energy harvesting
17:20	*R. Rinaldi* | Theranostic Polyelectrolyte Capsules for in vitro delivery and sensing	*S. Benedetti* | Substrate-driven self-assembling of metal nanocluster ordered arrays
17:45	**Poster session & aperitif**	
19:20	Walk to the Hotels	
20:15	***BUS TO DINNER (AGRITURISMO PERI AL VERDE, VIA EMILIA EST 1771, MODENA)***	

PROGRAM - TUESDAY JUNE 11, 2013

	I session | **Graphene & Co.** *chair M. Polini*
9:00	*S. Heun* | Hydrogen Storage on Graphene: an STM study
9:25	*D. Prezzi* | Electron and Optical Spectroscopies of Graphene Nanoribbons on Au
9:50	*A. Candini* | Tailoring the coupling between single molecule magnets and ferromagnetic substrate with a graphene layer
10:15	*V. Pellegrini* | Synthetic electron fluids based on graphene-GaAs double layers
10:40	*F. Taddei* | Charge pumping in superconducting wires with Majorana fermions
11:00	**Poster session & coffee**
13:15	***LUNCH***
14:15	General discussion
15:15	Parallel self-organized discussion meetings: 1. Thermoelectrics (host L. Sorba) 2. NanoBrain (host G. M. Ratto) 3. Multiscale computational platforms (hosts Tozzini-Corni).
17:00	Bus departure to Bologna Airport

SCIENTIFIC COMMITTEE

Milena De Giorgi, Lecce
Elisa Molinari, Modena
Marco Polini, Pisa

ORGANIZING COMMITTEE

Elisa Molinari and Lucia Sorba
Cnr Nano staff, Modena: Maria Grazia Angelini, Elisa Bolognesi, Luisa Neri, Anna Grazia Stefani
Communication: Maddalena Scandola
IT: Davide Calanca

ABSTRACTS| ORAL PRESENTATIONS

[O1] Light harvesting from first principles in the time-domain

C. A. Rozzi[1], S. M. Falke[2], N. Spallanzani[1,3], A. Rubio[4,5], E. Molinari[1,3], D. Brida[6], M. Maiuri[6], G. Cerullo[6], H. Schramm[7], J. Christoffers[7], and C. Lienau[2]

[1] Istituto Nanoscienze – CNR, Centro S3, Modena, Italy
[2] Institut für Physik and Center of Interface Science, Carl von Ossietzky Universität, Oldenburg, Germany
[3] Dipartimento FIM, Università di Modena e Reggio Emilia, Modena, Italy
[4] Dpto. Física de Materiales, Universidad del País Vasco, San Sebastián, Spain
[5] Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
[6] IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Milano, Italy
[7] Institut für Reine und Angewandte Chemie and Center of Interface Science, Carl von Ossietzky Universität, Oldenburg, Germany

Nature has developed sophisticated and highly efficient molecular architectures to convert sunlight into chemical energy. It is known that the primary steps, specifically both energy and charge transfer, occur on extremely fast time scales. These processes have traditionally been interpreted in terms of the incoherent kinetics of optical excitations and of charge hopping, but recently signatures of quantum coherence were observed in energy transfer in photosynthetic bacteria and algae [1,2]. We have studied the early steps of photoinduced charge separation in an an organic donor-bridge-acceptor supramolecular assembly [3] by combining Time-dependent Density Functional Theory simulations of the quantum dynamics and high time resolution femtosecond spectroscopy. We discuss the role of the electron-nuclei coupling and of the linking group in the photoinduced charge separation process. Our results provide evidence that the driving mechanism of the charge separation process is a quantum correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds, thus establishing the role of quantum coherence in artificial light harvesting [4].

References:

[1] G. S. Engel *et al.*, Nature 446 (2007) 782-786.
[2] E. Collini *et al.*, Nature 463 (2010) 644-647.
[3] G. Kodis *et al.*, J. Phys. Org. Chem. 17 (2004) 724-734.
[4] C. A. Rozzi *et al.*, Nat. Comm. 4 (2013) 1602.

[O2] Shock waves and solitons in a pond of exciton polaritons condensate

D. Ballarini[1,2], L. Dominici[1,2], M. De Giorgi[2], E. Cancellieri[3], F. Laussy[4], E. Giacobino[3], A. Bramati[3], G. Gigli[1,2,5], and D. Sanvitto[1,2]

[1] Istituto Italiano di Tecnologia, IIT-Lecce, Via Barsanti, 73010 Lecce, Italy
[2] NNL, Istituto Nanoscienze - CNR, Via Arnesano, 73100 Lecce, Italy
[3] Laboratoire Kastler Brossel, Université Pierre et Marie Curie-Paris 6, École Normale Supérieure et CNRS, Case 74, 4 place Jussieu, 75005 Paris, France
[4] Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, Spain
[5] Innovation Engineering Department, University of Salento, Via Arnesano, 73100 Lecce, Italy

Exciton polaritons are a powerful system for the study of nonlinear effects in quantum fluids, but also provide a promising potential for their application in optical devices of a new kind [1]. Here we report on the ultra-fast time-resolved analysis of the spatial dynamics of phase and density perturbations inside a polariton quantum fluid of small spatial extension, excited and shaked by a femptosecond laser pump. Oscillations reminiscent of those observed in a pond in which has been thrown a stone are observed as a result of the strong perturbation imparted by the pulsed resonant laser, but are, in our case, rooted in Rabi oscillations. The coherent state of exciton-polaritons thus formed rapidly evolves in time to exhibit other striking features, such as shock waves, soliton rings and a very localized, long-lived, bright standing soliton at the spot center.

Nonlinearities are at the base both of shock waves [2], moving with the sound velocity in the medium, and of solitons, characterized by time persistence and space localization of their shape when propagating. Recently propagating solitons have been revealed, under off-resonant pump plus resonant excitation condition, in an exciton-polariton system [3]; however, dynamics of standing solitons and shock waves formation have never been observed in these peculiar, non-equilibrium, quantum fluids. Here we show that depending on the excitation energy and power we can observe a transition from simply diffusing polaritons (Fig. 1 top raw) to self-focusing standing solitons (Fig. 1 bottom raw). In the intermediate regime we have simultaneous persistence of shock waves ejected in the outer region of the condensate, while a steady sharp soliton and solitonic bright and dark rings form in the inner region. These non-linear effects of a polariton quantum fluid are to ascribe to the peculiar polariton dispersion spectrum, which strongly depends on the condensate final state, density and excitation conditions.

References:

[1] D. Ballarini, M. De Giorgi, E. Cancellieri, R. Houdré, E. Giacobino, R. Cingolani, A. Bramati, G. Gigli, and D. Sanvitto, (2012) arXiv:1201.4071.
[2] M. A. Hoefer, M. J. Ablowitz, I. Coddington, E. A. Cornell, P. Engels, and V. Schweikhard, Phys. Rev. A 74 (2006) 023623.
[3] M. Sich, D. N. Krizhanovskii, M. S. Skolnick, A. V. Gorbach, R. Hartley, D. V. Skryabin, E. A. Cerda-Méndez, K. Biermann, R. Hey and P. V. Santos, Nat. Photonics 6 (2012) 50.

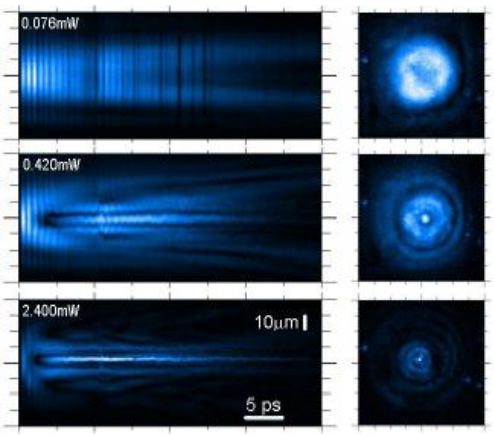


Fig. 1. In the left column, intensity cross section along the vertical diameter (y axis) versus time (x axis) are shown. The right columns are real space images of the polariton condensate 15ps after the pulse excitation. Rows correspond to different powers, increasing from top to bottom. At enough power, the central density rapidly decays to zero before starting to rise back in the form of a localized standing bright soliton, surrounded by a close ring. The central peak reaches its maximum after few ps and it is only weakly affected by the arrival of an eco pulse at 10ps. Such bright soliton remains of μm-size during its rise, stability and decay phases, while the external rings are expanding as shock waves at about the velocity of sound (1μm/ps) in the outer region.

[O3] Shaping light-matter interaction in four dimensions

S. Zanotto[1], J. Xu[1], M. Porer[2], J.-M. Ménard[2], G. Biasiol[3], L. Sorba[1], R. Huber[2], and A. Tredicucci[1]

[1] NEST, CNR-Istituto Nanoscienze and Scuola Normale Superiore, Pisa, Italy
[2] Department of Physics, University of Regensburg, Germany
[3] Laboratorio TASC, CNR-IOM, Trieste, Italy

Keywords: polaritons, intersubband transitions, photonic crystals, bistability, ultrafast phenomena.

Controlling the way light interacts with material excitations is at the heart of cavity quantum electrodynamics (cavity QED). In the strong coupling regime, an active material in a microresonator can absorb and spontaneously re-emit a photon many times before dissipation becomes effective, giving rise to mixed lightmatter eigenmodes. In the ultrastrong coupling regime, photon exchange occurs on time scales comparable with the oscillation period of light itself. In this limit, ultrafast modulation of the coupling strength has been suggested to pave the way towards unconventional QED phenomena [1]. While sophisticated light-matter coupling has been achieved in all three spatial dimensions, however, non-adiabatic control in the fourth dimension – time – has been developed only recently [2]. In such experiments, a quantum well waveguide structure is exploited to optically tune from weak to ultrastrong light-matter interaction and turn on maximum coupling within less than one cycle of light. In this regime, a novel class of extremely non-adiabatic phenomena becomes observable, and it is possible to monitor how a coherent photon population converts to cavity polaritons during abrupt switching.

In photonic crystals (PCs), on the other hand, a periodic spatial modulation of the refractive index is tailored to shape photonic band structures and mold the flow of light. Nonresonant light-matter interaction is sufficient to confine optical modes with subwavelength precision or to slow down the group velocity of radiation. Merging the concept of a PC with nonadiabatic and ultrastrong light-matter coupling allows approaching full spatial and temporal control of a photonic band structure with subcycle and subwavelength precision. In a one-dimensional surface plasmon PC [3,4], operated in straightforward transmission, with optically switchable intersubband (ISB) resonances of semiconductor QWs, phase- stable multi-terahertz pulses have been used to map out ultrafast snapshots of the photonic dispersion, while light-matter interaction is activated by a few-femtosecond control pulse [5]. These time-resolved measurements trace the nonadiabatic transition of the band structure from its unperturbed state to the ultrastrong coupling regime. The dynamics is characterized by an opening of a pronounced anticrossing, a dramatic flattening of the photonic bands, and a significant slow-down of the group velocity. A similar system offers the possibility to access the non-linear response of the polariton states, when the mid-IR pulse has sufficient energy to saturate the intersubband transition. In this condition polariton bleaching is observed [6], and the dynamics can be studied with a wavelet analysis, revealing the switching to the weak-coupling regime within the duration of the optical pulse. New PC designs with the presence of defect-like states will also be presented as a way to dramatically enhance the electric field intensity within the cavity.

Finally prospects for the observation of polariton states between Landau levels in a graphene-based metamaterial will be discussed.

References:

[1] S. De Liberato, C. Ciuti, and I. Carusotto, Phys. Rev. Lett. 98 (2007) 103602.
[2] G. Günter, A. A. Anappara, J. Hees, A. Sell, G. Biasiol, L. Sorba, S. De Liberato, C. Ciuti, A. Tredicucci, A. Leitenstorfer, and R. Huber, Nature 458 (2009).
[3] S. Zanotto, G. Biasiol, R. Degl'Innocenti, L. Sorba, and A. Tredicucci, Appl. Phys. Lett. 97 (2010) 231123.
[4] S. Zanotto, R. Degl'Innocenti, L. Sorba, A. Tredicucci, and G. Biasiol, Phys. Rev. B 85 (2012) 035307.
[5] M. Porer, J.-M. Ménard, A. Leitenstorfer, R. Huber, R. Degl'Innocenti, S. Zanotto, G. Biasiol, L. Sorba, and A. Tredicucci, Phys. Rev. B 85 (2012) 081302.
[6] S. Zanotto, R. degl'Innocenti, J.-H. Xu, L. Sorba, A. Tredicucci, and G. Biasiol, Phys. Rev. B 86 (2012) 201302.

[O4] Vortex electron beams and spin polarization

V. Grillo[1,2], L. Marrucci[3,4], E. Karimi[5], S. Frabboni[6], G. C. Gazzadi[1], and E. Santamato[3]

[1] CNR-Istituto Nanoscienze, Centro S3, Via G Campi 213/a, I-41125 Modena, Italy
[2] CNR-IMEM, Parco delle Scienze 37a, I-43100 Parma, Italy
[3] Dipartimento di Fisica, Università di Napoli "Federico II", Italy
[4] CNR-SPIN, Complesso Universitario di Monte S. Angelo, Napoli, Italy
[5] Department of Physics, University of Ottawa, Ottawa ON K1N 6N5 Canada
[6] Dipartimento FIM, Università Modena e Reggio Emilia, Via G Campi 213/a, I-41125 Modena, Italy

Keywords: Electron microscopy, Vortex beams, Spin polarization, magnetic dichroism, Spin-orbit interaction.

Few years ago, the existence of orbital angular momentum (OAM) for an electron beam was predicted theoretically [1], It is a rotational degree of freedom similar to that of electron orbiting an atom but without any external potential.
A couple of years later, two different techniques were used to generate electron beams carrying OAM from emerging electrons of Transmission Electron Microscopes (TEM) experimentally [2, 3]. Such a cool topic comes to interest of material scientists since opens up the road to magnetic circular dichroism on a very local scale [4].
Based on OAM beams a proposal for an electron-beam device that can act as an efficient spin-polarization filter has been recently put forward [5]. The filter (also named q-filter) is obtained by the use of quadrupolar magnetic field compensated by electric field that act as spin rotator, and by diffractive elements.
This result is particularly interesting since the polarization of an unpolarised beam was for long considered impossible as the same Bohr had initially declared. We are presently working on the practical implementation of such idea by studying the detailed behavior of OAM e-beams in a magnetic field. For this reason quantum simulation including spin of electron beams has been developed and experiments on vortex beam generation are being performed [6].
Fig 1 shows a quantum mechanics simulation of the beam evolution in the q-filter.
As for experiment we are working on Focused Ion Beam (FIB) nanofabrication of synthetic e-holograms capable to produce beams with different shape and tunable OAM and we are studying the experimental evolution of the e-beams using the TEM electron microscope as an effective optical bench for electrons. For this reason other experiments taken from light quantum optics could be transferred to a e-beams through a TEM but the use of charged particle should introduce important differences. A few application to material science will be also discussed.

References:
[1] K. Y.Bliokh, Y.P. Bliokh, S.Savalev, and F. Nori, Phys.Rev.Lett 99 (2007) 190404.
[2] J. Verbeeck, H. Tian, and P. Shattschneider, Nature 467 (2010) 301.
[3] B. J. McMorran, A. Agrawal, I. M. Anderson, A. A.Herzing *et al.*, Science 331(2011) 301.
[4] J. Verbeeck, P. Shattschneider *et al.*, Applied. Phys. Lett 99 (2011) 203109.
[5] E. Karimi, L. Marrucci, V. Grillo, E. Santamato, Phys. Rev. Lett 108 (2012) 044801.
[6] V. Grillo, L. Marrucci, E. Karimi *et al.*, arXiv:1301.3938.

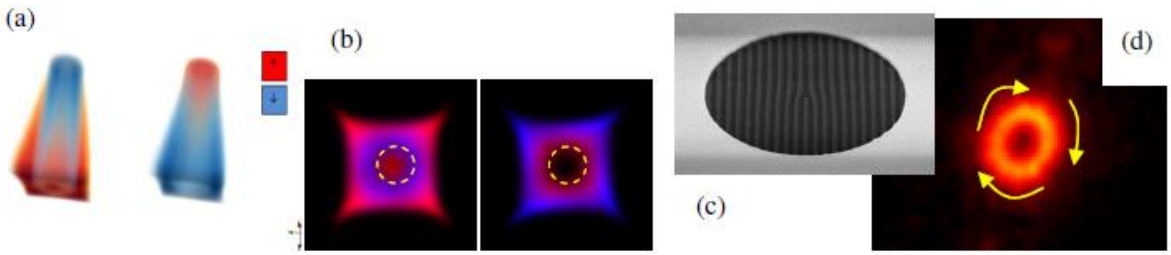


Fig. 1:a) 3D simulation of the z-evolution of different spin states (indicated by colors) for OAM beams in a q-filter b) snapshot of the wavefunction at the end of the filter. An appropriate pupil as indicated could be used to select the polarised fraction of the beam (c) Hologram fabricated by FIB for the production of OAM beams. d) Experimental TEM image of the OAM beams with OAM l=4ħ.

[O5] Nanowire and Graphene Terahertz Photodetectors

M. S. Vitiello[1], L. Viti[1], D. Coquillat[2], L. Vicarelli[1], L. Romeo[1], D. Ercolani[1], L. Sorba[1], M. Polini[1], A. Lombardo[3], A. C. Ferrari[3], V. Pellegrini[1], W. Knap[2], and A.Tredicucci[1]

[1] NEST, Istituto Nanoscienze – CNR and Scuola Normale Superiore, Piazza San Silvestro 12, Pisa, I-56127
[2] Université Montpellier 2, Laboratoire Charles Coulomb UMR 5221, F-34095, Montpellier, France
[3] Department of Engineering, Cambridge University, Cambridge, CB3 0FA, UK

Keywords: Terahertz photonics, plasma-waves field effect transistors, photodetectors.

Terahertz technology has become of large interest over the last few years for its potential in non-invasive imaging, spectroscopic and biological applications. In this context, the development of a breakthrough solid-state technology for fast and high-temperature THz detectors is highly desired.
Commercially available THz detectors are indeed based on thermal sensing elements being either very slow (10-400 Hz) (Golay cells, pyroelectric elements), or requiring deep cryogenic cooling (hot-electron bolometers), while those exploiting fast non-linear electronics (Schottky diodes) are mostly limited to the range < 1 THz.
The talk will offer an overview on our recent development of high detectivity, room-temperature THz detectors [1-6]. Antenna-coupled field effect transistors have been developed as plasma-wave THz detectors in both InAs nanowire and graphene channel material. Room temperature operation has been achieved up to frequencies of 3 THz, with noise equivalent powers as low as a few 10-11 W/Hz1/2, and high-speed response. Large area fast imaging applications of the detectors provided a reasonably good spatial resolution, making the proposed technology already exportable for practical applications across the far-infrared.

References:

[1] M. S. Vitiello, D. Coquillat, L. Viti, D. Ercolani, F. Teppe, A. Pitanti, F. Beltram, L. Sorba, W. Knap, and A. Tredicucci, Nano Lett. 12 (2012) 96.
[2] L. Vicarelli, M. S. Vitiello, D. Coquillat, A. Lombardo, A. C. Ferrari, W. Knap, M. Polini, V. Pellegrini and A. Tredicucci, Nature Materials 11 (2012) 865.
[3] M. S. Vitiello, L. Viti, L. Romeo, D. Ercolani, G. Scalari, J. Faist, F. Beltram, L. Sorba, and A. Tredicucci, Appl. Phys. Lett. 100 (2012) 241101.
[4] A. Pitanti, D. Coquillat, D. Ercolani, L. Sorba, F. Teppe, W. Knap, G. De Simoni, F. Beltram, A. Tredicucci, and M. S. Vitiello, Appl. Phys. Lett 101 (2012) 141103.
[5] L. Viti, M. S Vitiello, D. Ercolani, L. Sorba, and A. Tredicucci, Nanoscale Res. Lett. 7 (2012) 159.
[6] A. Pitanti, S. Roddaro, M. S. Vitiello, and A. Tredicucci, J. Appl. Phys 111 (2012) 064301.

[O6] Coherent caloritronics with Josephson nanocircuits

F. Giazotto and M. J. Martínez-Pérez

NEST, Istituto Nanoscienze CNR and Scuola Normale Superiore, Piazza San Silvestro 12, 56127 Pisa, Italy

Keywords: Mesoscopic physics, thermal transport, Josephson effect.

The Josephson effect [1] represents perhaps the prototype of macroscopic phase coherence and is at the basis of the most widespread interferometer, i.e., the superconducting quantum interference device (SQUID) [2]. Yet, in analogy to electric interference, Maki and Griffin [3] predicted in 1965 that thermal current flowing through a temperature-biased Josephson tunnel junction is a stationary periodic function of the quantum phase difference between the superconductors. The interplay between quasiparticles and Cooper pairs condensate is at the origin of such phase-dependent heat current, and is unique to Josephson junctions. In this scenario, a temperature-biased SQUID would allow heat currents to interfere [4, 5] thus implementing the thermal version of the electric Josephson interferometer. The dissipative character of heat flux makes this coherent phenomenon not less extraordinary than its electric (non-dissipative) counterpart. Surprisingly, this striking effect has never been demonstrated so far.

In this presentation we shall report the first experimental realization of a heat interferometer [6,7]. We investigate heat exchange between two normal metal electrodes kept at different temperatures and tunnel-coupled to each other through a thermal `*modulator*' [5] in the form of a DC-SQUID. Heat transport in the system is found to be phase dependent, in agreement with the original prediction. With our design the Josephson heat interferometer yields magnetic-flux-dependent temperature oscillations of amplitude up to ~21 mK, and provides a flux-to-temperature transfer coefficient exceeding ~60mK/Φ0 at 235 mK (Φ0 is the flux quantum). Besides offering remarkable insight into thermal transport in Josephson junctions, our results represent a significant step toward phase-coherent mastering of heat in solid-state nanocircuits, and pave the way to the design of novel-concept coherent caloritronic devices, for instance, heat transistors and thermal splitters which exploit phase-dependent heat transfer peculiar to the Josephson effect.

In this latter context, we shall also present the concept for a further development of a Josephson heat interferometer based on a double superconducting loop [8] which allows, in principle, enhanced control over heat transport. We shall finally conclude presenting some preliminary results on a quite different prototypical thermal interferometer which could add complementary flexibility in mastering heat flux at the nanoscale.

References:

[1] B. D. Josephson, Phys. Lett. 1(1962) 251.
[2] J. Clarke and A. I. Braginski, *The SQUID Handbook* (Wiley-VCH, 2004).
[3] K. Maki and A. Griffin, Phys. Rev. Lett. 15 (1965) 921.
[4] G. D. Guttman, E. Ben-Jacob, and J. Bergman, Phys. Rev. B 57(1998) 2717.
[5] F. Giazotto and M. J. Martínez-Pérez, Appl. Phys. Lett. 101 (2012) 102601.
[6] F. Giazotto and M. J. Martínez-Pérez, Nature 492 (2012) 401.
[7] R. W. Simmonds, Nature 492 (2012) 358.
[8] M. J. Martínez-Pérez and F. Giazotto, Appl. Phys. Lett. 102 (2013) 092602.

[O7] Magnetic cooling at single molecule level: a spectroscopic investigation on isolated molecules on surface

V. Corradini[1], A. Ghirri[1], A. Candini[1], R. Biagi[1,2], U. del Pennino[1,2], G. Dotti[1,2], E. Otero[3], F. Choueikani[3], R. J. Blagg[4], E. J. L. McInnes[4], and M. Affronte[1,2]

[1] S3 Centre, Institute Nanoscience - CNR, via G. Campi 213/A, 41125 Modena, Italy
[2] Dipartimento FIM, Università di Modena e Reggio Emilia, via G. Campi 213/A, 41125 Modena, Italy
[3] Synchrotron SOLEIL, L'Orme des Merisiers, 91120 Saint-Aubin, France
[4] School of Chemistry and Photon Science Institute, University of Manchester, Oxford Road, Manchester, M13 9PL, UK

Keywords: molecular nanomagnets, magnetocaloric effect, magnetic circular dichroism, surface deposition.

Magnetic cooling relies on large entropy variation of magnetic systems under the application of an external magnetic field. While giant magnetocaloric effect (MCE) in intermetallic compounds is related to the interplay between long range magnetic and lattice order, molecular nanomagnets have recently shown superior cooling performances at cryogenic temperatures. The molecular cage $Fe_{14}(bta)_6$ was one of the first examples on which enhanced MCE was experimentally observed in bulk samples [1] followed by a dozens of other cases in the recent years. Analysis of the low temperature thermodynamic properties of these molecular compounds shows that a large part of the entropy variation is due to the magnetic degeneracy of the ground molecular state and therefore high cooling power is expected at single molecule level, an interesting feature that can be exploited for applications down to the nanoscale. Yet, the deposition of large molecular cages on surfaces might be an non-innocent process since the interaction with the surface may provoke some drastic chemical changes or structural distortions that may alter the magnetic features and therefore the functionalities of the molecule. For this reason we checked if the functionality of potential molecular coolers is preserved when molecules are deposited on a substrate.
Here we report an investigation on the $Fe_{14}(bta)_6$ molecular nanomagnet to demonstrate that large MCE is a property held at single molecule level [2]. To this end we have characterized well isolated $Fe_{14}(bta)_6$ molecules deposited by liquid phase on a gold surface by a combined analysis carried out by STM, XPS, XAS and XMCD to independently measure how the chemical, electronic and magnetic features of the isolated molecules are modified by the interaction with the surface. The relevant point is that the MCE is directly observed in our experiments at a single molecule level. This demonstrates, for the first time, that an important contribution to magnetic refrigeration is an intrinsic molecular property and it opens the possibility of scaling cooling devices down to a molecular level with no need of a cooperative behavior.

References:

[1] M. Evangelisti, A. Candini, A. Ghirri, M.Affronte, E. K. Brechin, and E. J. L. McInnes, Appl. Phys. Lett. 87 (2005) 072504.
[2] V. Corradini, A. Ghirri, A. Candini, R. Biagi, U. del Pennino, G. Dotti, E. Otero, F. Choueikani, R. J. Blagg, E. J. L. McInnes, and M. Affronte, Adv. Mater. (2013). DOI: 10.1002/adma. 201205257.

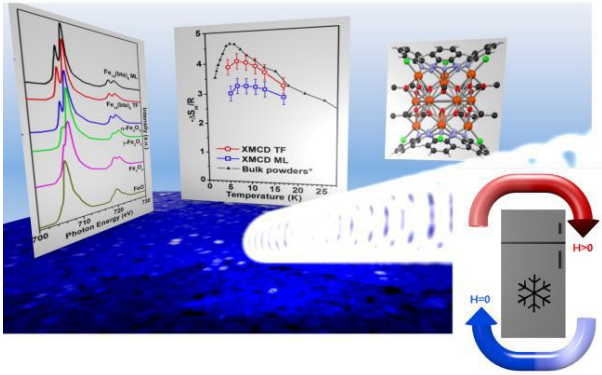


Fig. 1: A monolayer distributions of isolated molecular Fe14-bta nanomagnets is deposited intact on the Au(111) surface and investigated by XMCD spectroscopy. The entropy variation respect to the applied magnetic field is extracted from the magnetization curves, showing the preservation of the magnetocaloric effect at single-molecule level.

[O8] Field-effect manipulation of single-electron systems based on InAs/InP nanowires: hightemperature Coulomb blockade and electrostatically-driven spin transitions

S. Roddaro[1,*], A. Pitanti[1], L. Romeo[1], A. Pescaglini[1], D. Ercolani[1], L. Sorba[1], and F. Beltram[1,2]

[1] NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, P.za S. Silvestro 12, I-56127 Pisa, Italy
[2] CNI@NEST, Istituto Italiano di Tecnologia, P.za S. Silvestro 12, I-56127 Italy
[*] Present address: CNR-IOM, Laboratorio TASC, Area Science Park, Basovizza, I-34149 Trieste, Italy

Keywords: nanowire, quantum confinement, single-electron-transistor, spin, field-effect.

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 single electron 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 ~77K [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 ~75meV. In this configuration, a strong modulation of the device conductivity as a function of the electron filling is well visible up to 77K. 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 20K. 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.

References:

[1] Y. Li, F. Qian, J. Xiang, and C. M. Lieber, Materials Today 9 (2006) 18.
[2] M. S. Vitiello, D. Coquillat, L. Viti, D. Ercolani, F. Teppe, A. Pitanti, F. Beltram, L. Sorba, W. Knap, and A. Tredicucci, Nano Lett. 12 (2012) 96.
[3] Li Shi, Nanoscale and Microscale Thermophysical Engineering 16 (2012) 79.
[4] S. Roddaro, A. Pescalini, D. Ercolani, L. Sorba, and F. Beltram, Nano Lett. 11 (2011) 1695-1699.
[5] L. Romeo, S. Roddaro, A. Pitanti, D. Ercolani, L. Sorba, F. Beltram, Nano Lett. 12 (2012) 4490.

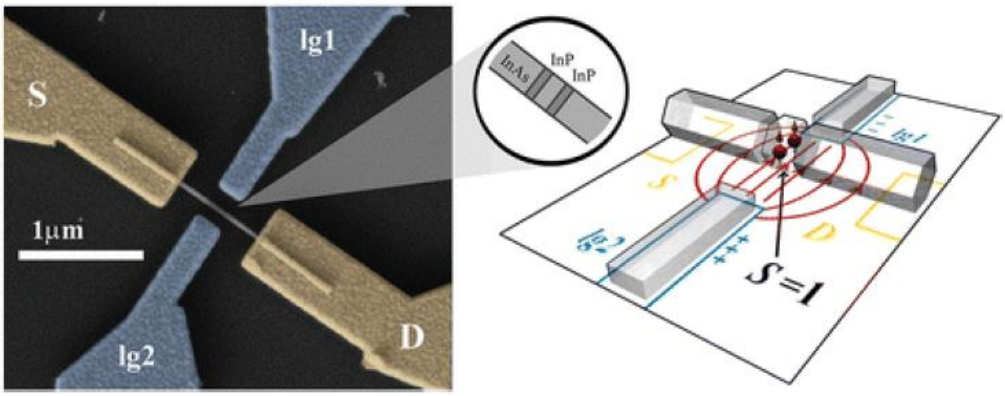


Fig.1. Scanning electron micrograph (left) and general sketch (right) of the device structure. A multipole gating technique allows the electrostatic control of the spin configuration of InAs/InP few-electron systems up to 20K. Image from [5].

[O9] Visualizing brain plasticity

S. Landi[1,2] and G. M. Ratto[2,1]

[1] NEST, Scuola Normale Superiore, Pisa, Italy
[2] NEST, Istituto Nanoscienze-CNR, Pisa, Italy

Keywords: brain plasticity, dendritic spines, extracellular matrix, two photon microscopy and electrophysiology.

A large part of brain communication occurs through structures, called dendritic spines, shaped as micrometric protusions of the neuronal membrane. Each excitatory neuron in the brain cortex includes thousands of spines each containing an excitatory synapse: changes in shape and dimensions of the dendritic spine strongly influences the synaptic currents generated during neuronal activity. Interestingly, the efficiency of a synapse depends on the size of the associated dendritic spine, with large spines sustaining stronger synaptic currents. Ultimately, the computation performed by the neuron depends on events occurring in the nano-domain enclosing the dendritic spine.

Many factors determines the capacity of the nervous system to learn and to adapt in response to changes of the external environment. In general, this capacity decreases with aging: this loss in plasticity on one side stabilizes the nervous system structure and function after the enhanced learning of young life, but, on the other side, it decreases the capacity of learning “new tricks” and, in general, is an obstacle to brain repair. The decrease of plasticity certainly depends on many developmental changes, that are, in most cases, very poorly understood. Controlling plasticity would impinge on our capacity of helping brain repair and in correcting defective brain circuitry established during early development as consequence of pathological conditions.

Here, we studied one of the less known elements of the environment surrounding a dendritic spine: the extracellular matrix. The composition of the matrix gradually matures during postnatal development, as the brain circuitry reaches its adult form. The fully developed extracellular environment stabilizes neuronal connectivity and decreases cortical plasticity as highlighted by the demonstration that treatments degrading the matrix are able to restore some synaptic plasticity in the adult brain. Up to know, the mechanisms through which the matrix inhibits cortical plasticity are not fully clarified. By means of in vivo and in vitro two-photon imaging and electrophysiology, we find that after enzymatic digestion of a component of the extracellular matrix (the chondroitin sulfate proteoglycans), cortical spines in the adult brain become more motile and express a larger degree of structural and functional plasticity, similarly to what happens in the young, immature cortex. Thus, manipulations of the extracellular matrix in the adult reinstate the juvenile phase of the brain life, reintroducing neuronal plasticity.

References:

[1] L. de Vivo, S. Landi, M. Panniello, L. Baroncelli, S. Chierzi, L. Mariotti, M. Spolidoro, T. Pizzorusso, L. Maffei, and G. M. Ratto, Nat Commun. 4 (2013) 1484.

[O10] Nanomechanical properties of lipid bilayers and their relevance for membrane proteins activity

A. Alessandrini[1,2], T. Caramaschi[2], and P. Facci[1]

[1] CNR Istituto Nanoscienze, S3, Modena
[2] Dip. Scienze Fisiche Informatiche e Matematiche, Università di Modena e Reggio Emilia, Modena

Keywords: supported lipid bilayers, nanomechanical properties, dynamic force spectroscopy, membrane proteins.

The mechanical properties of biological systems are emerging as fundamental aspects in determining their functional activity. In biological membranes, the activity of membrane related proteins are affected by the overall mechanical properties of the hosting environment. In recent years, the possibility of probing mechanical properties of lipid bilayers at the nanoscale has been promoted by the force spectroscopy potentiality of Atomic Force Microscopes (AFM). By acquiring force-curves on Supported Lipid Bilayers (SLBs) it is possible to probe the mechanical properties on a scale relevant to the interaction between membrane proteins and lipid bilayers and to monitor changes of these properties as a result of a changing environment.

Here, we study by force spectroscopy experiments on SLBs, the stability and the mechanical moduli of the lipid bilayer as a function of temperature and ionic strength of the solution. The properties are measured while monitoring the phase state of the lipid bilayer to highlight variation across the main phase transition of the bilayer [1,2]. The results show a softening behavior of the bilayer when it is in the phase transition state (Figure 1). The mechanical properties of the bilayer are compared to the transport properties of a single ion channel reconstituted in a bilayer of the same lipid composition [3]. Moreover, due to the strong analogy between the Atomic Force Microscopy tip penetration across a SLB and the pore formation process in an unsupported bilayer, we studied, by Dynamic Force Spectroscopy, the characteristics of the energy barrier of the process [4].

References:

[1] A. Alessandrini, H.M. Seeger, A. Di Cerbo, T. Caramaschi, and P. Facci, Soft Matter 7 (2011) 7054-7064.
[2] A. Alessandrini and P. Facci, Micron 43 (2012) 1212-23.
[3] H. M Seeger, L. Aldrovandi, A. Alessandrini, and P. Facci Biophys J. 99 (2011) 3675-83.
[4] A. Alessandrini, H.M. Seeger, T. Caramaschi, and P. Facci, Biophys J. 103 (2012) 38-47.

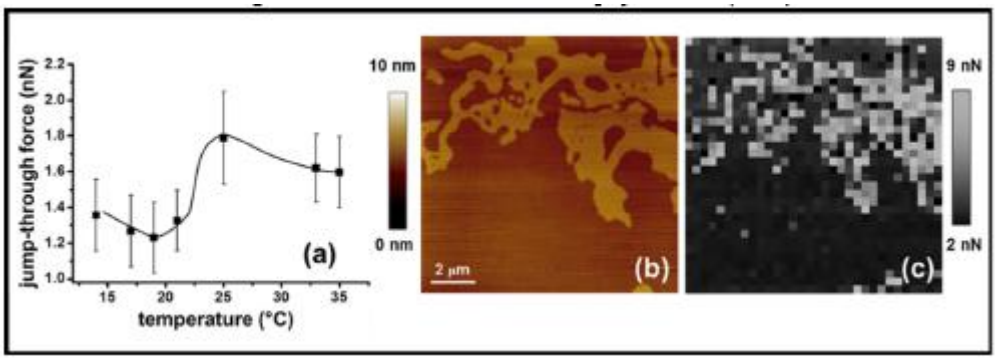


Figure 1: a) Dependence of the penetration force on the temperature for a POPE bilayer. b) Topographic image of the bilayer at 19°C in distilled water. The bilayer is the phase coexistence region of the liquid disordered and solid ordered phases. c) Map of the penetration force for the same area as in (a). The lighter area corresponds to the solid ordered phase of the bilayer, whereas the darker region corresponds to the still liquid disordered region of the bilayer where the force curves continue to be acquired.

[O11] Single-molecule folding mechanism of an EF-hand neuronal calcium sensor

P. O. Heidarsson[1], M. R. Otazo[2,3], L. Bellucci[2], A. Mossa[4], A. Imparato[4], E. Paci[5], S. Corni[2], R. Di Felice[2], B. B. Kragelund[1], and C. Cecconi[2]

[1] Structural Biology and NMR Laboratory, Department of Biology, University of Copenhagen, Denmark
[2] CNR Institute of Nanoscience S3, Via Giuseppe Campi, 41125 Modena, Italy
[3] Center of Applied Technologies and Nuclear Development (CEADEN), Department of Physics, Cuba
[4] Department of Physics and Astronomy, University of Aarhus, Ny Munkegade, Denmark
[5] Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds, United Kingdom

Keywords: single molecule protein folding; NCS-1; optical tweezers; molecular dynamics simulations; mechanical manipulation.

EF-hand calcium sensors respond structurally to changes in intracellular Ca^{2+} concentration triggering diverse cellular responses and resulting in broad interactomes. Despite impressive advances in decoding their structure-function relationships, the folding mechanism of neuronal calcium sensors is still elusive. We used single-molecule optical tweezers to study the folding mechanism of the human neuronal calcium sensor 1 (NCS1). Two intermediate structures induced by Ca^{2+} binding to the EF-hands are observed during refolding. The complete folding of the C-domain, which includes the sensory site, is obligatory for the folding of the N-domain, showing striking inter-domain dependence. Molecular dynamics results reveal the atomistic details of the unfolding process and rationalize the different domain stabilities during mechanical unfolding. Through constant-force experiments and hidden Markov model analysis, the free energy landscape of the protein was reconstructed (Fig. 1). Our results emphasize that NCS1 has evolved a remarkable complex inter-domain cooperativity and a fundamentally different folding mechanism compared to structurally related proteins.

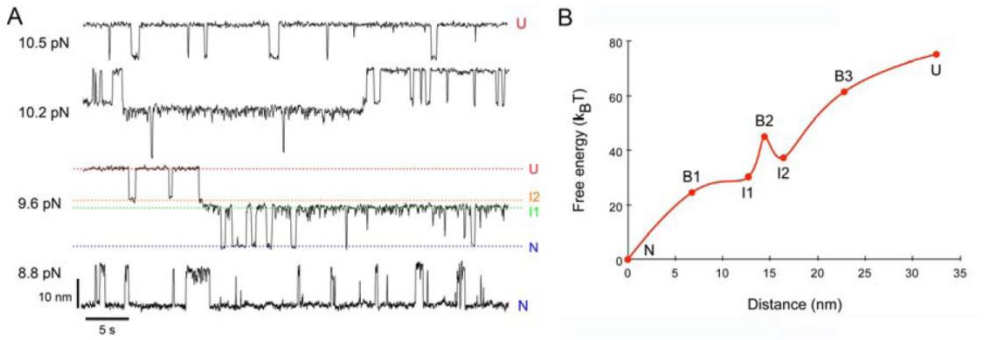


Figure 1. Equilibrium optical tweezers measurements. A) Extension vs. time traces of NCS1 at different preset force values. Force modulates the equilibrium between the unfolded state (U), intermediate state 2 (I2), intermediate state 1 (I1), and the native state (N). B) Sketch of the free energy landscape at zero applied force, reconstructed using Hidden Markov Model analysis. The different NCS1 structural states are indicated together with the transition state barriers (B1-B2-B3) that separate them.

[O12] Lab-on-chip devices for cancer diagnostics

G. Maruccio[1,2], V. Arima[1], A. Aloisi[1], A. Della Torre[1], E. Primiceri[1], M. S. Chiriacò[1,2], A. Zacheo[1,2], M. Bianco[1,2], A. Zizzari[1], E. Tarentini[1,2], and R. Rinaldi[1-3]

[1] NNL, Istituto Nanoscienze-CNR, Lecce, Italy
[2] Dipartimento di Matematica e Fisica "Ennio De Giorgi", Università del Salento, Lecce, Italy
[3] Scuola Superiore ISUFI, Università del Salento, Lecce, Italy

Keywords: diagnostics, lab-on-a-chip, microfluidics, cancer.

Application of lab-on-chip devices in cancer diagnostics is very promising with respect to conventional methods. It allows to achieve better performances in terms of speed, flexibility, automation and costs. In this respect, we recently optimized a multipurpose platform which can be configured for providing useful diagnostic and prognostic information for early detection and more accurate treatment of the disease. Here, its modular architecture and results on a few case studies will be discussed.

Our biochips essentially consist of two different components: (1) a PDMS microfluidic module obtained by replica molding from a SU-8 master and (2) the transducers, typically in the form of microelectrodes fabricated on glass substrates by optical lithography [1,2].

As a first demonstration, the application of such biochips for pancreatic cancer diagnosis will be reported.

Pancreatic ductal adenocarcinoma (PDAC) represents one of the principal causes of cancer death and is characterized by high aggressiveness, rapid progression, invasiveness, and resistance to treatments. This emphasizes the need for biomarkers and dedicated tools for early diagnosis, which are still missing but recently α-enolase (ENOA) was suggested as a marker with diagnostic and prognostic value. Our studies were carried out on serum samples. First a quartz crystal microbalance [3] was employed to detect ENOA and then dedicated impedimetric biochips [4] were implemented with better results than traditional techniques, such as ELISA. A similar study was also performed for the diagnosis of prostate cancer by evaluating percent amount of unbound PSA (free-to-total PSA ratio).

As a different approach, we will also mention a modified layout for on chip migration assays to quantify the invasive potential of cell lines by detecting the migratory activity of hepatocellular carcinoma (HCC) cells as a function of microenvironment [5, 6].

In all these applications, the integration of microfluidic components for sample handling and pre-processing is crucial. Thus separation tools and microfluidic valves were also optimized for their integration in our LOC platforms [7].

References:

[1] M. S. Chiriacò *et al.*, Lab on a Chip 11 (2011) 658.
[2] A. Aloisi *et al.*, in preparation.
[3] M. Bianco *et al.*, Biosensors and Bioelectronics 42 (2013) 646–652.
[4] M. S. Chiriacò *et al.*, Lab on a Chip 13 (2013) 730.
[5] E. Primiceri *et al.*, Biosensors and Bioelectronics 25 (2010) 2711.
[6] E. Primiceri *et al.*, Lab on a Chip 11 (2011) 4081.
[7] V. Arima *et al.*, Lab on a Chip (2013), DOI: 10.1039/C3LC00055A.

[O13] Theranostic Polyelectrolyte Capsules for in vitro delivery and sensing

S. Leporatti[1], L. L. del Mercato[1], F. Baldassarre[1], M. Ferraro[1], V. Vergaro[1], and R. Rinaldi[1,2]

[1] NNL, Istituto Nanoscienze-CNR, Lecce, Italy
[2] Scuola Superiore ISUFI, Università del Salento, Lecce, Italy

Keywords: polymer capsules, cancer therapy, drug delivery, sensing, optical reporters.

In the last years great attention has been focused on the development of novel theranostic platforms [1,2] wherein the carriers are decorated with the functionality for both diagnosis and therapy. In this context polymer capsules, fabricated via the Layer-by-Layer (LbL) technique [3], are emerging as ideal candidates owing to their high versatility which allow for the sequential performance of multiple functions including drug delivery, drug release, and sensing of important physiological processes [4-6].

We have designed and developed polyelectrolyte nano- and microcapsules that may act as vehicles for drug release and sensing inside living cells in a non-invasive way. Examples will be given in which **(i)** drug nano-colloids [7] and biodegradable capsules [8] are used for releasing antineoplastic drugs in cancer cells, **(ii)** colloidal quantum dots are used to label the walls of sensor capsules with unique optical bar codes [9], and **(iii)** pH-sensitive capsules are used to detect intracellular pH changes in complex cell lines [10].

These results show the practical applications of multilayer capsules and highlights their impact in the area of theranostics and nanomedicine.

References:

[1] L. Y. Rizzo, B. Theek, G. Storm, F. Kiessling, and T. Lammers, Curr. Opin. Biotechnol. 24 (2013).
[2] S. Mura and P. Couvreur, Adv. Drug Deliv. Rev. 64 (2012) 1394.
[3] G. Decher, Science 277 (1997) 1232.
[4] R. Xiong, S. J. Soenen, K. Braeckmans, and A. G. Skirtach, Theranostics 3 (2013) 141.
[5] V. Vergaro, F. Scarlino, C. Bellomo, R. Rinaldi, D. Vergara, M. Maffia, F. Baldassarre, G. Giannelli, X. C. Zhang, Y. M. Lvov, and S. Leporatti, Adv. Drug Deliv. Rev. 63 (2011) 847.
[6] L. L. del Mercato, P. Rivera-Gil, A. Z. Abbasi, M. Ochs, C. Ganas, I. Zins, C. Sönnichsen, and W. J. Parak, Nanoscale 2 (2010) 458.
[7] D. Vergara, C. Bellomo, X. Zhang, V. Vergaro, A. Tinelli, V. Lorusso, R. Rinaldi, Y. M. Lvov, S. Leporatti, and M. Maffia, Nanomedicine 8 (2011) 891.
[8] F. Baldassarre, V. Vergaro, F. Scarlino, F. De Santis, G. Lucarelli, A. Della Torre, G. Ciccarella, R. Rinaldi, G. Giannelli, and S. Leporatti, Macromol. Biosci. 12 (2012) 656.
[9] L. L. del Mercato, A. Z. Abbasi, M. Ochs, and W. J. Parak, ACS NANO 5 (2011) 9668.
[10] L. L. del Mercato, M. Ferraro, M. De Luca, C. Bucci, and R. Rinaldi, in preparation.

[O14] High Efficiency ITO-free flexible white organic light-emitting diodes based on multi-cavity technology

M. Mazzeo[1,2], F. Mariano[2], A. Genco[2], S. Carallo[1], and G. Gigli[1,2]

[1] NNL CNR-Istituto Nanoscienze, c/o Distretto Tecnologico, via per Arnesano km. 5, 73100 Lecce, Italy
[2] Dipartimento di Matematica e Fisica "E. De Giorgi", via Arnesano, 73100 Lecce, Italy

Keywords: White OLEDs, microcavity.

White Organic light-emitting diodes (WOLEDs) are promising light sources which could offer an important progress in indoor lighting, where luminous efficacy (LE) higher than 60 lm W^{-1} and color rendering index (CRI) larger than 80 are needed [1]. The potential of WOLEDs lies in the low cost of manufacturing, LE overcoming 100 lm W^{-1}[2], CRI near the limit of 100 [3], and the possibility to use lightweight flexible plastic substrates [4,5]. Nevertheless the simultaneous achievement of high luminous efficacy (LE), high color rendering index (CRI), very low manufacturing costs and compatibility with flexible thin substrates is still a great challenge. Indeed, very high efficiency devices show usually low values of CRI, not suitable for lighting applications, and use expensive indium tin oxide (ITO) electrodes which are not compatible with low cost and/or flexible products. Here we show a novel low cost ITO-free WOLED structure based on a multi-cavity architecture [6] with increased photonic mode density and still broad white emission spectrum, which allows for simultaneous optimization of all device characteristics. Without using out-coupling optics or high refractive index substrates, CRI of 85 and LE as high as 33 lm/W and 14 lm/W have been demonstrated on ITO-free glass and flexible substrates, respectively.

References:

[1] M. C. Gather, A. Kohnen, and K. Meerholz, Adv. Mater. 23 (2011) 233-248.
[2] S. Reineke, F. Lindner, G. Schwartz, N. Seidler, K. Walzer, B. Lüssem, and K. Leo, Nature 459 (2009) 234-238.
[3] J.-H. Jou, S.-M. Shen, C.-R. Lin, Y.-S. Wang, Y.-C. Chou, S.-Z. Chen, and Y.-C. Jou, Org. Electr.12 (2011) 865-868.
[4] T.-H. Han, Y. Lee, M.-R. Choi, S.-H. Woo, S.-H. Bae, B. H. Hong, J.-H. Ahn, and T.-W. Lee, Nature Photonics 6 (2012) 105-110.
[5] J.-H. Jou , C.-P. Wang, M.-H. Wu, H.-W. Lin, H. C. Pan, and B.-H. Liu, Journal of Materials Chemistry, 20 (2010) 6626-6629.
[6] M. Mazzeo, F. Della Sala, F. Mariano, G. Melcarne, S. D'Agostino, Y. Duan, R. Cingolani, and G. Gigli, Adv. Mater. 22 (2010) 4696-4700.

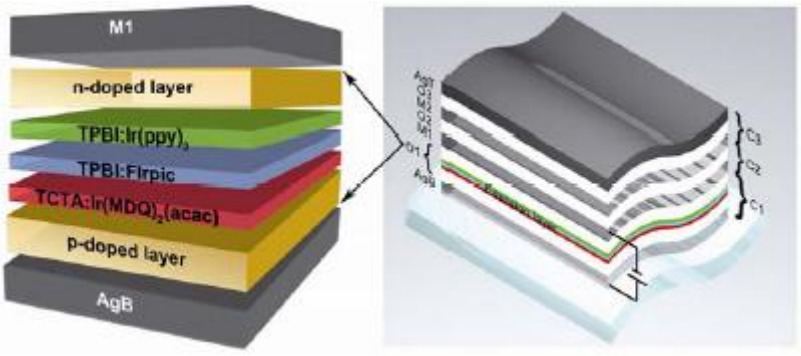


Fig. 1: Coupled micro-cavity White OLED architecture.

[015] Carrier multiplication in isolated and interacting silicon nanocrystals for photovoltaic applications: ab-initio results

I. Marri[1,2], M. Govoni[3], and S. Ossicini[1,3]

[1] Dipartimento di Scienze e Metodi dell'Ingegneria, Università degli Studi di Modena e Reggio Emilia, Italy
[2] CNR-NANO Research Center S3, Via Campi 213/A, 41125 Modena, Italy
[3] Department of Chemistry, University of California Davis, USA

Keywords: Solar cells, Carrier Multiplication, Silicon.

An important challenge of the scientific research is promoting the establishment of clean, cheap and renewable energy sources. One of the most appealing and promising technology is solar based, i.e. photovoltaics. For optimal energy conversion in photovoltaic devices one important requirement is that the full energy of the photon is used. However in such systems a single electron-hole pair of specific energy is generated only when the incoming photon energy is above a certain energy threshold, with the excess energy being lost to heat. Efficiency bottleneck caused by heat generation induced by phonon-assisted carrier relaxation processes can be partially reduced promoting fast and non-dissipative mechanisms that impede or strongly reduce the occurrence of thermalization processes. In this context Carrier Multiplication can be used to increase solar cell performances by promoting a net reduction of loss mechanisms; it results in the generation of multiple electron-hole pairs after absorption of one single photon. Carrier Multiplication was observed in a large range of systems despite a microscopic interpretation of such effect is still missing. Recently a new carrier multiplication scheme was hypothesized by Timmerman et. al. [1] and by Trinh et. al. [2] in order to explain results obtained from photoluminescence and induce absorption experiments conducted on dense arrays of silicon nanocrystals. In the interpretation of these experiments, a Coulomb-driven energy transfer process (defined Space Separated Quantum Cutting) between interacting silicon nanocrystals were hypothesized to generate different electron-hole pairs distributed on separated silicon nanocrystals after absorption of a single photon. In this talk we will analyze results obtained by first principle calculations in the study of carrier multiplication processes in silicon nanocrystals. After a brief analysis on carrier multiplication processes in isolated silicon nanocrystals (one-site carrier multiplication processes), we will investigate effects induced by nanocrystal-nanocrystal interaction on carrier multiplication dynamics. A detailed analysis of space separated quantum cutting processes will be pointed out and the condition that maximize such effects will be emphasized. A new Carrier Multiplication effect, defined Coulomb Driven Charge Transfer, will be introduced and quantified. A model based on the occurrence of one-site mechanisms, space separated quantum cutting and Auger recycling [3] will be presented in order to interpret results of Ref. [1,2].

References:

[1] D. Timmerman, I. Izeddin, P. Stallinga, I. N. Yassievich, and T. Gregorkiewicz, Nat. Photon. 2 (2008) 105.
[2] M. T. Trinh, R. Limpens, W. D. A. M. de Boer, J. M. Schins, L. D. A. Siebbeles, and T. Gregorkiewicz Nature Photon. 6 (2012) 316321.
[3] M. Govoni, I. Marri, and S. Ossicini, Nature Photon. 6 (2012) 672.

[016] Hybrid and Organic Photovoltaics

S. Colella[1], A. Loiudice[1,2], A. Rizzo[1], and G. Gigli[1,2]

[1] NNL CNR-Istituto Nanoscienze, c/o Distretto Tecnologico, via per Arnesano km. 5, 73100 Lecce, Italy
[2] Dipartimento di Matematica e Fisica "E. De Giorgi", via Arnesano, 73100 Lecce, Italy

Keywords: hybrid solar cells, flexible devices, colloidal nanocrystals.

The donor/acceptor inter-mixing in bulk heterojunction (BHJ) solar cells is a critical parameter, often leading to irreproducible performance of the finished device. We propose an alternative fabrication strategy towards a better control of the micro/nano-structured morphology consists in a sequential coating of the donor (P3HT) and acceptor (PCBM) from orthogonal solvents. We demonstrate that this technique allows to obtain a graded vertical phase-separated junction, resulting from the diffusion of the PCBM in the P3HT bottom layer. We are able to control the diffusion of PCBM, which occurs preferentially in the amorphous P3HT domains, by easily varying the ratio between crystalline/amorphous domains in the P3HT.[1] Most notably we exploit the potentiality of such novel device configuration to study the p-doping effect on polymer photovoltaic devices. We report, for the first time, improved conversion efficiency by p-type doping of the donor species in polymer solar cells.[2]

To improve the stability of such solar cells, we explore semiconductor nanocrystals (NCs) as promising building blocks for future-generation photovoltaic devices.[3] Solution processed NCs offer the potential to fabricate solar cells on large areas at low cost and with improved efficiency. Their wide spectral tunability, originating in the quantum size effect, may enable efficient light harvesting of the sun's full energy spectrum spanning across the visible and infrared spectrum. We demonstrate the fabrication of high-efficiency all-inorganic solar cells by a novel approach that involves processing of colloidal PbS QDs and anisotropic TiO_2 NCs under room-temperature conditions. Our results fully meet one of the major pursued goals in the design and fabrication of NC-based solar cells, that is the development of a facile and mild-room temperature solution-based route to the assembly of solar cells via utilization of "inorganic inks" that combine the advantages of low-temperature solution-processable organic compounds and the chemical-physical properties of semiconductor NCs.

References:

[1] A. Loiudice, A. Rizzo, G. Latini, C. Nobile, M. de Giorgi, and G. Gigli, Sol. Energ. Mat. Sol. Cells 100 (2012) 147-152.
[2] A. Loiudice, A. Rizzo, M. Biasiucci, and G. Gigli, J. Phys. Chem. Lett. 3 (2012), 1908–1915.
[3] A. Loiudice, A. Rizzo, G. Grancini, M. Biasiucci, M. R. Belviso, M. Corricelli, M. L. Curri, M. Striccoli, A. Agostiano, P. D. Cozzoli, A. M. Petrozza, G. Lanzani, and G. Gigli, Energy Environ. Sci. (2013) DOI:10.1039/c3ee23928d.

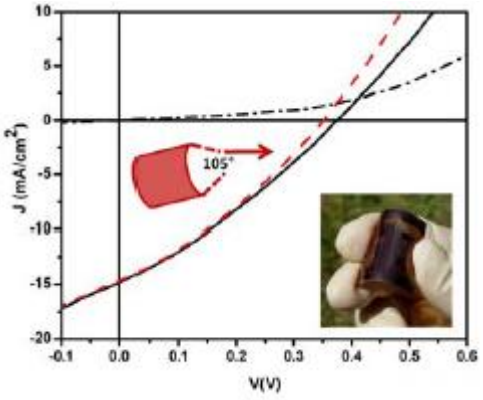


Fig. 1: TiO_2-NR/PbS-QD NC photovoltaic devices on a plastic substrate.

[O17] Nanofiber-based Devices for Energy Harvesting

L. Persano[1], C. Dagdeviren[2], Y. Su[3,4], Y. Zhang[3,4], S. Girardo[1], D. Pisignano[1,5], Y. Huang[4], and J. A. Rogers[2]

[1] National Nanotechnology Laboratory of Istituto Nanoscienze-CNR, Università del Salento, via Arnesano, I-73100 Lecce, Italy
[2] Department of Materials Science and Engineering, Frederick Seitz Materials Research Laboratory, and Beckman Institute for Advanced Science, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA
[3] Center for Mechanics and Materials, Tsinghua University, Beijing 100084, China
[4] Department of Civil and Environmental Engineering and Department of Mechanical Engineering, Northwestern University, Evanston, IL 60208, USA
[5] Dipartimento di Matematica e Fisica "Ennio De Giorgi", Università del Salento, via Arnesano I-73100 Lecce (Italy)

Keywords: Nanofibers, Energy harvesting, Piezoelectricity, Flexible devices.

The development of multifunctional, portable and flexible devices for applications which involve the integration with the human body or, in the field of robotics, in efforts to optimize human-like manipulation schemes are particularly valuable in the emerging field of self-powered electronics. For these and related applications, piezoelectric polymers, in forms that enable bending and stretching, are attractive for pressure/force sensors and mechanical energy harvesters [1]. Here we introduce our work on large area, flexible piezoelectric materials that consist of a free-standing, three-dimensional architectures of aligned piezoelectric polymer nanofibers. These enable ultra-high sensitivity in the low pressure regime (0.1 Pa) [2]. Experimental and theoretical studies reveal both the intrinsic properties as well as the behaviour of various realized devices. Quantitative analysis provides detailed insights into the pressure sensing mechanisms, and engineering design rules for applications that range from self-powered micro-mechanical elements, self-balancing robots and sensitive impact detectors. Our experiments show the feasibility for use in solid-state accelerometers, capable of measuring physical movements, pulsations and changes in orientation.

Acknowledgement : L.P. and D. P. acknowledge the European Research Council for supporting, under the European Union's Seventh Framework Programme (FP7/2007–2013), the ERC Starting Grant 'NANO-JETS' (Grant Agreement no. 306357).

References:

[1] J. A. Rogers, Nature 468 (2010) 177; Z. L. Wang *et al*., Materials Today 15 (2012) 532.
[2] L. Persano *et al.*, Nat. Commun. 4 (2013) 1633; doi: 10.1038/ncomms2639.

[O18] Substrate-driven self-assembling of metal nanocluster ordered arrays

S. Benedetti[1], S. Valeri[1], F. Stavale[2], N. Nilius[2], H.-J. Freund[2], J. Goniakowski[3], and C. Noguera[3]

[1] Centro S3, Instituto Nanoscienze-CNR and Dipartimento di Scienze Fisiche Informatiche e Matematiche, Università di Modena e Reggio Emilia, via Campi 213/a, Modena, 41125, Italy
[2] Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, Berlin, 14195, Germany
[3] CNRS and Université Pierre et Marie Curie-Paris 6, INSP, UMR7588, 4 place Jussieu, Paris cedex 05, 75252 France

Keywords: epitaxy, metal nanoparticles, thin films, self-assembly, metal-oxide interactions.

Ordered arrays of metal nanoclusters are of great interest for their applications in nanomagnetism, optics and catalysis. Amongst possible fabrication methods, the exploitation of a thin film as a support is appealing, where the nanopatterning induced by a misfit dislocation network can guide the nanocluster self-assembly into an ordered array [1].

In this work we combine experimental and theoretical investigation of nanoparticle self-ordering on a MgO film on Mo(001), where the presence of an interfacial dislocation network induces a surface periodic deformation connected with a modification in the workfunction (Fig. 1a) [2]. The deposition of Fe atoms leads to the spontaneous formation of nanoclusters disposed in a square array, with about 6 nm average distance, corresponding to the dislocation periodicity (Fig. 1b) [3]. Increasing MgO film thickness, the order of metal nanoparticles fades away and completely disappears for 40 ML MgO. DFT calculations clarify the mechanisms that determine ordered Fe nucleation. The modulations in the adsorption potential induce Fe atoms to preferentially bind to regions of high workfunction that enable electron transfer from the ad-species into the support. Particle growth, on the other hand, preferentially occurs in zones of contracted lattice parameter, where metal-metal and metal-oxide interactions can be optimized simultaneously. Both constraints favor particle growth in the Mg-Mo domains of the coincidence lattice (Fig. 1c).

The observed ordering effect on the MgO thin films is therefore caused by interplay of geometric and electronic properties at the metal-oxide interface. This growth-template allows us to produce extended particle arrays with narrow size distribution. This opens an experimentally simple route to address fundamental questions in heterogeneous catalysis, magnetism and nano-optics.

References:
[1] H. Brune *et al*., Nature 394 (1998) 451.
[2] S. Benedetti *et al*., Phys. Rev. B 78 (2008) 195411; H. M. Benia *et al.*, Surf. Sci 604 (2010) 435.
[3] S. Benedetti et al., Adv. Func. Mater. 23 (2013) 75.

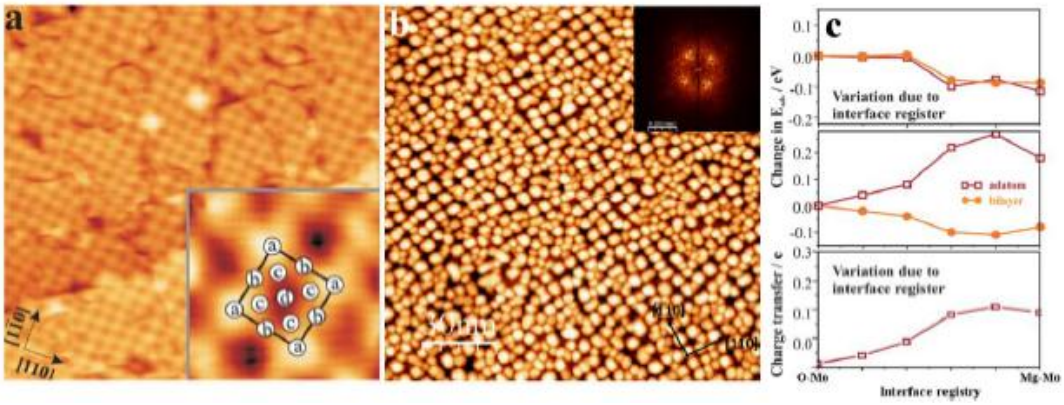


Fig. 1: a) STM image of a 10 ML thick MgO/Mo(001) film showing the typical coincidence lattice (80 × 80 nm^2). The inset shows a close-up with the superstructure unit-cell (12 × 12 nm^2); b) STM image of 3 ML Fe on MgO film; inset shows the FFT of the image; c) Calculated relative binding energies (per atom) with respect to the O-Mo domain and charge transfer for Fe adatoms and bilayers adsorbed on a 3 ML thick MgO/Mo(001) film shown as a function of interface register .

[O19] Hydrogen Storage on Graphene: an STM study

S. Goler[1,2], C. Coletti[2], V. Tozzini[1], V. Piazza[2], T. Mashoff[2], M. Takamura[3], S. Tanabe[3], H. Hibino[3], F. Beltram[1,2], V. Pellegrini[1], and S. Heun[1]

[1] NEST, Istituto Nanoscienze – CNR and Scuola Normale Superiore, Piazza San Silvestro 12, 56127 Pisa, Italy
[2] Center for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro 12, 56127 Pisa, Italy
[3] NTT Basic Research Laboratories, NTT Corporation, 3-1, Morinosato Wakamiya, Atsugi, Kanagawa 243-0198, Japan

Keywords: Graphene, Hydrogen, Hydrogen Storage, Functionalization, Scanning Tunneling Microscopy.

The realization of innovative hydrogen storage materials has worldwide strategic importance. In this context, graphene has recently attracted attention as a promising hydrogen storage medium. Indeed, graphene is lightweight, chemically stable, and exhibits attractive physico-chemical properties for hydrogen adsorption. Furthermore, the interaction between hydrogen and graphene can be controlled by chemical functionalization. However, experimental demonstrations of graphene-based hydrogen storage devices have yet to be reported.

The energetics of the chemisorption of hydrogen on graphene can be modified by the local curvature of the graphene sheet [1]. Based on scanning tunneling microscopy (STM) techniques, we report on site-selective adsorption of atomic hydrogen on convexly warped regions of monolayer graphene grown on SiC(0001). This system exhibits an intrinsic curvature owing to the interaction with the substrate [2]. We show that at low coverage hydrogen is found on convex areas of the graphene lattice. No hydrogen is detected on concave regions. These findings are in agreement with theoretical models which suggest that both binding energy and adsorption barrier can be tuned by controlling the local curvature of the graphene lattice [1]. This curvature-dependence combined with the known graphene flexibility may be exploited for storage and controlled release of hydrogen at room temperature.

Theoretical studies regarding metal atoms (e.g. Ti) deposited on graphene suggest that such materials can adsorb up to 8 wt% gravimetric density of hydrogen. We investigated the deposition of titanium on graphene and its potential for hydrogen storage. As shown in Fig. 1a, the titanium atoms form small islands (diameter ~ 10 nm). The Ti-covered graphene was exposed to molecular hydrogen (5 min at $1x10^{-7}$ mbar deuterium). The sample temperature was then increased up to 550ºC with a constant heating rate of 10 K/s while measuring the mass-sensitive desorption. The desorption spectra show two peaks at 210ºC and 290ºC (see Fig. 1b). Their intensity increases with increasing Ti coverage. Our data demonstrate the stability of hydrogen binding at room temperature and show that the hydrogen desorbes at moderate temperatures – both ideally matching technical requirements for hydrogen storage.

References:

[1] V. Tozzini and V. Pellegrini, J. Phys. Chem. C 115 (2011) 25523.
[2] S. Goler, C. Coletti, V. Piazza, P. Pingue, F. Colangelo, V. Pellegrini, K. V. Emtsev, S. Forti, U. Starke, F. Beltram, and S. Heun, Carbon 51 (2013) 249.

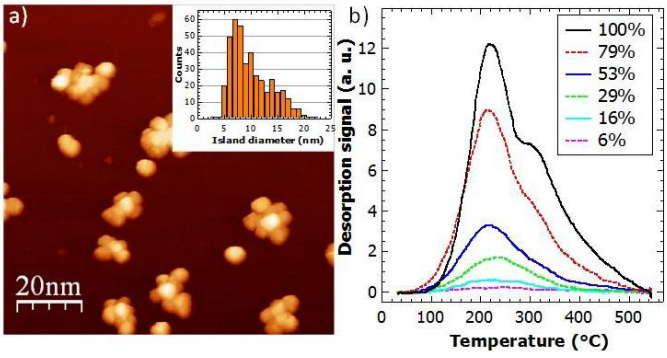


Fig. 1: a) 100 x 100 nm^2 UHV-STM image of a graphene surface with a titanium coverage of 16% (V = 2 V, I = 280 pA). The titanium atoms form small islands with a size distribution as shown in the inset. b) Desorption spectra measured for different coverages of titanium. The amount of stored hydrogen increases with Ti-coverage.

[O20] Electron and Optical Spectroscopies of Graphene Nanoribbons on Au(111): Insights from Ab-Initio Calculations

D. Prezzi[1], A. Ferretti[1], S. D. Wang[1], A. Ruini[1,2], E. Molinari[1,2], P. Ruffieux[3], J. Cai[3], N. C. Plumb[4], L. Patthey[4], X. Feng[5], K. Müllen[5], C. A. Pignedoli[3], and R. Fasel[3,6]

[1] Centro S3, CNR-Istituto Nanoscienze, Modena, Italy
[2] Dipartimento di Scienze Fisiche, Informatiche e Matematiche, UNIMORE, Italy
[3] Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland
[4] Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland
[5] Max Planck Institut for Polymer Research, Mainz, Germany
[6] Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland

Keywords: graphene nanoribbons, substrate, quasiparticle and excitonic effects.

Graphene nanostructures have striking properties related to their lateral confinement, that can open a band gap and induce a semiconducting behavior. Key features connected to the tunability of electronic and optical properties as a function of structural parameters, e.g. width and edge structure of graphene nanoribbons (GNR), have been predicted theoretically [1]; however, only recently atomic control of GNR geometry was demonstrated on Au(111) susbtrate [2]. These advancements have allowed the first measurements of the band gap and the topology of the occupied bands by STS and ARPES techniques [3].

In this work we combine cutting edge theoretical and experimental techniques to study the electronic and optical properties of a specific armchair nanoribbon (7-AGNR). Quasiparticle energies and excitonic effects are computed within the so-called GW-BSE scheme for the isolated N=7 AGNR; the presence of the substrate is accounted for by means of a classical image charge model for the screened Coulomb interaction. Our findings show that the metallic substrate induces a significant reduction of the energy gap as compared to the isolated 7-AGNR, bringing the GW gap from 3.7±0.1 eV to 2.3-2.7 eV on Au(111). On the contrary, the position of the optical peaks remains unaltered. Our results are in very good agreement with the experimental values obtained by STS [3] and differential reflectance data [4], indicating that this scheme can provide quantitative predictions for electron and optical spectroscopies of nanoribbons on weakly coupled substrates such as Au.

References:

[1] D. Prezzi, D. Varsano, A. Ruini, A. Marini, and E. Molinari, Phys. Rev. B 77 (2008) 041404(R); D. Prezzi, D. Varsano, A. Ruini, and E. Molinari, Phys. Rev. B 84 (2011) 041401(R).
[2] J. Cai *et al*, Nature, 466 (2010) 470.
[3] P. Ruffieux, J. Cai, N. C. Plumb, L. Patthey, D. Prezzi, A. Ferretti, E. Molinari, X. Feng, K. Müllen, C. A. Pignedoli, and R. Fasel, ACS Nano 6 (2012) 6930.
[4] P. Ruffieux *et al*., to be published.

[O21] Tailoring the coupling between single molecule magnets and ferromagnetic substrate with a graphene layer

A. Candini[1], V. Corradini[1], D. Klar[2], V. Bellini[1,3], R. Biagi[1,4], V. de Renzi[1,4], S. Klyatskaya5, H. Wende[2], M. Ruben[5], U. del Pennino[1,4], and M. Affronte[1,4]

[1] Centro S3 Istituto Nanoscienze – CNR, Modena, Italy
[2] Universität Duisburg-Essen, Duisburg, Germany
[3] Istituto Struttura dei Materiali, ISM-CNR, Trieste Italy
[4] Università di Modena e Reggio Emilia, Modena, Italy
[5] Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

Keywords: single molecule magnets, graphene, x-ray magnetic circular dichroism, spintronics.

Future spintronics devices will require the realization of novel hybrid metal-organic nano-architectures where single magnetic molecules are employed as active elements. Understanding and controlling the interaction between the molecules and metallic substrate is therefore of crucial importance. We address here the role of graphene as a buffer layer to tune the coupling between SMMs (namely TbPc2) and the magnetic substrates (Ni(111) single crystal).

Graphene monolayer is prepared on Ni(111) single crystal under UHV conditions by exposure to propane at high temperature. The integrity and quality of the graphene film are checked by STM, XPS and LEED. TbPc2 molecules are then deposited in situ by sublimation. The morphological, electrical and magnetic properties of the metallic-organic magnetic multilayer are studied by STM, XPS and UPS and by means of circular and linear X-ray dichroism at synchrotron facilities.

We observe that the molecules graft oriented with the Pc plane flat on the substrate (with and without graphene) and do not form 3D aggregation, thus remaining flat in contact with the substrate. When the molecules are in direct contact with the ferromagnetic Ni(111) surface an antiferromagnetic exchange coupling exists between the Tb magnetic moment and the substrate. This coupling is still present, although reduced, even after the insertion of the graphene layer, without changing sign.

We qualitatively modeled the interaction considering the organic part of the magnetic molecules, where a free electron links the magnetic center with the substrate. Our model is corroborated also by ab-initio DFT calculations. The presence of the magnetic coupling even when the graphene layer is inserted between the molecules and the surface is a consequence of the spin-properties of the molecular/graphene/Ni(111) interface.

[O22] Synthetic electron fluids based on graphene-GaAs double layers

V. Pellegrini

[1] CNR-NANO and Scuola Normale Superiore, Pisa, Italy

We propose a new double layer system 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. In this talk we shall discuss ongoing research efforts including experiments on Coulomb drag and time-resolved photoluminescence. These synthetic systems open new research opportunities for fundamental studies of electron-electron interaction effects and exciton condensation in two spatial dimensions.

Acknowledgement: Work done in collaboration with A. Gamucci, D. Spirito, B. Karmakar, M. Carrega, A. Principi, R. Azgari, M. Polini, A. Lombardo, M. Bruna, A. Ferrari, F. Koppens

[O23] Charge pumping in superconducting wires with Majorana fermions

F. Taddei[1], M. Gibertini[2], M. Polini[1], and R. Fazio[1]

[1] NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Pisa, Italy
[2] École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Keywords: electronic transport in mesoscopic systems; proximity effects; Andreev reflection; SN and SNS junctions

Since the first prediction [1] of real solutions to the Dirac equation, known as Majorana fermions, there have been many attempts to demonstrate their occurrence in nature, but clear evidence is still lacking. It has been recently suggested that Majorana fermions can exist as exotic excitations in certain condensed-matter systems, such as spin-orbit coupled semiconducting nanowires in a magnetic field with proximity-induced s-wave superconducting pairing [2-3]. The importance of finding Majorana fermions in condensed-matter systems is not only related to their fundamental interests. It is also rooted in the non-Abelian braiding statistics of these particles, which could be exploited as a basis for decoherence-free topological quantum computation [4].

This contribution will focus on the spectroscopic and transport properties of topological superconducting heterostructures. In particular, it will be shown that topological adiabatic pumping of charges occurs in a superconducting nanowire connected to a metallic lead, provided that a single mode of the latter is affected by the presence of Majorana fermions present at the endpoints of the super- conducting nanowire [5]. This is the case, for example, when the lead supports a single propagating mode or when the nanowire is coupled to the lead through a quantum point contact. The topological nature of pumping consists in the fact that any continuous deformation of the pumping path in parameter space does not change the charge pumped in a cycle. The necessary condition to achieve a finite quantized value of the pumped charge is that the phase diagram presents a non-simply connected structure, where isolated non-topological regions are surrounded by connected topological ones. This is possible by allowing both a non-uniform pairing amplitude and a tilted Zeeman field. Non-contractible pumping paths in parameter space can thus be identified within the topological phase. We have furthermore verified that the quantization of the pumped charge is robust against disorder.

References:

[1] E. Majorana, Nuovo Cimento 14, 171 (1937).
[2] R. M. Lutchyn, J. D. Sau, and S. Das Sarma, Phys. Rev. Lett. 105 (2010) 077001.
[3] Y. Oreg, G. Refael, and F. von Oppen, Phys. Rev. Lett. 105 (2010) 177002.
[4] C. Nayak, S. H. Simon, A. Stern, M. Freedman, and S. Das Sarma, Rev. Mod. Phys. 80 (2008) 1083.
[5] M. Gibertini, R. Fazio, M. Polini, and F. Taddei, arXiv:1302.2736.

ABSTRACTS| POSTER PRESENTATIONS

[P1] Spin dynamics in the molecular antiferromagnetic nanomagnet Ni_7: a 1H NMR study

P. Arosio[1], S. Sanna[2], A. Lascialfari[1,2], M. Mariani[2,6], E. Garlatti[1,3], S. Carretta[3], P. Santini[3], M. Affronte[4], and E. C. Sañudo[5]

[1] Dipartimento di Fisica, Università degli Studi di Milano, Milano, and S3-CNR, Istituto di Nanoscienze, Modena, Italy
[2].Dipartimento di Fisica, Università degli Studi di Pavia, Pavia, Italy
[3] Dipartimento di Fisica, Unità CNISM di Parma, Università di Parma, Parma, Italy
[4] Dipartimento di Fisica, Università degli Studi di Modena, and S3-CNR, Istituto di Nanoscienze, Modena, Italy
[5] Department of Inorganic Chemistry, University of Barcelona, Barcelona, Spain
[6] Dipartimento di Fisica, Università degli Studi di Bologna, Bologna, Italy

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 ^{1}H-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 ^{1}H NMR nuclear spin-lattice relaxation rate $1/T_1$ 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 $1/T_1$ 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]

References:

[1] E. K. Brechin, S. G. Harris, S. Parsons, and R. E. P. Winpenny, Angew. Chem. Int. Edn. 36 (1997) 1967.
[2] E. Garlatti, S.Carretta, M. Affronte, E. C. Sañudo, G. Amoretti, and P. Santini, J. Phys.: Condens. Matter 24 (2012) 10740063.
[3] F. Borsa, A. Lascialfari, and Y. Furukawa, Novel NMR and ERP Techniques, Springer, New York (2006).
[4] P. Santini, S. Carretta, E. Liviotti, G. Amoretti, P. Carretta, M. Filibian, A. Lascialfari, and E. Micotti, Phys.Rev.Letters 94, 077203 (2005)
[5] I. Rousochatzakis, Phys.Rev.B 79 (2009) 064421.

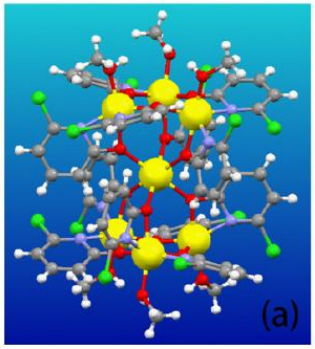


Fig. 1. The structure of Ni_7, where the yellow spheres represent the Ni ions (reprinted from ref. 2).

[P2] Mechanical features of Neuronal calcium sensor-1 revealed by molecular simulations

L. Bellucci[1], C. Cecconi[1], P. O. Heidarsson[2], B. B. Kragelund[2], S. Corni[1], E. Paci[3], and R. Di Felice[1]

[1] Centro S3, Istituto Nanoscienze Consiglio Nazionale delle Ricerche (CNR-NANO), 41125 Modena, Italy
[2] SBiNlab Department of Biology University of Copenhagen, Ole Maaløes Vej 5 DK-2200 Copenhagen, Denmark
[3] Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds, UK

Keywords: NCS-1, molecular dynamics simulations.

Understanding the mechanisms of protein folding is a long-standing objective of a multidisciplinary research community. Knowledge of intermediate states that occur during unfolding may shed light on the folding process. Recent progress in this field has been obtained by single-molecule experiments, especially by measurements carried out with the optical-tweezers technique [1,2].

In the work presented in this poster we have used molecular dynamic simulations (MD) to study the structure and unfolding process of the Neuronal Calcium Sensor-1 (NCS-1). NCS-1 is a protein able to trigger signal transduction processes by binding a large number of substrates and re-shaping its structure depending on the environment conditions and calcium ion concentration. The structure and dynamical properties of this protein appear to be crucial for its function. However, experimental data obtained with X-ray crystallography and NMR differ. The X-ray crystal structure of the NCS-1 shows a large solvent-exposed hydrophobic crevice (HC) occupied by PEG molecules, whereas in the NMR solution structure, the C-terminal tail partially occupies the HC [3]. To rationalize the structural differences observed with the two experimental techniques, we have performed two MD simulations, one starting from the NMR structure and the other starting from the X-ray structure without PEG molecules docked into HC. The relaxation of the two systems has generated a collection of structures in which the C-terminal tail occupies the HC.

A series of optical-tweezers (OT) measurements showed that NCS-1 unfolds in a three state manner, where the N-domain is the first to unfold followed, at higher forces, by the C-domain. To gain insights into the atomistic details of the unfolding process of this protein we have performed steered molecular dynamics simulations (SMD) [4,5] in explicit solvent. The results of our simulations are consistent with those obtained with OT and reveal a series of residue-residue interactions that appear to play a crucial role for the mechanical stability and unfolding process of this protein. Specifically, analysis of the MD unfolding trajectory reveals a key role played by the triple-helix structure H6-H9-H8 that appear to be a main determinant of the mechanical stability of the C-domain [6]. It is worth noting that H9 is linked to the C-terminal tail that, as shown by our relaxation studies, plays an important role for the mechanical stabilization of the C-domain.

References:

[1] C. Cecconi, E. Shank, C. Bustamante and S. Marqusee, Science 309 (2005).
[2] P. O. Heidarsson, I. Valpapuram, C. Camilloni, A. Imparato *et al.*, J Am Chem Soc 134 (2012).
[3] P. O. Heidarsson, I. Bjerrum-Bohr, G. Jensen, O. Pongs, B. Finn *et al.*, J Mol Biol 417 (2012).
[4] E. Paci and M. Karplus, Proc. Natl. Acad. Sci. USA 97 (2000).
[5] M. Schlierf, Z. T. Yew, M. Rief, and E. Paci, Biophys J. 99 (2010).
[6] P. O Heidarsson, M. R. Otazo, L. Bellucci *et al.*, Structure (2013) submitted.

[P3] Exciton Transfer of Azobenzene Derivatives in Self-Assembled Monolayers

E. Benassi and S. Corni

Centro S3 CNR Istituto Nanoscienze, via G. Campi 213/a, 41125 Modena, Italy

Keywords: azobenzene, exciton transfer, Self-Assembled Monolayers.

Di-phenyl-diazene and its derivative bis[(1,1')-biphenyl-4-yl]diazene (see Scheme, X = H, SH) were found to have innovative technological applications when arranged in Self-Assembled Monolayers (SAMs). This is due to their switching capability between two different configurations via photoisomerisation, that is preserved also when they are in a close-packed assembly over the metal surface forming SAMs. One of the possible phenomena that can hinder the photo-isomerisation process is the intermolecular excitonic transfer. Understanding this possibility is therefore of utmost importance. For doing so, we tackled a QM study, that begins from the exploration of the electronic excited states properties of a single molecule, to the intermolecular exciton couplings computed at different theory levels, till the excitonic diffusion dynamics, evaluated both within a frozen SAM portion and as average along a MD simulation. A simple kinetic model has been also developed in order to understand the time evolution of the populations after interaction with the electromagnetic radiation.

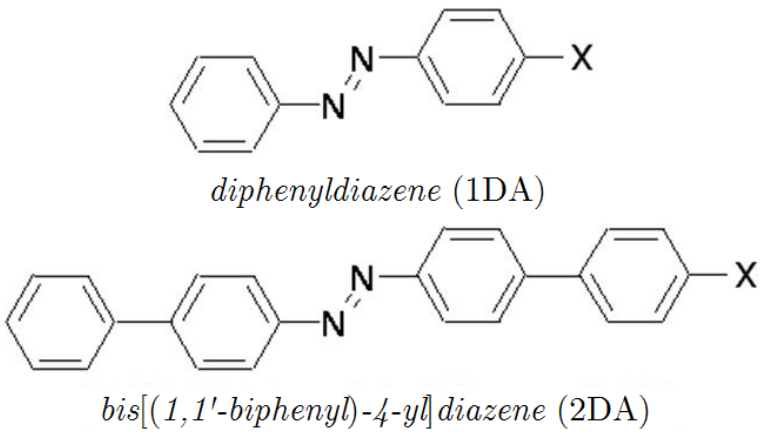


Fig. 1: Scheme.

[P4] Can azobenzene photoisomerise when chemisorbed on a Gold surface?

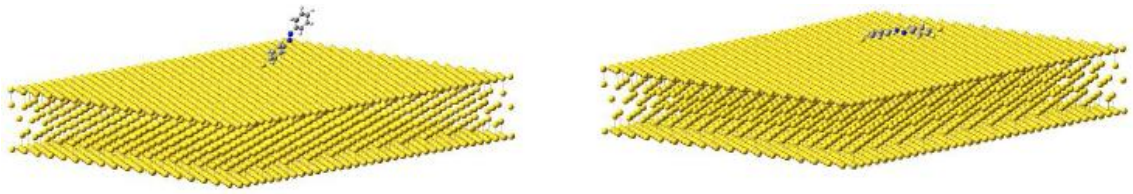
E. Benassi[1], G. Granucci[2], M. Persico[2], and S. Corni[1]

[1] Centro S3 CNR Istituto Nanoscienze, via G. Campi 213/a, 41125 Modena, Italy
[2] Dep. of Chemistry and Industrial Chemistry, University of Pisa, via Risorgimento 35, 56126 Pisa, Italy

Keywords: azobenzene, QM-MM, photoisomerisation, Self-Assembling Monolayers.

During the last years, the design and the production of molecular and super-molecular reversible switchable devices has been a very active field of research. Thanks to their reversible *trans-cis* photoisomerisation capability and the large geometrical and optical changes after isomerization, azobenzene (*alias* diphenyldiazene) and its derivatives represent one of the most attractive class of organic compounds for these aims. For practical applications, the molecular switcher is usually anchored on a noble metal surface, forming Self-Assembling Monolayers (SAMs). The surface presence affects the photoswitching behaviour, because of (i) geometric constraints imposed by the substrate or by neighbouring molecules, (ii) energy delocalisation and phase relaxation within the molecule by coupling to substrate phonons, substrate electron-hole pairs, and other adsorbates, or (iii) active implication of the surface. These effects can hinder the switching processes, but to date the mechanism is not clarified yet. In this study we employ a hybrid Quantum Mechanical / Molecular Mechanical (QM/MM) approach to evaluate the photodynamics of the azo-derivatives, when they are chemisorbed on a Gold surface.

The main objectives of this work are two: (i) estimate the extent of the effects due to the presence of the surface on the photoisomerisation process; (ii) verify whether it is possible that, when doubly anchored to the Gold surface, the azobenzene can photoisomerise preserving the two bonds with the surface. In fact, it has been experimentally observed that the *p,p'*-dithio-diphenyldiazene is able to photoisomerise when adsorbed on a Gold surface. This may be heuristically explained invoking two possible mechanisms: (i) because of the strength due to the photoisomerisation, one or two bonds with the surface are broken when the photoisomerisation process begins to occur, and finally, when the *cis* conformation has been reached, the molecule newly forms the bonds with the surface; (ii) the flexibility of the central moiety of the azobenzene enables the molecule to photoisomerise without any bond breaking.



[P5] Amyloid peptides at gold/water interface: insights from atomistic simulations

L. Bellucci[1], G. Bussi[2], R. Di Felice[1], and S. Corni[1]

[1] Centro S3, Istituto Nanoscienze Consiglio Nazionale delle Ricerche (CNR-NANO), 41125 Modena, Italy
[2] Scuola Internazionale Superiore di Studi Avanzati (SISSA), 34136 Trieste, Italy

Keywords: Amyloid-β peptide, adsorption process, gold nanoparticles.

Understanding adsorption processes of bio-molecules to the inorganic surfaces constitute the first step to rationalize the behavior of the new generation of nanoscale-based systems, which are of great importance in many emerging disciplines spanning from the nanotechnology to the nanomedicine. In particular recent experimental works tackled the effect, in vitro, of nanoparticles (NPs) on protein fibrillation. Protein fibrillation is involved in many human diseases, including Alzheimer's, Parkinson's, Creutzfeld-Jacob's and dialysis-related amyloidosis. Molecular adsorption on solid surface or NPs is a complex process that involves many dynamical steps from the initial recognition of the molecule by the surface, to the equilibrium conformational rearrangement of the adsorbed molecule. The rationalization of such aspects represent one of the major challenge of the experimental and theoretical investigation methods, however, specific dynamical aspects can be investigated by using advanced molecular dynamics (MD) simulations.

Using computational tools developed and validated so far [1,2,3], we studied the adsorption of the alanine dipeptide on the gold surface in water. The alanine di-peptide represent one of the most simple molecule that exhibits the mainly features shown by larger bio-molecules. This simple prototype system was used to evaluate a detailed three dimensional free energy surface (3D-FES) of the adsorption process by using metadynamics technique [4]. Analyzing the 3D-FES, we were able to track the shape modulation of the dialanine free energy landscape by the presence of the gold surface.

Exploiting such tools and by using high performance computing (HPC) resources [5], we are studying the interaction between the gold surface, and amyloid β-peptide (Aβ) and amyloid-like peptide segments in water. It is widely accepted that the Aβ in water solution is intrinsically unstructured and it can be described as an ensemble of highly dynamic conformational species in equilibrium with each other. The gold surface or NPs could easily modify the equilibrium among these conformations, making the Aβ monomer peptide an ideal platform (i) to study the conformational changes due to interaction with the Au surface and (ii) to unravel microscopic mechanisms that affect the fibrillation propensity of amyloidogenic peptide when contacting inorganic NPs.

References:

[1] F. Iori, R. Di Felice, E. Molinari, and S. Corni, J. Comput. Chem. 30 (2009) 1465.
[2] M. Hoefling, F. Iori, S. Corni, and K.E. Gottschalk, ChemPhysChem 11 (2010) 1763.
[3] L. Bellucci, G. Brancolini, A. Calzolari, O. Carrillo Parramon, S. Corni, R. Di Felice, "Proteins and Peptides at Gold Surfaces: Insights from Atomistic Simulations", in *Proteins at Interfaces III State of the Art*, eds. T. Horbett, J. L. Brash, W. Norde, Vol 1120, ACS Symposium Series (2012) 229.
[4] A. Laio, M. Parrinello, PNAS 99 (2002) 12562.
[5] PRACE, the Partnership for Advanced Computing in Europe infrastructure.

[P6] Quartz Crystal Microbalance as tool to probe (bio) molecular interactions in real-time

M. Bianco[1], R. Rinaldi[1,2], and V. Arima[1]

[1] National Nanotechnology Laboratory (NNL) - CNR-Istituto Nanoscienze, U.O.S. Lecce, Via per Arnesano 16, 73100 Lecce, Italy
[2] Università del Salento, Dipartimento di Matematica e Fisica "E. De Giorgi", ex Collegio Fiorini Campus extraurbano, via per Arnesano, 73100, Lecce, Italy

The detection of antigens, antibodies and toxins relevant to human health in trace as well as the accurate tuning of the chemical/physical properties of innovative biomaterials, need the evaluation of (bio)molecular interactions with highly sensitive and specific tools [1].
For the recognition of (bio)molecular interactions, several methods are available (i.e. NMR, X-ray crystallography, ELISA); unluckily, most of them are limited in sensitivity, are expensive, and difficult to be adapted to a huge number of applications [2-4]. In contrast, Quartz Crystal Microbalance (QCM) has sub-nanogram detection capabilities, is label-free and can be readily modified with a number of diverse surface chemistries to detect and characterize various interactions [5].

In the studies here reported we aim at investigating diverse applications of QCM, which include the detection of antigen–antibody interactions in pancreatic ductal adenocarcinoma (PDAC), detection of ochratoxin A (OTA) in fresh pork meat and the adsorption of tear fluid (TF) proteins on novel fluoropolymer coated contact lenses (CLs). A preliminary characterization of the (bio)molecular thin films deposited on the QCM surface was performed using Atomic Force Microscopy (AFM) and Dynamic Contact Angle (DCA).
The target of one QCM application was to develop specific protocols for detecting PDAC markers with un-labeled biosensors by optimizing surfaces less sensitive to non-specific interactions and to study the interactions between synthetic phosphorylated and un-phosphorylated peptides with sera of healthy and PDAC patients. The synthetic peptides were immobilized on the gold surface of the QCM sensor via a self-assembled alkanethiol monolayer [6-8].
A second QCM application was to develop suitable protocols for low cost, specific and sensitive detection of OTA, the most toxic member of a family of fungal metabolites frequently found in a variety of foodstuffs (including coffee, wine, blood derived meat products, particularly pork) [9]. We monitored the presence of OTA by immobilizing several DNA-aptamers and developing different functionalizations on the gold surface of the QCM sensor.
The objective of the third QCM application here reported was to deposit CL-derived polymers on QCM surface and to exploit the adsorption of the main TF components in absence or in presence of a thin film coating based on fluoropolimers (named P(S3-b-Sz)10 (P10) and P(S3-b-Sz)20 (P20)) [10-11]. The results of this study provide evidences that fluoropolymers allow to extend CL lifetime reducing proteins adsorption from TF.

References:
[1] C.I. Cheng, Y.P. Chang and Y.H. Chu, Chem. Soc. Rev 41 (2012) 1947.
[2] D. L. Minor, Jr., Neuron 54 (2007) 511.
[3] K. Takeuchi and G. Wagner, Curr. Opin. Struct. Biol 16 (2006) 109.
[4] S. Jager, L. Brand and C. Eggeling, Curr. Pharm. Biotechnol 4 (2003) 463.
[5] M. C. Dixon, J. Biomol. Tech 19 (2008) 151.
[6] M. Bianco, A. Aloisi, V. Arima, M. Capello, S. Ferri-Borgogno, F. Novelli, S. Leporatti, R. Rinaldi, Biosens. Bioelectron 42 (2013) 646.
[7] M. Capello, S. Ferri-Borgogno, P. Cappello, F. Novelli, FEBS Journal 278 (2011) 1064.
[8] F. Novelli, B. Tomaino, P. Cappello, (2011) WIPO Patent Application WO/2011/030302.
[9] A. el Khoury and A. Atoui, Toxins 2 (2010) 461.
[10] R. Mapstone, Br J Ophthalmol 52 (1968) 729.
[11] M. Rodahl and B. Kasemo, Review of Scientific Instruments 67 (1996) 3238.

[P7] Local magnetic properties in Cr_8, Cr_7Cd and Cr_7Ni molecular rings from 19F-NMR

L. Bordonali[1,3,6], C.M. Casadei[1,3], M. Corti[1,4], M. Moscardini[1], E. Garlatti[2], Y. Furukawa[3], F. Borsa[1,3,4], A. Lascialfari[2,4], G. Timco[5], and R. Winpenny[5]

[1] CNISM and Department of Physics , Università degli Studi di Pavia, I-27100,Pavia,Italy
[2] Department of Molecular Physics, Università degli Studi di Milano, I-20134,Milano,Italy and S3-CNR, Istituto Nanoscienze, Modena, Italy
[3] Department of Physics and Astronomy, Ames Laboratory, Iowa State University, 50011 Ames, Iowa, USA
[4] Consorzio INSTM, Via Giusti 9, I-50121 Firenze, Italy
[5] The Lewis Magnetism Laboratory, The University of Manchester, M13 9PL Manchester, United Kingdom
[6] Department of Physics "E. Amaldi," Università Uniroma TRE, Roma, Italy

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 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 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 MnF_2, for F-Ni^{2+} in $KNiF_3$ and NiF_2 and for F-Cr^{3+} in $K2NaCrF_6$.

References:

[1] C. M. Casadei *et al.*, J. Phys.: Condens. Matter 24 (2012) 406002.

[P8] The redox functionality of a protein is determined by its dynamic interaction with the surrounding solvent

C. A. Bortolotti[1,2], M. Sola[1,2], L. Paltrinieri[3], M. Borsari[3], I. Daidone[4], and S. Corni[2]

[1] Department of Life Sciences, University of Modena and Reggio Emilia, Italy
[2] Center S3, CNR Institute of Nanoscience, Modena, Italy
[3] Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia, Italy
[4] Department of Chemistry, University of L'Aquila, Italy

Keywords: Electron transfer, Redox Proteins, PMM/MD, Solvent, Dynamics.

The number of conformations experienced by a protein under physiological conditions is much larger than what is shown by the static, although obviously extremely informative, X-ray structure. To understand a biomolecule in action, a fourth dimension, time, must be taken into account, updating the usual structure-function paradigm to include dynamics. Experimental techniques are hindered by spatial and temporal resolution limits that do not allow us to watch individual atoms move within a protein. Within this respect, molecular dynamics (MD) simulation provide a powerful tool to investigate the effects of dynamics on the functionality of a protein. We have investigated native and mutant species of two electron transfer (ET) proteins, azurin and cytochrome *c*, by means of MD simulation and Perturbed Matrix Method (PMM) approach, a QM/MM-like theoretical method allowing for the calculation of electronic properties in complex systems based on a wide configurational sampling. For both species, we find that the dynamic interplay between protein and solvent is the key factor determining the redox properties of these hallmark ET systems. In particular, we find that the solvent accessibility to heme in cytochtome *c* affects not only its reorganization energy [1] but also its redox potential [2] through the reversible opening of solvent accessible cavities in the protein matrix that lead to hydration of the heme propionates which raises the protein E^0. In the case of azurin, we show how the dynamics of the small, metal-binding loop region controls the outer-sphere reorganization energy not only by determining the exposure of the active site to solvent but also through the modulation of the redox-dependent rearrangement of the whole protein scaffold and of the surrounding water molecules [3]. These results show the importance of the inclusion of protein-solvent dynamic effects to understand the fundamentals of biological ET, but also to improve the rational design of engineered biomolecules with tailored redox properties for nanobiotechnological applications.

References:

[1] C. A. Bortolotti, M. E. Siwko, E. Castellini, A. Ranieri, M. Sola, and S. Corni, J. Phys. Chem. Letters 2 (2011) 1761.
[2] C. A. Bortolotti, A. Amadei, M. Aschi, M. Borsari, S. Corni, and I. Daidone, J. Am. Chem. Soc. 134 (2012) 13670.
[3] L. Paltrinieri, M. Borsari, A. Ranieri, G. Battistuzzi, S. Corni, and C. A. Bortolotti, J. Phys. Chem. Letters 4 (2013) 710.

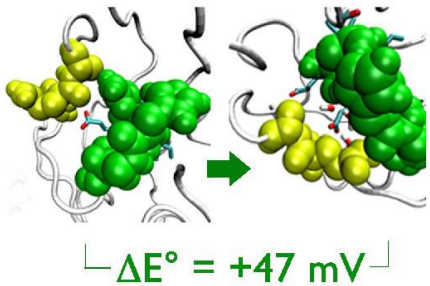


Fig.1: The effect of the opening of a solvent accessible cavity on the reduction potential of cytochrome *c*.

[P9] Molecular Simulations of β2-Microglobulin

G. Brancolini[1], O. Carrillo Parramon[1], A. Bochicchio[2], V. Tozzini[2], and S. Corni[1]

[1] CNR-NANO S3, Institute of Nanoscience, via Campi 213/A, 41125 Modena, Italy
[2] NEST-CNR, Institute of Nanoscience, P.zza San Silvestro 12, 56127 Pisa, Italy

Keywords: Docking, Molecular Dynamics, Gold, Protein Aggregation.

The pathological self-aggregation of β2-microglobulin (β_2m) has been investigated experimentally in the past, starting from some relevant structural aspects of the protein. The characterization of β_2m aggregates by direct investigation through electron microscopy, atomic force microscopy, solid state NMR and other solid state techniques has provided important structural and morphological information on the assembly, but no clues about the mechanism of the aggregation process. [1]

Computer simulations at the atomistic level [2,3] are a powerful tool that can effectively complement the experimental studies on the pathological self-aggregation of β_2m, as well as its systemic deposition of fibrils. To elucidate the atomistic processes involved in the mechanism of aggregation and to interpret the hypothesis that the effect of the environment may physiologically support the deposition, [1] we perform a series of simulations by using different levels of theory (ab initio quantum mechanical, classical Molecular Dynamics and Brownian Dynamics) that cover multiple length- and time-scales. [4] Relevant effects of the environment on protein conformational stability will be described involving: (I) protein in solution (II) protein in proximity of charge arrays e.g. bare gold surfaces (Fig. 1) and gold surfaces covered with charged surfactants, (III) functionalized gold nanoparticles. On the basis of the preferred protein-gold encounter complexes resulted from docking, MD simulations of the complexes anchoring the protein to gold through the C-terminal tail, showed strong fluctuation of the D-strand and DE-loop which are known to play an important role in the amyloid structure formation.

References:

[1] G. Esposito *et al*., Subcell Biochem. 65 (2012) 165-83.
[2] R. A. Latour, Biointerphases 3 (2008) FC2.
[3] F. Iori *et al.*, J. Comput. Chem. 30 (2009) 1465.
[4] G. Brancolini *et al.*, ACS Nano 6 (2012) 9863.

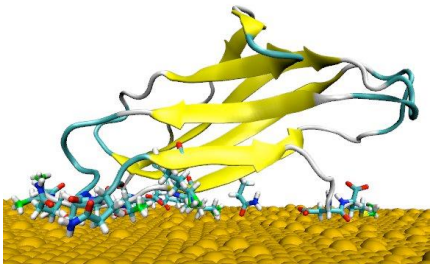


Fig. 1

[P10] Coarse-grained methods for the study of amyloid proteins

O. Carrillo[1], G. Brancolini[1], V. Tozzini[2], and S. Corni[1]

[1] Centro S3, CNR-Istituto Nanoscienze, Modena, Italy
[2] Laboratorio NEST, CNR-Istituto Nanoscienze, Pisa, Italy

Coarse-grained (CG) methods have shown to be useful tools to model biological systems. They replace groups of atoms of an atomistic structure with single interaction sites, the so-called coarse-grained beads and they map inter-atomistic interactions to effective ones between these CG units. This reduction of degrees of freedom increases the speed of the simulation which allows the study of new relevant biological problems that were unconceivable some years ago by only considering a classical Molecular Dynamics (MD). Literature is rich of different CG methods and different applications that extend to a large variety of systems [1].

One of the less explored applications is the study of a protein structure transition. These transitions happen in the so called amyloid proteins, who can undergo misfolding and eventually aggregation to form fibrillar structures. In this work, we are interested in one of these proteins: β2-microglobulin [2]. We study its propensity of misfolding by using different CG methods. In the one hand, we study its behaviour under the interaction with a gold surface by considering a CG method based on the Essential Dynamics of the protein. In a recent work we presented a new method that is used to study the behaviour of coarse-grained proteins on a gold surface. It uses the Essential Dynamics results of the free protein to build a harmonic potential (ED/MD potential [3]) that accounts for all bonded, non-bonded forces of the structure and solvation effects. This force field is more simple than the all atomistic one and makes molecular dynamics simulations be more computationally efficient. At this point, the interaction of a given protein and a gold surface can be modeled just adding to this ED/MD potential an effective Lennard-Jones interactions [4]. Results are found by numerically solving the corresponding Langevin Equation of the system. In the case of β2-microglobulin, as well as Lennard-Jones potential, a coulombic interaction is considered.

In the other hand, Kovacs' CG model [5] is used in order to study the free β2-microglobulin. Its particular harmonic-type bead-bead interactions allows us to redefine them as residue-residue dependent in order to change the interactions between different parts of the protein. As it can be found in the literature, misfolding of amyloid proteins starts when the interaction pattern of protein is changed. By changing the interaction pattern in the Kovacs CG model, a change in the correlation map of the system is found which makes β2-microglobulin to misfold as expected.

Moreover, we are also exploring the use of single bead CG models using interbead potentials able to switch between two configurations of the protein (e.g., native vs misfolded), to verify how the interaction with the environment (e.g., with metal surfaces and nanoparticles) can modify the native-misfolded equilibrium.

References:

[1] V. Tozzini, Curr. Op. In Struct. Biol. 15 (2005) 144.
[2] F. Fogolari, A. Corazza, P. Viglino, P. Zuccato, L. Pieri, P. Faccioli, V. Bellotti, and G. Esposito, Biophys. J. 92 (2007) 1673.
[3] O. Carrillo, C. A. Laughton, and M. Orozco, J. Chem. Theor. Comp. 8 (2012) 792.
[4] D. B. Kohn, S. Corni, P. J. Winn, M. Hoefling, K. E. Gottschalk, and R. C. Wade, J. Chem. Theor. Comp. 6 (2010) 1753.
[4] D. B. Kohn, S. Corni, P. J. Winn, M. Hoefling, K. E. Gottschalk, and R. C. Wade, J. Chem. Theor. Comp. 6 (2010) 1753.

[P11] Triphenylamine-based dyes as fluorophores for dye sensitized solar cells and for labeling and imaging of living cells' cytoplasm

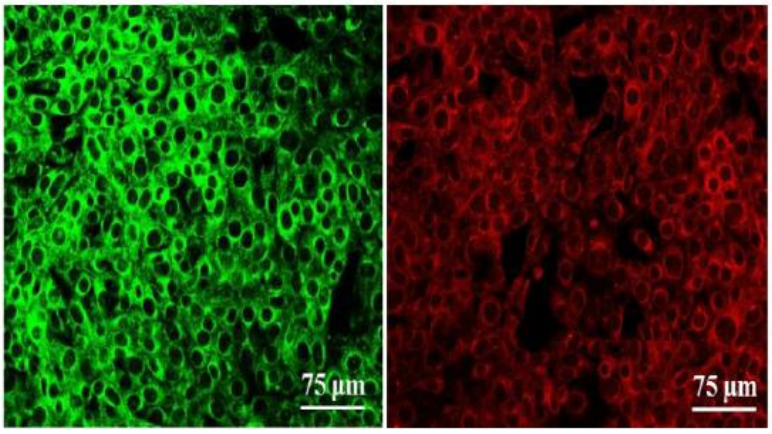
A. Scrascia[1], L. De Marco[2], I. E. Palamà[1], S. Laricchia[2], R. A. Picca[3], C. Carlucci[1,4], E. Fabiano[1], A. L. Capodilupo[1], F. Della Sala[1,2], G. Gigli[1,2,4], and G. Ciccarella[1,4]

[1] Istituto Nanoscienze – CNR, National Nanotechnology Laboratory (NNL), Via Arnesano, 73100 Lecce, Italy. E-mail: giuseppe.ciccarella@unisalento.it)
[2] Center for Biomolecular Nanotechnologies @UNILE, Istituto Italiano di Tecnologia (IIT), Via Barsanti, 73010 Arnesano (LE), Italy
[3] Dipartimento di Scienza dei Materiali, Università del Salento, via Monteroni 73100 Lecce, Italy
[4] Dipartimento di Ingegneria dell'Innovazione, Università del Salento, Via Monteroni, 73100, Lecce, Italy

Keywords: Triphenylamine-based dyes, dye sensitized solar cells, imaging of living cells' cytoplasm.

Novel triphenylamine (TPA)-based organic dyes were synthesized and assessed for their performance in dye-sensitized solar cells (DSSCs). In the considered dyes the TPA group and the cyanoacetic acid have the role of electron-donor and -acceptor, respectively, whereas a thienyl, phenyl and thienyl-fluoro-phenyl-substituted as p-linker were introduced to improve the dye performance in DSSCs. Experimental characterization and density functional theory calculations suggest that the presence of electron withdrawing substituents in the linker close to the electron-acceptor moiety leads to a more efficient intramolecular photo-induced charge transfer. In fact, photovoltaic experiments reveal that the DSSCs based on the thienyl-fluoro-phenyl substituted dyes yield a better solar-energy-to-electricity conversion efficiency with respect to not fluorinate-dyes, with an increase of 1%. This confirms that the thienyl-fluoro-phenyl substitution provides an effective strategy for promoting the DSSCs performance. For each dye were carried out photophysical and electrochemical characterization and theoretical investigation. The performance of the new sensitizers was investigated by constructing test devices and the photovoltaic parameters in terms of short circuit current (J_{sc}), open circuit voltage (V_{oc}), fill factor (FF), and the power conversion efficiency (η) reaching efficiencies around 6%.

The chemistry of small molecule as fluorophores is exciting and is playing an important role also in cellular biology research, in particular in cell viability and revealing cytotoxicity, following proliferation, and monitoring cell adhesion and spreading. Thus, it was developed the idea of applying our dyes typically studied for energy in biological systems. it was investigated the cytoplasm labeling of two cell lines (3T3 fibroblasts and C2C12 myoblasts) with conjugated triphenylamine-based fluorophores. The dyes revealed biocompatible and spontaneously crossing the membrane of living cells. The obtained results concerning our dyes are the proof that the fluorescent molecules are cell-permeant and non-toxic and can be used as cell tracing to different component of cellular cytoplasm.



[P12] An interfacial electrochemical sensor for biomembrane-interacting chemicals

D. Q. Colosso[1], M. Onofri[2], and G. Zuccheri[1,2]

[1] Department of Pharmacy and Biotechnologies at the University of Bologna, Via Belmeloro, 6 Bologna, Italy, 40126
[2] Interdepartmental Center for Industrial Research on Life Science and Technologies at the University of Bologna, Italy

Keywords: Electrochemical biosensors, tethered lipid membranes, chemical pollutants.

Interaction of a molecule or macromolecule with a biological membrane can include transient or permanent surface binding, transient of permanent insertion, disruption of the membrane order or other physical properties, including punching holes or the extraction of lipids. Such processes can also be simultaneous or occur for the same substance in different regimes. It is important not only to understand the mechanism of interaction of the different membranes with the molecules to which they could be exposed, but also to have reliable and simply deployable means for monitoring such interaction in real-life conditions, and also for complex analytical matrices. Here the effective result might depend on the simultaneous presence of different phenomena, thus the availability of an experimental net-effect determination could be of value.

In order to test and monitor the possible interaction of synthetic chemicals and environmental matrixes with the biological membranes, several possible model systems have been proposed. Soluble/suspended or surface-associated model membranes can be exposed to the potentially interacting chemical and the effect could then be evaluated.

Here, we show our results for the implementation of an electrochemical biosensor based on a covalently tethered lipid bilayer anchored on a flat gold electrode (tBLM, in short). The electrical properties of the complex electrode-bilayer-environment interface depends on the state and integrity of the tethered membrane. A change in the membrane properties commonly leads to a change in the average electrical capacitance or resistivity of the membrane. Such measurement is simple to perform via electrochemical impedance spectroscopy or related techniques [1], and it is simply amenable of parallelization and automatization, so as to become a fast screening method for libraries of compounds or libraries of membranes of different lipid composition.

The system was tested by monitoring in time the interactions of pollutant-models such as dinitrophenol (reversible), cyclohexane (non-reversible or partially so) or of biological toxins such as melittin and gramicidin, demonstrating the possible use of the device in environmental or drug-screening applications.

References:

[1] R. Naumann, S. M. Schiller, F. Giess, B. Grohe, K. B. Hartman, I. Karcher, I. Koper, J. Lubben, K. Vasilev, W. Knoll, Langmuir 19 (2003) 5435.

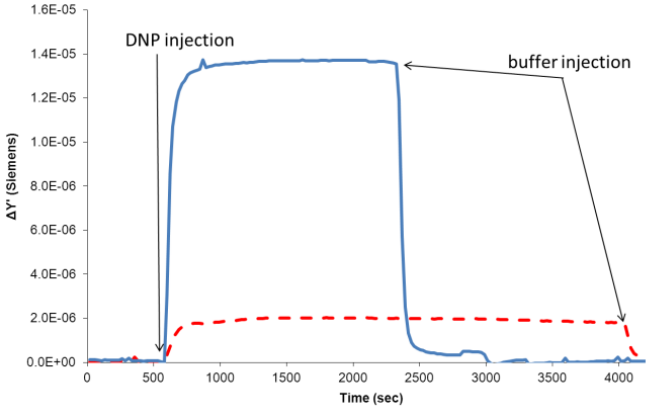


Fig. 1:Time course of the measurement of the electrical interface admittance (the inverse of the electrical impedance) of tethered lipid bilayers exposed to 50 µM 2,4-dinitrophenol (solid trace) and 15 µM 2,4-dinitrophenol (dashed trace).

[P13] Multiphoton Molecular Photorelease by Functionalized Gold Nanoparticles: Microscopic Insights by Electromagnetic and Molecular Dynamics simulations

L. Bergamini[1,2], V. Voliani[3], R. Nifosì[4], and S. Corni[1]

[1] Center S3, CNR Institute of Nanoscience, Modena, Italy
[2] Dept. of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia, Modena, Italy
[3] Universidad de Valencia, Instituto de Ciencia Molecular (ICMol), Valencia, Spain
[4] NEST, Institute of Nanoscience, Pisa, Italy

Keywords: nanoparticles, controlled drug delivery, plasmonics, simulations.

Recently, functionalized nanoparticles (NPs) have demonstrated a clear potential for drug delivery. On one hand, by exploiting proper functionalization strategies, they can be targeted to the specific cells where the drug should be delivered, maximizing the therapeutics efficiency by minimizing side effects. On the other hand, nanoparticles can also have an active role in the drug release, being able to transduce an external stimulus (e.g., light) in the liberation of the drug and thus in its bioavailability at a specific and externally controlled time and location. A proof of principle that such remotely-controlled delivery is possible has been previously given with gold nanoparticle functionalized with a peptide spacer connected by click-chemistry to a payload (a fluorescent molecule) via a 1,2,3-triazole photocleavable unit [1]. In particular, the experimental data showed that the photodissociation involves a three-photon absorption process. An interplay between the plasmonic gold nanoparticle and the photocleavable unit is required to enhance the multiphoton absorption cross section and thus explain the release event.

In this work, we investigated the possible extent of three-photon absorption enhancement due to the gold nanoparticles by means of fully-retarded electromagnetic simulations based on the Boundary Elements Methods [2]. In particular, we considered the enhancement achievable when the nanoparticles are well-separated in solution and when they form aggregates of a few nanoparticles with various shapes. In the latter case, electromagnetic hot-spot between NPs are found, providing very high electromagnetic enhancements. As expected, results are highly sensitive to the position and the orientation of the photocleavable moiety with respect to the metal surface. We addressed the distribution of relative positions of such moiety by performing atomistic molecular dynamics simulations of the peptide spacer layer on a gold surface. The results of our simulations clarify the microscopic picture behind the experimental results, allowing for improved design of such promising synergistic multiphoton photorelease nanosystems.

References:

[1] V. Voliani, F. Ricci, G. Signori, R. Nifosì, and F. Beltram, Small 7 (2011) 3271.
[2] F. García de Abajo and A. Howie, Phys. Rev. B 65 (2002) 115418.

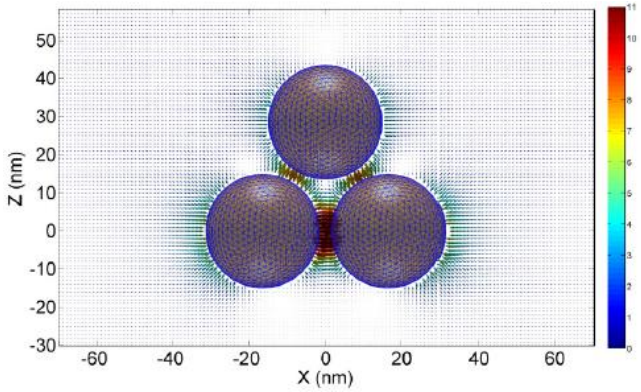


Fig. 1: Graphical representation of the total electric field at a given instant produced by a linearly polarized plane wave impinging on a gold three-NP aggregate. The plan wave is traveling along the Z direction and the electric field is polarized along X. The color scale represent the electric field intensity in units of the impinging wave electric field.

[P14] Modeling opto-electronic properties of a dye molecule in the vicinity of a semiconductor nanoparticle

A. Delgado[1], S. Corni[1], and G. Goldoni[1,2]

[1] CNR-NANO S3, Institute for Nanoscience, Via Campi 213/A, 41125 Modena, Italy
[2] University of Modena and Reggio Emilia, Via Campi 213/A, 41125 Modena, Italy

Keywords: optical properties, charge-transfer excitations, solvent and environmental effects.

A general methodology is presented to model the opto-electronic properties of a dye molecule modified by a TiO_2 semiconductor nanoparticle (NP), a model system resembling the architecture of dye-sensitized solar cells[1]. The total reaction potential due to the polarization of the solvent (acetonitrile) and the metal oxide is calculated by extending the PCM integral equation formalism (IEF-PCM) [2]. The general electrostatic problem is solved numerically by an external code interfaced to a modified version of the GAMESS program [3]. The developed method is applied to compute the excited state oxidation potential (ESOP) of the L_0 organic dye [4] at different distances and configurations respect to the NP surface. Results are reported for the protonated and deprotonated forms of L0. The stronger renormalizations of the ESOP values due to the presence of the TiO_2 nanostructure are found for the protonated dye, reaching a maximum of about -0.16 eV. The role of protonation effect is discussed in terms of the atomic Löwdin charges of the oxidized and reduced species. The ground state energies are computed by using density functional theory (DFT) while the vertical electronic excitations are obtained by time-dependent DFT in a state-specific corrected linear response scheme [5]. We observed a weak effect on the L_0 optical excitation gap due to the polarization response of the NP.

References:
[1] Nature 414 (2001) 338; Solar Energy 85 (2011) 1172.
[2] J. Chem. Phys. 107 (1997) 3032.
[3] J. Comp. Chem. 14 (1993) 1347.
[4] J. Org. Chem. 72 (2007) 9550.
[5] J. Chem. Phys. 124 (2006) 124520.

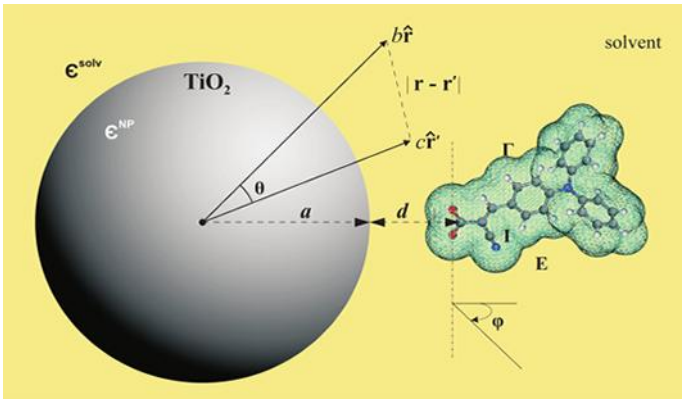


Fig. 1: sketch of the model system, a dye molecule close to a spherical nanoparticle embedded in a solvent solution. G represents the cavity hosting the deprotonated L_0 dye. The color code for the elements is red for O, blue for N, grey for C, and white for H.

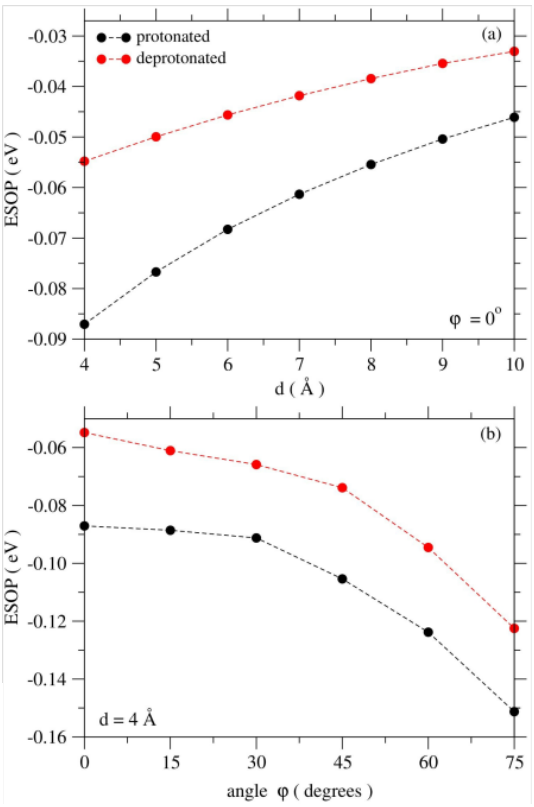


Fig. 2: Calculated excited state oxidation potential (ESOP) as a function of the distance d between the dye and the NP (a) and the rotation angle φ (b).

[P15] Nitro-catechol/ZnO(10-10): molecular dipole and energy level alignment in a model system for Dye/ metal oxides interfaces

V. De Renzi[1,2], G. Arnaud[1,2], U. del Pennino[1,2], V. Corradini[2], R. Biagi[1,2], A Calzolari[2], A. Ruini[1,2], and A. Catellani[2]

[1] Dipartimento di Scienze Fisiche, Informatiche e Matematiche dell' Università di Modena e Reggio Emilia

[2] Centro S3, CNR-Istituto di Nanoscienze, Via G. Campi 213/A , 41125 Modena, Italy

Keywords: DSSC, interface electronic properties, electron spectroscopies, DFT

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 alignment of the empty states relative to the substrate bands. DFT calculations allow the understanding of electronic structure 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.

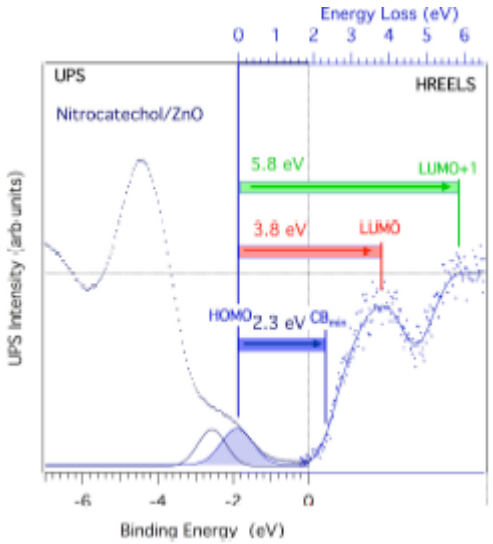


Fig. 1: UPS and HREELS spectra of one monolayer nitrocathecol/Zno(10-10) . The HOMO state lies 1.1 eV above the valence band maximum. Three HREELS features at 2.3 eV, 3.8 eV and 5.8 eV are attributed to HOMO-Conduction band minimum, HOMO-LUMO and HOMO-LUMO+1 transitions, respectively.

[P16] Control of DNA Minor Groove Width and Fis Protein Binding by the Purine 2-amino Group

S. P. Hancock[1], T. Ghane[2], D. Cascio[3], R. Rohs[4], R. Di Felice[2], and R. C. Johnson[5]

[1] Department of Biological Chemistry, David Geffen School of Medicine at the University of California at Los Angeles, Los Angeles, CA 90095-1737, USA
[2] Center S3, CNR Institute of Nanoscience, Via Campi 213/A, 41125 Modena, Italy
[3] University of California at Los Angeles-Department of Energy Institute of Genomics and Proteomics, University of California at Los Angeles, Los Angeles, California 90095-1570, USA
[4] Molecular and Computational Biology Program, Department of Biological Sciences, Department of Physics and Department of Chemistry, University of Southern California, Los Angeles, CA 90089, USA
[5] Molecular Biology Institute, University of California at Los Angeles, Los Angeles, California 90095, USA

Keywords: protein-DNA binding, biochemical synthesis, X-ray structures, molecular dynamics.

The width of the DNA minor groove varies with sequence and can be a major determinant of DNA shape recognition by proteins. For example, the minor groove within the center of the Fis-DNA complex narrows to about half the mean minor groove width of canonical B-form DNA (Figure 1) in order to fit onto the protein surface. G/C base pairs within this segment, which is not contacted by the Fis protein, reduce binding affinities up to 2000-fold over A/T-rich sequences. We show here [1] through multiple X-ray structures and binding properties of Fis-DNA complexes containing base analogs that the 2-amino group on guanine is the primary molecular determinant controlling minor groove widths. Specifically, we have investigated the role of the purine 2-amino group in controlling the shape of the minor groove by evaluating Fis binding efficiency and DNA structures in Fis-bound complexes when guanine or inosine are substituted for adenine within the center of the binding site. Molecular dynamics simulations of free DNA targets with canonical and modified bases further demonstrate that sequence-dependent narrowing of minor groove widths is modulated almost entirely by the presence of purine 2- amino groups.

References:

[1] S. P. Hancock, T. Ghane, D. Cascio, R. Rohs, R. Di Felice, and R. C. Johnson, Nucl. Acids Res. (2013) in press.

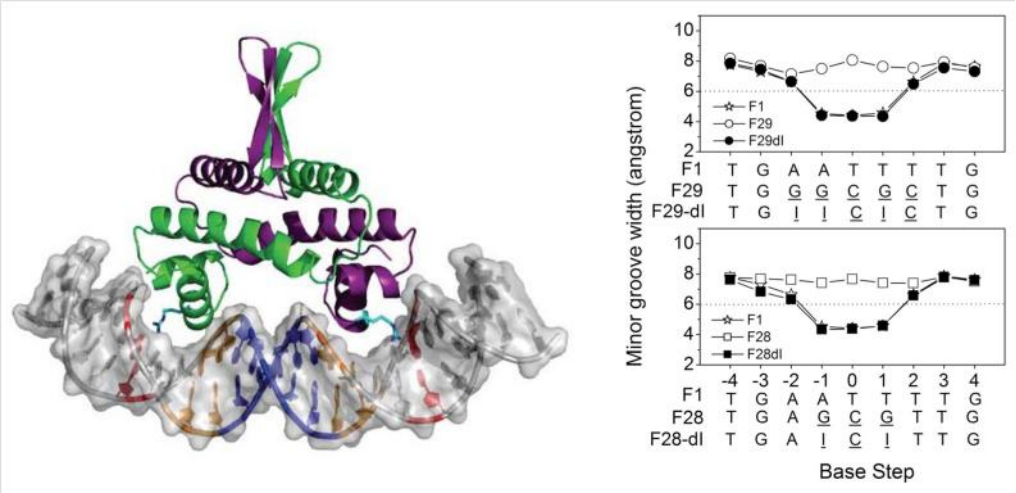


Fig. 1: Left: three-dimensional structure of the Fis-DNA complex resolved by X-ray. Right: minor groove widths from molecular dynamics simulations, which match the trends in the X-ray structures.

[P17] Electron transport properties of a redox molecule with a pH-dependent gate

A. Alessandrini[1,2], P. Petrangolini[1,2], and P. Facci[1]

[1] CNR Istituto Nanoscienze, S3, Modena
[2] Dipartimento di Scienze Fisiche Informatiche e Matematiche, Università di Modena e Reggio Emilia, Modena

Keywords: molecular electron transport, Electrochemical Scanning Tunneling Microscopy, electrolyte gating, pH gating.

The electron transport properties of the hydroquinone/benzoquinone redox couple have been investigated in the Electrochemical-Scanning Tunneling Microscopy (EC-STM) set-up. The redox couple at issue is characterized by an oxidation state variation which involves the transfer of two electrons and two protons. The electrochemical analysis of the redox couple in aqueous solutions shows that the intermediate state between the fully reduced and fully oxidized species is not stable, leading to only one reduction and only one oxidation waves, which involve the exchange of two electrons. When the transport properties of a single or a few hydroquinone molecules are studied by EC-STM, the electrolyte gating effect on the tunneling current is observed . Interestingly, the sweeping of the electrode potential on which the molecules are immobilized, while keeping the substrate/tip voltage bias constant shows the presence of two regions of tunneling current enhancement (Figure 1) [1,2]. This behavior is interpreted as related to the three redox states, even the intermediated one, of the redox molecule sandwiching the two metal electrodes.

A spectroscopic study of the molecular junction is performed both at constant tip/substrate bias and while sweeping the bias voltage to perform the classical I-V curves. According to different experimental conditions, transistor, Negative Differential Resistance (NDR) and switching properties are observed for the same molecular species. Moreover, the proton exchange involved in the redox reaction introduces a pH dependence for the regions of tunneling current enhancement, implementing a pH controlled gating effect.

References

[1] P. Petrangolini, A. Alessandrini, L. Berti, and P. Facci, J Am Chem Soc. 132 (2010) 7445-53.
[2] P. Petrangolini, A. Alessandrini, M. L. Navacchia, M. L. Capobianco, and P. Facci, J. Phys. Chem. C 115 (2011) 19971-19978.

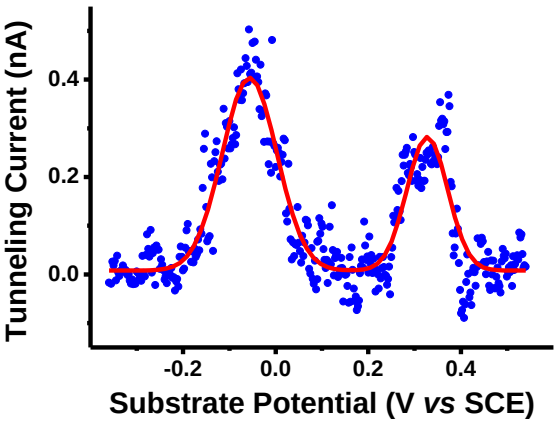


Fig. 1: Behavior of the tunneling current as a function of the substrate potential with respect to the reference electrode while keeping the tip/substrate bias voltage constant.

[P18] Applications of Magnetic Nanoparticles to Biomedicine

A. Lascialfari[1,2], M. Corti[3], T. Orlando[3], P. Arosio[1], and F. Orsini[1]

[1] Dipartimento di Fisica, Università degli studi di Milano, Milano, and INSTM, Milano, Italy
[2] Centro S3, CNR-Istituto Nanoscienze, Modena, Italy
[2] Dipartimento di Fisica, Università degli studi di Pavia, Pavia, and INSTM, Italy

In the last decade we studied novel multifunctional nanostructures based on magnetic nanoparticles (MNP) useful as agents for Magnetic Resonance Imaging, Optical Imaging and Magnetic Fluid Hyperthermia, carriers for drugs and molecular targeting vectors. Most of the systems that will be presented can be used mainly as MRI contrast agents and magnetic fluid hyperthermia mediators, where in the last case radio-frequency fields are used to produce heat on tumour cells, possibly inducing their death. Some other applications of novel systems based on MNP activated by different magnetic field effects and to be used in the field of (nano) medicine therapy and diagnosis, will be also briefly reported. Among these, magnetic field biosensors for detection of antibody-antigene (virus-antivirus, etc.) molecular interactions and the new system Sentimag® for detecting the sentinel lymphnodes will be briefly described.

[P19] Mechanisms of membrane penetration by peptides: insights from molecular dynamics simulations

R. Nifosì[1], F. Salomone[1,2] and F. Cardarelli[2]

[1] NEST, CNR-Istituto Nanoscienze and Scuola Normale Superiore Pisa, Italy
[2] Center for Nanotechnology Innovation @NEST, IIT, Pisa, Italy

Keywords: antimicrobial peptides, molecular dynamics simulations, cell penetrating peptides.

Peptides able to cross the cellular membrane are actively studied and designed as means to transport bioactive molecules (proteins, DNA/RNA, drugs) into the cytoplasm. Tat11, a HIV1 Tat derived peptide, is efficiently internalized by endocytosis. However, it undergoes entrapment in the endosome (a membrane bound compartment participating in the endocytic pathway from the membrane to the lysosome) and subsequent metabolic degradation. The fusion of Tat11 with an antimicrobial peptide (CM18, a cecropin mellitin hybrid peptide) promotes escape from the endosome while preserving internalization [1]. The mechanisms by which CM18 and the analogous 3-aa shorter CM15 interact with the membrane were investigated by molecular dynamics simulations in the presence of explicit bilayers, formed either by pure POPC lipids or by a mixture of POPC and POPG. These two membrane models mimic respectively the eukaryotic and the bacterial membrane. The interaction with the bilayer was evaluated at changing peptide/lipid ratio (1, 2 or 3 peptide copies and 128 lipids) and with different force fields, the all-atom Charmm36 and the united-atom Gromos54A7. Thanks to their detailed description, MD simulations afford an invaluable window into peptide/membrane interactions and a precious tool for the design of novel cell-penetrating peptide sequences.

References:

[1] F. Salomone, F. Cardarelli, M. Di Luca, C. Boccardi, R. Nifosì, G. Bardi, L. Di Bari, M. Serresi, and F. Beltram, J Control Release 163 (2012) 293.

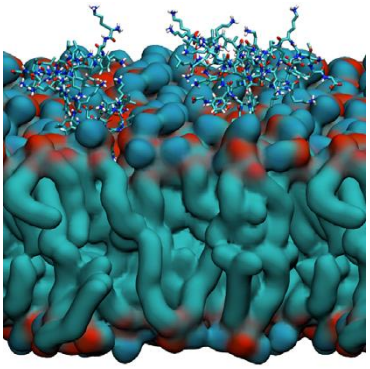


Fig. 1: Snapshot from a molecular dynamics simulation showing CM18 peptides interacting with a POPC bilayer.

[P20] NMR Investigation of Spin Dynamics in Maghemite-Gold Nanoparticles

A. Capozzi[1], T. Orlando[2], M. Mariani[3], E. Umut[4], F. Pineider[5], C. Sangregorio[5], M. Corti[3], F. Tabak[4], A. Lascialfari[3,6], and P. Ghigna[7]

[1] Institute of Physics of Biological Systems, EPFL, Lausanne, Switzerland
[2] Dipartimento di Fisica, Università degli Studi di Pavia, and Consorzio INSTM, Italy
[3] Dipartimento di Fisica e Astronomia, Università di Bologna, Italy
[4] Physics Engineering Department, Hacettepe University, Beytepe-Ankara, Turkey
[5] Dipartimento di Chimica, Università di Firenze and Consorzio INSTM, Italy
[6] Dip. di Fisica, Università degli Studi di Milano, Consorzio INSTM and CNR-S3, Istituto Nanoscienze, Italy
[7] Dipartimento di Chimica, Università degli Studi di Pavia, and Consorzio INSTM, Italy

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 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÷300 K, for two different magnetic fields, H=0.65 T and H=1.65 T. 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.

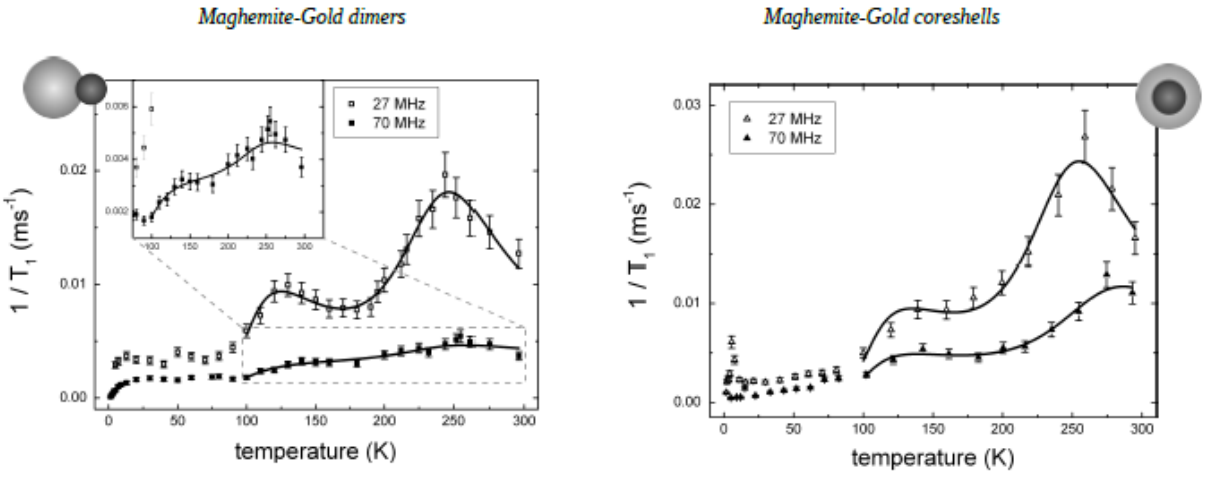
We can explain this behaviour by taking into account three different contributions to the spectral spin density, each one following the Bloemberger-Purcell-Pound (BPP) equation and characterized by a specific correlation time (τ_c). Indeed, we hypothesize that: the peak at high temperatures is associated 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, whilst of still unclear origin, could be related to the surface spins dynamics (τ_c^{SSD}).

Therefore, our heuristic model can be written as:

$$\frac{1}{T_1} = A\frac{\tau_c^{rot}}{1+(\tau_c^{rot})^2\,\omega_L^2} + B\chi T\left(\frac{\tau_c^{SPM}}{1+(\tau_c^{SPM})^2\,\omega_L^2} + C\frac{\tau_c^{SSD}}{1+(\tau_c^{SSD})^2\,\omega_L^2}\right)$$

where ω_L is the proton Larmor frequency and *A, B, C* are arbitrary constant. For the *SPM* and the *SSD* peaks, the spectral density is multiplied by the effective magnetic moment of the nanoparticles, χT, which represent the static contribution to the nuclear relaxation rate.

Cariplo Foundation (Project no. 2010-0612) is thanked for funding the research.



[P21] Uptake of imatinib-loaded polyelectrolyte nanocomplexes for sustained targeting of BCR-ABL+ leukemia stem cells

I. E. Palamà[1*], A. M. L. Coluccia[2], S. D'Amone[1], and G. Gigli[1,3,4]

[1] NNL, Institute of Nanoscience CNR, Lecce, ITALY
[2] Hematology and Clinical Proteomics Unit, "Vito Fazzi" Hospital, University of Salento, ITALY
[3] Dipartimento di Matematica e Fisica "Ennio De Giorgi", University of Salento, Lecce, ITALY
[4] Center for Biomolecular Nanotechnologies (CNB) of IIT, Arnesano (Le), ITALY
*ilariaelena.palama@nano.cnr.it

Keywords: Chronic myeloid leukemia, Imatinib mesylate, Polyelectrolyte complexes, PEC, nanoscale delivery carriers.

Introduction. The chimeric oncoprotein BCR-ABL by the Philadelphia chromosome, Ph) is an ideal target for molecular targeted therapy, because it is expressed only in primitive CD34+ hematopoietic stem cells which cause Chronic Myeloid Leukemia (CML) in humans. Imatinib mesylate (IM, STI571, Gleevec/Glivec) is a small-molecule drug that selectively binds to the ABL tyrosine kinase ATP-binding site, thus preventing the constitutive autophosphorylation of BCR-ABL and, in turn, the aberrant activation of its downstream signaling substrates. The current recommendations for CML state a lifelong continuance of therapy with IM, as the drug minimally affects the viability of primitive CML stem cells, whilst it efficiently eradicates all BCR-ABL+ mature blood cells. This commonly leads to IM dose escalation or early disease relapses when therapy is stopped or discontinued in CML resistant/refractory patients. Other concerns regarding the potential risk of adverse effects with long-term treatment with IM and issues of non-compliance have refocused the interest of researchers towards micro/nanoscaled delivery carriers to increase drug's retention effects and anti-leukemic activity in viable residual CML-initiating cells. At this regard, we previously validated IM-loading into biodegradable carriers [1,2] based on hollow polyelectrolyte microcapsules with an average diameter of 3 μm (PMC) as a feasible, safe and effective purging agents to aid CML stem cell eradication from patient-derived blood specimens.

Materials & Methods. We tested how and whether the particle size could impact the uptake modality and therapeutic index of IM in CML-patient derived stem/myeloid cells, by using novel polyelectrolyte nanocomplexes (PEC) with average diameters of 250 nm obtained via electrostatic interactions between dextran sulphate (DXS) and poly(allylamine hydrochloride) (PAH) as model carriers for IM [3].

Results & Discussion. The nanoscale complexes (PEC) were effective in promoting a permanent BCR-ABL kinase inactivation that is mandatory to eradicate quiescent CML stem cells, at about 2-fold lesser intracellular IM dose compared with their microscale (PMC) counterpart.

Conclusion. IM-loaded PEC can be used as a highly efficient delivery device for overcoming inherent drug resistance of CML stem cells ex vivo, through a long-acting and irreversible blockage of BCR-ABL oncogenic activity at sub-therapeutic dosages of freely-soluble IM as single agent.

References:

[1] I. E. Palamà *et al.*, Nanomedicine, 5(3) (2010) 419-431.
[2] I. E. Palamà *et al.*, Science of Advanced Materials 2 (2010) 1-9.
[3] I. E. Palamà *et al.*, Journal of Drug Delivery 1-7 (2011).

[P22] Classical atomistic simulations of azobenzene-based self-assembled monolayers

S. Pipolo, E. Benassi, G. Brancolini, and S. Corni

CNR Nano S3 Center Via Campi 213/A, 41125 Modena, Italy

Keywords: azobenzenes, self-assembling monolayers, force field parameterization.

The possibility of performing controlled movements of nano-sized objects is one of the more fascinating target of nanotechnology, not only as a proof of principle but mostly for the high potential at the application level. The design of a nanoscopic system capable to trans-form radiative energy into mechanical work [1] has engaged the mind of scientists of different research areas in the last decades. Self Assembling Monolayers (SAMs) of Azobenzene molecules are an example of such photomechanic nanostructures that employ an efficient cis/trans photoisomerization that is controlled by UV and visible light [2].

Accordingly they can be exploited to set up tools performing light driven motion of nano-sized objects [3]. A classical Molecular Dynamics study of the Azobenzene SAMs is presented and discussed, based on a dedicated force field developed using ab-initio Potential Energy Surfaces [4]. Different aspects are investigated, ranging from the structure of the SAMs [5] to their wettability [6] and stiffness [7] properties. Besides, the work presented here shows the usefulness and the reliability of classical force field simulations with ab-initio parametrized potentials, providing a detailed description of a set of physical properties of the studied systems in line with experimental data. Furthermore it opens new perspectives on future computational investigations on the azobenzene based SAMs in the field of nanomechanics.

References:

[1] T. Hugel, N. Holland, A. Cattani, L. Moroder, M. Seitz, and H. Gaub, Science 296 (2002) 1103.
[2] G. Pace, V. Ferri, C. Grave, M. Elbing, C. Von Hänisch, M. Zharnikov, M. Mayor, M. Rampi, and P. Samorì, PNAS 104 (2007) 9937.
[3] V. Ferri, M. Elbing, G. Pace, M. Dickey, M. Zharnikov, P. Samorì, M. Mayor, and M. Rampi, Angew. Chem. 120 (2008) 3455.
[4] S. Pipolo, E. Benassi, G. Brancolini, M. Val ´ ˇek, M. Mayor, and S. Corni, TCAC 131 (2012) 1.
[5] S. Pipolo, E. Benassi, and S. Corni, (2013) in preparation.
[6] S. Pipolo and S. Corni, (2013) in preparation.
[7] E. Tirosh, E. Benassi, S. Pipolo, M. Mayor, M. Valsek, V. Frydman, S. Corni, and S. Cohen, Beil. J. Nanotech. 2 (2011) 834.

[P23] Visualizing electron correlation in molecules using a scanning tunneling microscope: An ab initio prediction

M. Rontani, D. Toroz, and S. Corni

CNR-NANO Research Center S3, Via Campi 213A, 41125 Modena, Italy

Keywords: Scanning tunneling spectroscopy, molecular imaging, ab-initio calculations, post-Hartree-Fock methods, coordination complexes.

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 (see fig. 1). 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.

References:

[1] J. Repp, G. Meyer, S. M. Stojkovic, A. Gourdon, and C. Joachim, Phys. Rev. Lett. 94 (2005) 026803.
[2] M. Rontani and E. Molinari, Phys. Rev. B 71 (2005) 233106; M. Rontani, Nature Mat. 10 (2011) 173.
[3] D. Toroz, M. Rontani, and S. Corni, J. Chem. Phys. 134 (2011) 024104; Phys. Rev. Lett. 110 (2013) 018305.

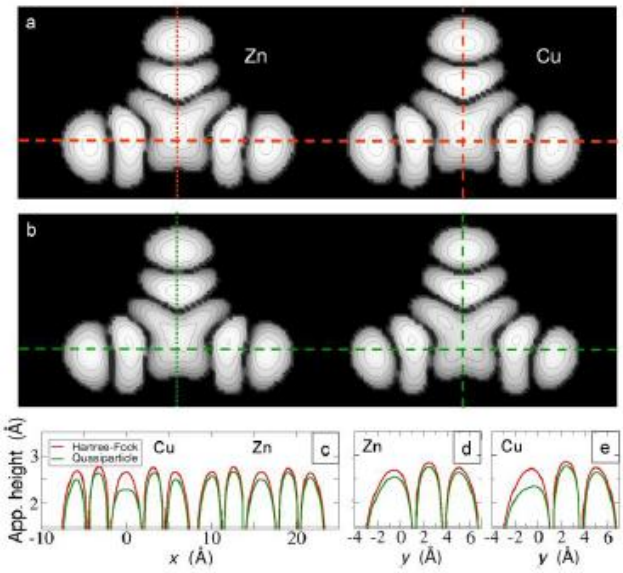


Fig. 1: Calculated STS images of positively ionized zinc-saloph and copper-saloph in the constant-current mode. Contour plot images of (a) Hartree-Fock highest occupied molecular orbitals and (b) quasiparticle wave functions (i.e., including many-body effects) in the xy plane. Slices of the Hartree-Fock (red curves) and quasiparticle (green curves) images obtained along the (c) horizontal and (d-e) vertical dashed lines shown in panels a and b. As shown by the map slices, copper- and zinc-saloph share the same morphology but only copper-saloph changes at the many-body level. Therefore, the comparison between the molecular images provides the experimental means to uncover the many-body effect.

[P24] The interaction of nucleic acid bases with the Au(111) surface

M. Rosa, S. Corni, and R. Di Felice

Center S3, CNR Institute of Nanoscience, Via Campi 213/A, 41125 Modena, Italy

Keywords: DNA, gold, adsorption, DFT, vdW.

The fate of an individual DNA molecule when it is deposited on a hard inorganic surface in a "dry" environment is unknown, while it is a crucial determinant for nanotechnology applications of nucleic acids. In the absence of experimental approaches that are able to unravel the three- dimensional atomic structure of the target system, here we tackle the first step towards a computational solution of the problem. By using first-principles quantum mechanical calculations of the four nucleobases on the Au(111) surface, we propose a simple force field that will enable classical simulations of DNA on Au(111) to investigate the structural modifications of the duplex in these non-native conditions. Furthermore, we fully characterize each system at the individual level. We find that van der Waals interactions are crucial for a correct description of the geometry and energetics. However, the mechanism of adsorption is well beyond pure dispersion interactions. Indeed, we find charge transfer between the substrate and the adsorbate, the formation of hybrid orbitals and even bonding orbitals. Yet, this association is qualitatively distinct from the thiol adsorption mechanism [1,2]: we discuss such differences and also the relation to the adsorption mechanism of pure aromatic molecules.

Thanks to quantum mechanical results, we were able to parametrize a force field suitable for molecular dynamics calculations of more complex DNA structures adsorbed on gold. To verify our method and the results obtained, we make a comparison between DFT, MD and experimental results on DNA bases monolayers adsorbed on Au(111) and we were able to find a remarkable agreement.

References:

[1] M. C. Vargas, P. Giannozzi, A. Selloni, and G. J. Scoles, Phys. Chem. B 105 (2001) 9509.
[2] R. Di Felice, A. Selloni, and E. Molinari, J. Phys. Chem. B 107 (2003) 1151.

[P25] Detecting entanglement in molecular nanomagnets

I. Siloi[1,2] and F. Troiani[1]

[1] S3-Istituto Nanoscienze-CNR, 41125 Modena, Italy
[2] FIM, Università di Modena e Reggio Emilia, 41125 Modena, Italy

Keywords: entanglement, molecular nanomagnets.

Molecular nanomagnets (MNs) represent a varied class of spin systems, whose physical and structural properties can be tailored by chemical synthesis. This – together with quantum coherence at low temperature – makes these systems an ideal test bed for generating quantum entanglement [1]. In spite of these potentialities, entanglement in MNs is still a largely unexplored subject. Here we theoretically show how the introduction of a spin impurity, in homometallic molecules, induces a clear oscillatory dependence of spin-pair entanglement as a function of position. Besides, the amplitude and phase of the oscillations display a clear dependence on the specific magnetic impurity (see Figure 1) [2]. This suggests that (suitably combined) chemical substitutions can be an effective means to engineer entanglement in MNs [3]. The above features persist at finite temperature, where they can be effectively detected by the exchange energy of individual spin pairs. These quantities are now experimentally accessible through inelastic neutron scattering [4]. Quite remarkably, exchange energy allows to detect also multipartite (*k*-spin) entanglement. Applying a recently developed method [5], we establish the threshold temperatures for *k*-spin entanglement in clusters of arbitrary spins, and highlight the dependence of multipartite entanglement on the chemical substitution [6].

References:

[1] F. Troiani *et al.*, Nanotechnology 21 (2010) 274009.
[2] I. Siloi and F. Troiani, Phys. Rev. B 86 (2012) 224404.
[3] G. Lorusso *et al.*, Phys. Rev. B 86 (2012) 184424.
[4] M. L. Baker *et al.*, Nat. Phys 8 (2012) 906-911.
[5] F. Troiani and I. Siloi, Phys. Rev. A 86 (2012) 032330.
[6] I. Siloi and F. Troiani, submitted.

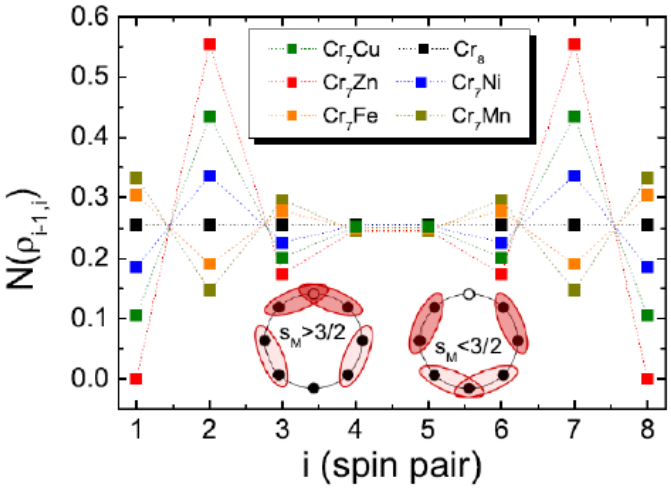


Fig. 1: Negativity of neighboring spin pairs in Cr_7M rings (M=Cu,Zn,Fe,Ni,Mn). The values refers to the ground state of antiferromagnetic spin Hamiltonian. The inset shows a pictorial representation of the entanglement localization induced by the defect M: the shaded area highlight the most entangled spin pairs.

[P26] The role of linker in Charge Transfer process in DNA-gold interface

W. Sun, A. Ferretti, G. Brancolini, S. Corni, and R. Di Felice

CNR Institute of Nanoscience, S3 Center, Via Campi 213/A, 41125 Modena, Italy

Keywords: vdw-DF, Charge transfer, DNA, gold surface.

Experimentally, the strategy of attaching thiol groups directly to the nucleic acid backbone in order to have an efficient electrical contact was mostly unsuccessful, probably due to the electrostatic repulsion between the negatively charged DNA and the negatively charged electrode surface. Thus, alkyl chains had to be used. On the other hand, PNA (peptide nucleic acid), with its neutral peptide backbone, can in principle act as a direct linker when a cysteine residue terminates the chain. Herein, we report on van der Waals corrected density functional calculations to disclose the role of the length and chemistry of the linker in the realization of the guanine-gold contact. We have investigated two linkers, namely a cysteine that terminates the N-(2- aminothyl)-glycine chain in a PNA-like guanine and alkane (CH2)3 molecule that terminates a ribose sugar backbone. We find that the first flexible linker could make the interface more stable and generate large charge transfer from the gold surface to guanine, compared with the its alkane counterpart. After replacing guanine with the size-expanded guanine (xG4), both the binding energy and amount of charge transfer significantly increase, due to the expanded π conjugation. Interestingly, the lowest unoccupied molecular orbital (LUMO) moves downward across the Fermi level after adsorption as a consequence of introducing the two NH- groups in spacer ring.

References:
[1] B. Xu, P. Zhang, X. Li, and N. Tao, Nano Letters 4 (6) 1105.
[2] H. Cohen, C. Nogues, R. Naaman, and D, Porath, Proc. Natl. Acad. Sci. USA 102 (33) 11589.
[3] W. Sun and R. Di Felice. J. Phys. Chem. C 116 (47) 24954.

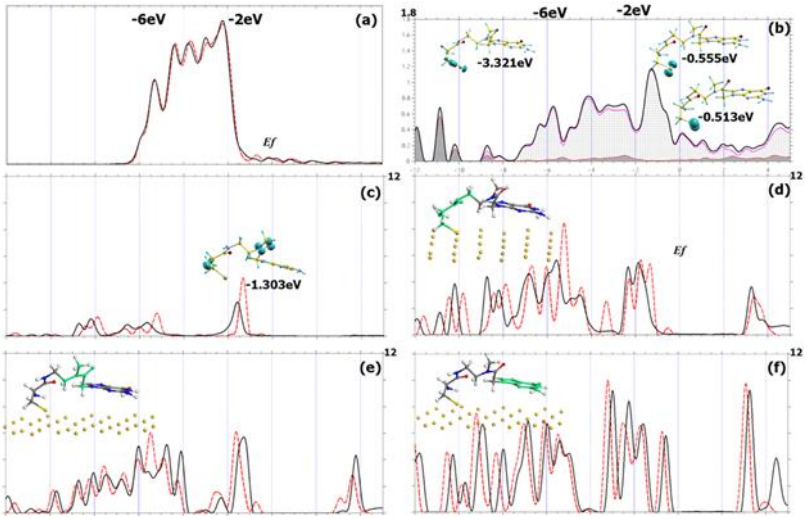


Fig. 1: PDOS of pn-G/Au(111) interface. Selected parts are highlighted in green in the inserts. In all panels, red and black lines represent the PDOS before and after adsorption, respectively. The Fermi level is aligned with the origin of the energy scale.

[P27] Interaction of neural cells with nanotopographies: from mechanotransduction in nerve regeneration to neurite contact guidance in patho-physiological models

I. Tonazzini[1], E. Jacchetti[1], S. Meucci[1], G. M. Van Woerden[2], S. Raimondo[3], S. Geuna[3], Y. Elgersma[2], F. Beltram[1], and M. Cecchini[1]

[1] NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, 56127 Pisa, Italy
[2] Department of Neuroscience, Erasmus Medical Center, 3015AA Rotterdam, the Netherlands
[3] Neuroscience Institute of the Cavalieri Ottolenghi Foundation, University of Turin, 10043 Orbassano, Italy

Keywords: mechanotransduction, nanotopography, contact guidance, neurite, neuronal differentiation.

Controlling neuronal cell adhesion, migration and axonal outgrowth via contact interactions with biomaterials is a critical element for tissue engineering applications and for developing artificial neuronal interfaces. To this end, one promising approach relies on the exploitation of nanostructured surfaces, which were demonstrated to be capable of tuning neural differentiation, polarity, migration and neurite orientation.
By nanoimprint lithography techniques, we engineered biocompatible plastic nanogratings (NGs), anisotropic topographies composed by alternating lines of grooves and ridges with submicrometer lateral dimension, suitable for high-resolution microscopy. NGs with different line-widths (0.5-10 5m), depths (0.35-2.5 5m) and directionalities were produced to investigate the molecular processes regulating mechano-transduction in different types of neural cells, from PC12 and human neuroblastoma SH-SY5Y differentiating cells to primary hippocampal neurons and glial cells.
Neuronal mechano-transduction was studied as axon guidance and its tolerance to nanotopographical noise, in a PC12 neuronal model: topographical signal integration is determined by focal adhesion (FA) sensing and it is enhanced by increasing cell contractility. Specifically, by total-internal-reflection-fluorescence (TIRF) microscopy we demonstrated a non-linear behavior of axon guidance vs. substrate directionality correlating with FA shaping.
SH-SY5Y-cell contact guidance was studied in proliferating conditions and after differentiation with RA/BDNF. Our results demonstrate that SH-SY5Y can effectively retrieved substrate topographical signals, in particular during differentiation: RA/BDNF improved the responsiveness of tubulin cytoskeleton organization to NG directional cues, significantly enhancing cell alignment.
NGs were coupled with Wild-Type (WT) and Ubiquitin ligase E3a (Ube3a)-KO primary mouse hippocampal neurons (a model for a neurocognitive disorder, Angelman syndrome). We found impaired mechanotransduction in Ube3a-KO neurons, which is in agreement with the hypothesis that the loss of Ube3a would result in abnormal neuronal micro-connectivity leading to pathological neuronal plasticity.
We finally studied Schwann cell migration as a function of substrate directionality. We measured single-cell migration response to nanotopographies by time-lapse microscopy, in order to found optimal scaffold geometry to enhance nerve regeneration. Overall, our data shows that directional nanotopographies can induce similar effects on neurite cytoskeleton organization and network growth in several neuronal models in vitro, according to their periodicity and cell characteristics. These results might help the rational engineering of neuro-regenerative scaffolds to improve peripheral nerve wound healing as well as to investigate the basic mechanisms of neuronal wiring.

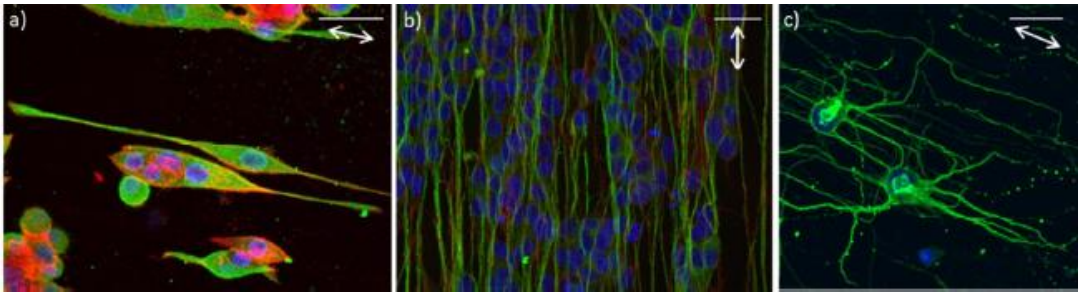


Fig. 1: Confocal images of different neuronal models cultured on NGs. PC12 (**a**), SH-SY5Y (**b**) and mouse hippocampal (**c**) neuronal cells grown on 500nm-ridge NGs and immunostained for βIII-tubulin (*green*), actin (*red*) and nuclei (*blue*); scale bars = 30 μm; white arrows = NG direction.

[P28] A platform for Multi-Scale bio-molecular systems modeling

V. Tozzini[1,2], F. Trovato[1,2,3], G. Maccari[3], G. Spampinato[1], F Tavanti[1], P Mereghetti[3], and R Nifosi[1,2]

[1] NEST - Istituto Nanoscienze - Cnr Pisa, Italy
[2] Scuola Normale Superiore, Pisa, Italy
[3] CNI@NEST, Istituto Italiano di Tecnologia, Pisa, Italy

Keywords: Molecular Dynamics Simulations, QM/MM, Coarse Grained models, Bioinformatics, Biological macromolecules.

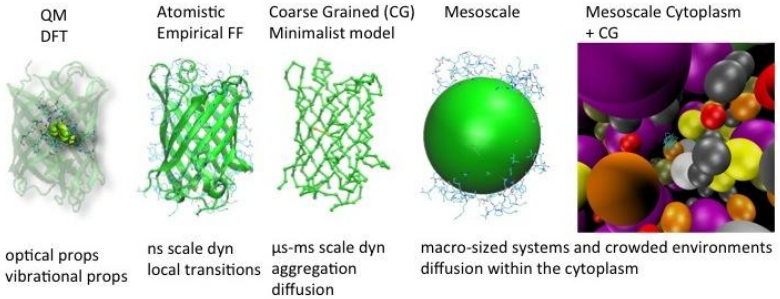
The biological matter has an intrinsic hierarchical organization, spanning ~10-15 orders of magnitude in the size and time domains, from the ultra-fast reactions localized in active sites, to the macroscopic level (cells or organs). Therefore, bio-systems modelers are often forced to adopt different approaches representing a given system to different levels of resolution. These are typically the atomistic level (with (QM) or without (MM) explicit electrons), super-atomistic (Coarse Grained, CG, or mesoscale, MS), and continuum approaches (e.g. for the solvent, for the membranes or eventually for the particles fluxes). These are used either "in parallel" in the same simulation of a given system (as in the QM/MM approach), or "serially", in separate simulations. In either cases a specific effort is necessary to maintain the coherency between the representations, which involves the parameterization of the "coarser" levels, the reconstruction of the "finer" structures from the coarser, and in general exchange of coordinates, velocities and forces along the simulations.

In the course of the last years we have been involved in solving a number of tasks related to the multi-scale modeling: we developed GC[2,3] and MS[4] models for proteins and nucleic acids[5,6] and strategies for their parameterization [7,8]; finally, we combined atomistic and CG-MS representations in "parallel" approaches [4,9]. All of these tasks have involved programming proprietary codes or modifying open source existing ones. E.g., the CG and MS models dynamics was implemented within the multi-purpose code DL_POLY[10]. The ensemble of these codes constitutes a package, which covers basically all the tasks of multi-scale simulations. However it is difficult to distribute, because it lacks a unitary organization. In addition, only a small part of the codes has a web graphical interface.

In this presentation we aim to show the structure of this package, i.e. the function, connections and dependencies of the different codes among each other. We also indicate the strategy to build a unitary graphical interface that would make this package user friendly and easily distributable.

References:

[1] V. Tozzini, Accounts Chem Res 43 (2010) 220.
[2] V. Tozzini, Quart Rev Biophys 43 (2010) 333-371.
[3] F. Trovato and V. Tozzini, AIP Conf. Proc. 1456 (2012) 187-200.
[4] F. Trovato and V. Tozzini, A meso-scale model for the Cytoplasm of Escherichia Coli in preparation.
[5] F. Trovato and V. Tozzini, J Phys Chem B (2008).
[6] F. Leonarski, F. Trovato, V. Tozzini, and J. Trylska, Abs of the Papers of the ACS 241 (2011) 285-COMP.
[7] F. Leonarski, F. Trovato, V. Tozzini, and J. Trylska, Proc EvoBIO'11, 6623 (2011) 147-152.
[8] G. Spampinato, G. Maccari, and V. Tozzini, Selection and statistical analysis of secondary structures in Proteins Data Bases in preparation.
[9] F. Tavanti and V. Tozzini, A multi-scale and multi-stable model for the photocyle of rhodopsins, in preparation.
[10] DL_POLY http://www.stfc.ac.uk/CSE/randd/ccg/software/DL_POLY/25526.aspx.



[P29] Nuclear-induced decoherence of chirality qubits

F. Troiani[1], D. Stepanenko[2], and D. Loss[2]

[1] S3-Istituto Nanoscienze-CNR, 41125 Modena, Italy
[2] University of Basel, Basel, Switzerland

Keywords: decoherence, chirality, molecular nanomagnet.

Molecular nanomagnets represent a varied class of spin clusters, whose physical properties can be extensively engineered by chemical synthesis. This makes them a potential alternative to other spin systems for the implementation of spin-cluster qubits. While most of the attention has been so far focused on the use of the total-spin projection (Sz) as a computational degree of freedom, it has been recently realized that alternative encodings would enable the use of electric—rather than magnetic—fields for the qubit manipulation [1,2]. In particular, transitions between states of opposite spin chirality (Cz) can be induced, with estimated gating times τg in the ns range.

In order to assess the suitability of spin chirality for applications in quantum-information processing, τg has to be contrasted with a characteristic decoherence time τd. Here we theoretically estimate the characteristic time scale of hyperfine-induced decoherence, and investigate its dependence on the qubit encoding within a prototypical spin-cluster qubit, consisting of an antiferromagnetic spin triangle, coupled to a bath of nuclear spins. In particular, we consider three different encodings, based on Sz, Cz, and the partial spin sum S12, whose value—as that of Cz—can be controlled through spin-electric coupling. Values of the decoherence times approaching the ms are found for the spin chirality. S12 is instead characterized by decoherence times comparable to those of the total-spin projection. We conclude that an effective decoupling of the molecular spin cluster from the nuclear spin bath requires the logical states to be indistinguishable both in terms of the total- and of the individual-spin expectation values.

References:

[1] M. Trif, F. Troiani, D. Stepanenko, and D. Loss, Phys. Rev. Lett. 101(2008) 217201.
[2] M. Trif, F. Troiani, D. Stepanenko, and D. Loss, Phys. Rev. B 82 (2010) 045429.
[3] F. Troiani, D. Stepanenko, and D. Loss, Phys. Rev. B 86 (2012) 161409(R).

[P31] Modeling electron transfer between Cytochrome c and a gold electrode: a perturbative approach

L. Zanetti-Polzi[1], A. Amadei[2], M. Aschi[3], I. Daidone[3], and S. Corni[1]

[1] Center S3, Institute of Nanoscience – CNR, Modena, Italy
[2] Dipartimento di Scienze e Tecnologie Chimiche, University of Rome "Tor Vergata", Rome, Italy
[3] Dipartimento di Scienze Fisiche e Chimiche, University of L'Aquila, Coppito (AQ), Italy

Keywords: Electron transfer, Cytochrome c, gold electrode, Perturbed Matrix Method.

Electron transfer (ET) reactions are key events in the energy transduction pathways in living organisms, where they play a central role in a variety of fundamental biological processes [1,2]. Moreover, ET proteins immobilized on electrode surfaces can be used as active constituents in bioelectronic devices of actual importance for biotechnological applications [3]. However, for rational design of such devices, a deeper insight into the molecular processes of immobilized proteins is required. In this framework, the coupling of experimental and simulation techniques, providing dynamical information at the molecular level, is a promising approach to attain deeper knowledge of such biological processes. Nevertheless, a reliable modeling of chemical reactions taking place in complex systems is one of the challenges of theoretical chemistry and biophysics. The primary difficulty is represented by the need of maintaining the electronic detail of the chemical reaction within a configurationally complex atomistic environment. Mixed quantum mechanics/ molecular dynamics (QM/MD) methodologies are commonly used to model complex system and, among others, a QM/MD theoretical-computational approach based on the perturbed matrix method [4,5] was recently used to model ET reactions in complex systems [6,7].

In PMM calculations, similarly to other QM/MM procedures, a portion of the system to be treated at electronic level is predefined (the quantum center, QC), with the rest of the system described at a classical atomistic level exerting an electrostatic perturbation on the QC electronic states. The essence of PMM is to use high-quality unperturbed electronic states as a basis set to express the Hamiltonian matrix of the quantum center including the electric field perturbation resulting from the atomic environment. With a relatively low computational cost, the PMM can be therefore applied to a very large set of molecular configurations.

The aim of the work we are currently carrying on, is to use the PMM to model the ET reaction between yeast iso-1-cytochrome c (YCC) and a gold electrode. YCC is generally considered to be a suitable candidate for bioelectronic applications since it contains a single surface cysteine residue that can be exploited for specific tethering, ensuring unique orientation of the protein. Recently, YCC has been covalently bound on bare glod surfaces via Cys102, obtaining a fast and reversible ET with retention of protein functionality [8]. By means of molecular dynamics simulations and PMM calculations, the reduction potential of YCC interactiong with a gold surface can be calculated and compared to previous results on cyt c in water obtained with the same methodology [9]. These results could be able to clarify the ET reaction between proteins and electrodes at the molecular level, gaining insight into such a complex biological process with very interesting technological fallouts.

References:

[1] C. C. Moser, J. M. Keske, K. Warncke, R. S. Farid, and P. L. Dutton, Nature 355 (1992) 796.
[2] H. B. Gray and J.R. Winkler, Q. Rev. Biophys. 36 (2003) 341.
[3] R. R. Birge, “Molecular and Biomolecular Electronics”, Oxford University Press (New York, 1994).
[4] M. Aschi, R. Spezia, A. Di Nola, and A. Amadei, Chem. Phys. Lett. 344 (2001) 374.
[5] A. Amadei, I. Daidone, A. Di Nola, and M. Aschi, Curr. Opin. Struct. Biol. 20 (2010) 155.
[6] M. D'Abramo, M. Aschi, and A. Amadei, Phys. Chem. Chem. Phys. 11 (2009) 10614.
[7] A. Amadei, I. Daidone, and M. Aschi, Phys. Chem. Chem. Phys. 14 (2012) 1360.
[8] H. A. Heering, F. G. M. Wiertz, C. Dekker, and S. de Vries, J. Am. Chem. Soc. 126 (2004) 11103.
[9] C. A. Bortolotti, A. Amadei, M. Aschi, M. Borsari, S. Corni, M. Sola, and I. Daidone, J. Am. Chem. Soc. 134 (2012) 13670.

[P32] Towards triplex-based intracellular pH biosensors based on self-assembled DNA nanostructures

P. Angelini[1], C. Bergamini[2] , K. J. Rhoden[2,3], R. Fato[1,2], A. M. Porcelli[1,2], and G. Zuccheri[1,2,4]

[1] Department of Pharmacy and Biotechnologies at the University of Bologna, Via Belmeloro, 6 40126 Bologna, Italy
[2] Interdepartmental Center for Industrial Research on Life Science and Technologies at the University of Bologna, Italy
[3] Department of Medical and Surgical Sciences at the University of Bologna, Italy
[4] Institute of Nanosciences of the National Research Council (CNR-NANO), S3 Unit, Italy

Keywords: DNA Nanostructures, biosensors, self-assembly, live-cell imaging, single-cell measurements.

There is a significant interest in extending the tools of single-cell biology, towards studying the complex phenomena that take place in a live human cell without the need to disrupt the cell or to extract single-cell results from the behavior of a cell population.

Recently, a few research groups have showed that it is possible to introduce self-assembled DNA nanostructures in live cells without significantly disrupting their viability [1-3]. Furthermore, it was showed that such nanostructures can be taken up by the cells spontaneously, even without the need to deliver them, so enabling the minimal possible perturbation of the cell physiology.

The ability to design DNA-based nanostructures leads to the possibility to introduce multiple functionalities on them. As these groups showed, dynamic nanostructures have been inserted in live cells: their design yielded a conformation change that can take place in the presence of an analyte [3]. Such dynamic behavior turns the DNA nanostructure into a logic gate or possibly into a biosensor, which can then be introduced in a live cell and lead to intracellular sensing. If the conformational change leads to a change in the fluorescence properties of the nanostructure, the sensing can then be performed non-destructively and in real-time. It is nowadays possible to devise a number of possible chemical and biochemical sensing elements based on DNA or proteins that could be used to enhance such DNA-based nanostructures.

Some time ago, we devised a simple DNA nanoswitch that can respond dynamically to a change in the pH of the solution [4]. Its structure can switch between a double and a triple DNA helix, leading to a change in size and compaction that can also be made to lead to a change in fluorescence emission, upon proper decoration with fluorophores. Such nanodevice can respond within a fraction of a second to a change in pH across its transition point. We have also showed that such nanodevice can function and be detected at very high dilution, all the way to the single-molecule level [4-5].

We here report on the design and experiments towards developing a DNA nanoswitch with a conformational transition across pH=7. This switch is then introduced in a DNA-based nanosized tetrahedron, so that this structure can work as a nanosized pH sensor that can be then introduced in a small population of cells. It would then be possible to measure the intracellular pH in live cells and follow its evolution in real-time. We have been performed preliminary experiments in order to characterize the cellular uptake of the DNA tetrahedrons on different cell lines. A relevant question to be answered is the intracellular localization and life-time of such nanodevices, as this would significantly affect their usefulness in research.

References:

[1] A. S. Walsh, H. F. Yin, C. M. Erben, M. J. A. Wood, and A. J. Turberfield, Acs Nano 5 (2011) 5427.
[2] J. Li, H. Pei, B. Zhu, L. Liang, M. Wei, Y. He, N. Chen, D. Li, Q. Huang, and C. H. Fan, Acs Nano 5 (2011) 8783.
[3] H. Pei, L. Liang, G. B. Yao, J. Li, Q. Huang, and C. H. Fan, Angewandte Chemie-International Edition 51 (2012) 9020.
[4] M. Brucale, G. Zuccheri, and B. Samorì, Org Biomol Chem 3 (2005) 575.
[5] B. Kolaric, M. Sliwa, M. Brucale, R. A. L. Vallee, G. Zuccheri, B. Samori, J. Hofkens, and F. C. De Schryver, Photochemical & Photobiological Sciences 6 (2007) 614.

[P33] Graphene-mediated exchange coupling between cobaltocene and magnetic surfaces

S. Marocchi[1,2], P. Ferriani[3], N. M. Caffrey[3], S. Heinze[3], F. Manghi[1,2], V. Bellini[2,4]

[1] Dipartimento di Fisica, Università di Modena e Reggio Emilia, Modena, Italy
[2] CNR – Istituto di Nanoscienze – S3, Modena, Italy
[3] Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany
[4] CNR—Istituto di Struttura della Materia, sede distaccata di Trieste, Italy

Keywords: magnetic molecules, exchange interactions, graphene.

The ability to improve the current electronic devices appear to be increasingly connected with the development of the molecule-based electronics [1] and spintronics [2]. Among the molecules which exhibit magnetic properties, metallocenes, i.e. MCp2, where M= metal ion and Cp= cyclopentadienyl ring, offer a case study to perform systematic investigations, and experiments attempting to deposit intact metallocenes on metal surfaces could be found in the literature [3].

We have concentrated our study, employing state-of-the-art density-functional theory calculations, on the structural and magnetic properties of the Cobaltocene (CoCp2) adsorbed on graphene deposited on slab of Ni(111). This molecule has been chosen because of its electronic structure rather unique among the metallocenes [4]. In its ground state a single electron can go, according to the Jahn-Teller effect, in one of the two orbitals dyz and dxz, producing respectively the two states 2A2 or 2B2 [5]. The slightly distorted geometry of these two states produces very different magnetic density distributions through the molecule. In several article has been pointed also out that graphene on Nickel (111) has mainly two energetically favored adsorption modes, namely top-fcc and bridge-top [6,7]. We will show how the magnitude of the magnetic coupling is influenced by the structural factors named above. We further show how this coupling could be tuned by the intercalation of a magnetic monolayer, e.g. Fe and Co, between graphene and the Ni subtrate, and discuss the role of the graphene layer.

References:

[1] X. Y. Zhu, Surf. Sci. Rep. 56 (2004) 1.
[2] S. Sanvito, Chem. Soc. Rev. 40 (2011) 3336.
[3] B. Heinrich, L. Limot, M. Rastei, C. Iacovita, J. Bucher, D. Djimbi, C. Massobrio, *et al.*, Phys. Rev. Lett. 107 (2011) 216801.
[4] Y. Li, X. Chen, G. Zhou, W. Duan, Y. Kim, M. Kim, and J. Ihm, Phys. Rev. B 83 (2011) 195443.
[5] Z. F. Xu, Y. Xie, W. L. Feng and H. F. Schaefer, J. Phys. Chem. A 107 (2003) 2716.
[6] W. Zhao, S. M. Kozlov, O. Hofert, K. Gotterbarm, M. P. A. Lorenz, F. Vin, C. Papp, et al., J. Phys. Chem. Lett. 2 (2011) 759.
[7] M. Weser, N. E. Voloshina, K. Horn and Y. S. Dedkov, Phys. Chem. Chem. Phys. 13 (2011) 7534.

[P34] Substrate-driven self-assembling of metal nanocluster ordered arrays

S. Benedetti[1], S. Valeri[1], F. Stavale[2], N. Nilius[2], H.-J. Freund[2], J. Goniakowski[3], and C. Noguera[3]

[1] Centro S3, Instituto Nanoscienze-CNR and Dipartimento di Scienze Fisiche Informatiche e Matematiche, Università di Modena e Reggio Emilia, via Campi 213/a, Modena, 41125, Italy
[2] Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, Berlin, 14195, Germany
[3] CNRS and Université Pierre et Marie Curie-Paris 6, INSP, UMR7588, 4 place Jussieu, Paris cedex 05, 75252 France

Keywords: epitaxy, metal nanoparticles, thin films, self-assembly, metal-oxide interactions.

Ordered arrays of metal nanoclusters are of great interest for their applications in nanomagnetism, optics and catalysis. Amongst possible fabrication methods, the exploitation of a thin film as a support is appealing, where the nanopatterning induced by a misfit dislocation network can guide the nanocluster self-assembly into an ordered array [1].

In this work we combine experimental and theoretical investigation of nanoparticle self-ordering on a MgO film on Mo(001), where the presence of an interfacial dislocation network induces a surface periodic deformation connected with a modification in the workfunction (Fig. 1a) [2]. The deposition of Fe atoms leads to the spontaneous formation of nanoclusters disposed in a square array, with about 6 nm average distance, corresponding to the dislocation periodicity (Fig. 1b) [3]. Increasing MgO film thickness, the order of metal nanoparticles fades away and completely disappears for 40 ML MgO. DFT calculations clarify the mechanisms that determine ordered Fe nucleation. The modulations in the adsorption potential induce Fe atoms to preferentially bind to regions of high workfunction that enable electron transfer from the ad-species into the support. Particle growth, on the other hand, preferentially occurs in zones of contracted lattice parameter, where metal-metal and metal-oxide interactions can be optimized simultaneously. Both constraints favor particle growth in the Mg-Mo domains of the coincidence lattice (Fig. 1c).

The observed ordering effect on the MgO thin films is therefore caused by interplay of geometric and electronic properties at the metal-oxide interface. This growth-template allows us to produce extended particle arrays with narrow size distribution. This opens an experimentally simple route to address fundamental questions in heterogeneous catalysis, magnetism and nano-optics.

References:
[1] H. Brune *et al*., Nature 394 (1998) 451.
[2] S. Benedetti *et al*., Phys. Rev. B 78 (2008) 195411; H. M. Benia *et al.*, Surf. Sci 604 (2010) 435.
[3] S. Benedetti *et al.*, Adv. Func. Mater. 23 (2013) 75.

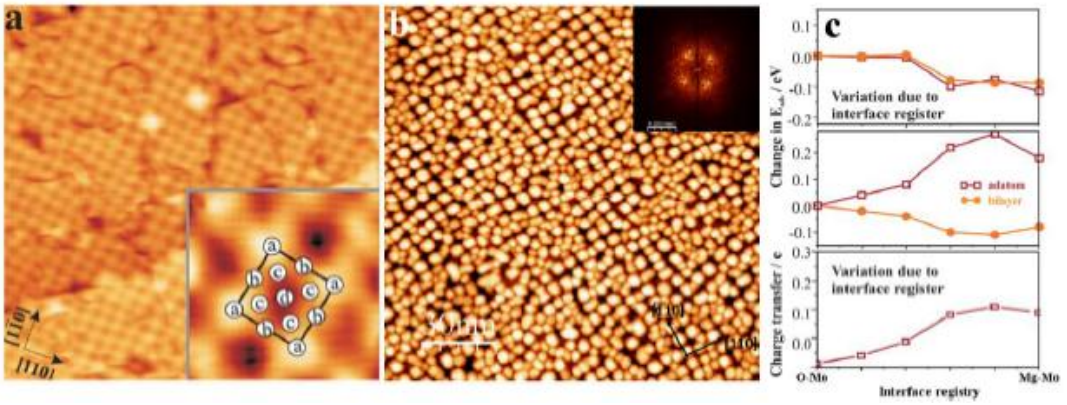


Fig. 1: a) STM image of a 10 ML thick MgO/Mo(001) film showing the typical coincidence lattice (80 × 80 nm^2). The inset shows a close-up with the superstructure unit-cell (12 × 12 nm^2); b) STM image of 3 ML Fe on MgO film; inset shows the FFT of the image; c) Calculated relative binding energies (per atom) with respect to the O-Mo domain and charge transfer for Fe adatoms and bilayers adsorbed on a 3 ML thick MgO/Mo(001) film shown as a function of interface register .

[P35] Near-infrared plasmonic activity in metal-doped ZnO derivatives

A. Calzolari[1], A. Ruini[1,2], and A. Catellani[1]

[1] CNR-NANO Istituto Nanoscienze, Centro S3, Modena, Italy
[2] Dipartimento FIM, Università di Modena e Reggio Emilia, Modena, Italy

Noble metals such as gold and silver are conventionally used as the primary plasmonic building blocks in the fields of the telecommunications and energy conversion. Both localized surface plasmons in nanoparticles and surface plasmon polaritons (SPPs) propagating at metal/semiconductor interfaces are of interest for optoelectronic applications: the formers can be exploited in photovoltaic systems as amplifier optical antenna that increase the absorption of incident solar light through excitation of particle plasmon resonances; the latters provide the opportunity of confining light in very small dimensions, thus acting as subwavelength scattering elements to couple and trap freely radiations and propagating over long spatial range [1].

However, metals are plagued by large losses, especially in the UV–vis and IR spectral ranges, arising in part from interband electronic transitions and in part from dissipative scattering events. These losses are detrimental to the performance of plasmonic devices, seriously limiting the feasibility of many plasmonic applications. As an alternative, heavily doped semiconductors can exhibit a small negative real permittivity (i.e. high conductivity) and very small losses at the infrared and longer wavelengths.

Here we present a first principles investigation of the optical and plasmonic properties of metal-doped ZnO systems [2-4], based on density functional theory, within the Random-Phase-Approximation. We first show the formation of SPP resonances at Al: ZnO/ZnO interfaces, and their dependence on doping dosage. These systems present tunable plasmonic activity in the near-IR range and in particular at wavelength relevant for telecommunications (1,5 μm) [5]. Then we characterize the plasmon properties of In-doped nanowires that have been envisaged as plasmonic nanoparticles in solar or fuel cells for energy conversion [6].

References:

[1] W. A. Murray and W. L. Barnes, Adv. Mater. 19 (2007) 3771.
[2] M. Bazzani, A. Neroni, A. Calzolari, and A. Catellani, Appl. Phys. Lett. 98 (2011) 121907.
[3] A. Catellani, A. Ruini, G. Cicero, and A. Calzolari, Phys. St. Sol. (2013) in press.
[4] A. Calzolari, A. Ruini, and A. Catellani, preprint (2013).
[5] G. Naik *et al.*, PNAS 109 (2012) 8834.
[6] H. A. Atwater and A. Polman, Nat. Mater. 9 (2010) 205.

[P36] Plasmons and Coulomb drag in Dirac/Schroedinger hybrid electron systems

M. Carrega[1], A. Principi[1], R. Asgari[2], V. Pellegrini[1], and M. Polini[1]

[1] NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy
[2] School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran 19395-5531, Iran

Keywords: graphene, hybrid system, plasmons, transport properties.

We show that the plasmon spectrum of an ordinary two-dimensional electron gas (2DEG) hosted in a GaAs heterostructure is significantly modified when a graphene sheet is placed on the surface of the semiconductor in close proximity to the 2DEG. Long-range Coulomb interactions between massive electrons and massless Dirac fermions lead to a new set of optical and acoustic intra-subband plasmons. Here we compute the dispersion of these coupled modes within the Random Phase Approximation, providing analytical expressions in the long-wavelength limit that shed light on their dependence on the Dirac velocity and Dirac-fermion density.

Moreover, we theoretically evaluate the transresistivity in a Coulomb-drag transport setup. At low temperature in the Fermi liquid regime we demonstrate that the drag resistivity of this hybrid system shows peculiar power-law dependence on carrier densities and interlayer distance.

These Dirac/Schroedinger hybrid electron systems are experimentally feasible and open new research opportunities for fundamental studies of electron-electron interaction effects in two spatial dimensions.

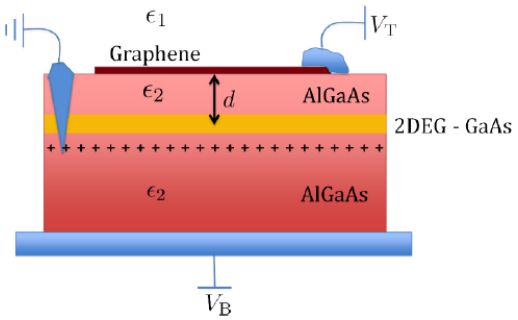


Fig. 1: Schematics of the double-layer massless Dirac/Schroedinger hybrid electron system studied in this work. A grapheme sheet is deposited on the surface of a semiconductor, underneath which a GaAs quantum well (at distance *d* from the surface) hosts a high-mobility two-dimensional electron gas (2DEG). Carriers in the two layers are induced by conventional gating techniques (the + signs below the quantum well indicate the doping layer). In the presence of Coulomb coupling between the subsystems, optical and acoustic hybrid collective modes emerge, which can be probed by resonant inelastic light scattering.

[P37] Optical excitations in edge-functionalized graphene nanostructures

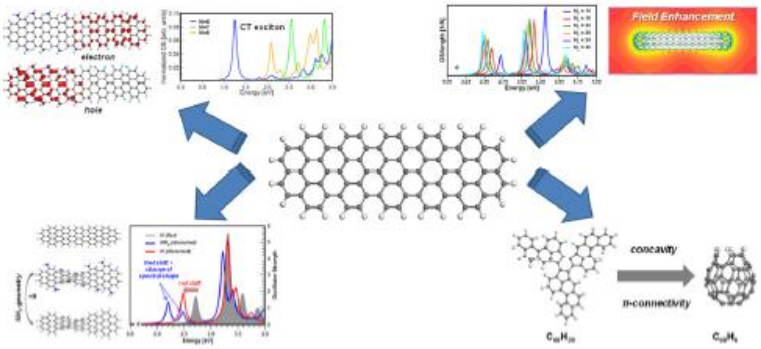
C. Cocchi[1], M. De Corato[2], D. Prezzi[2], A. Ruini[2,3], M. J. Caldas[4], A. Fasolino[5], S. Corni[2], and E. Molinari[2,3]

[1] Humboldt-Universität zu Berlin, Institut für Physik und IRIS Adlershof, Berlin, Germany
[2] Centro S3, CNR-Istituto Nanoscienze, Modena, Italy
[3] Dipartimento di Scienze Fisiche, Informatiche e Matematiche, UNIMORE, Italy
[4] Instituto de Física, Universidade de São Paulo, São Paulo, Brazil
[5] Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands

Keywords: graphene nanostructures, optical properties, edge functionalization.

The fabrication of nanoscale graphene ribbons of finite length is now reaching atomic scale accuracy and extreme edge control [1]. Here we present a theoretical investigation of the optical excitations of elongated nanoflakes. We focus both on intrinsic field enhancement effects and on the modification of the optical properties by means of edge modulation, functionalization and distortions [2]. We employ either quantum chemistry semi-empirical approaches [2-5] or ab-initio many-body perturbation theory techniques [6,7], depending on the system type. We find [5] that the optical spectra of elongated graphene flakes are dominated at low energy by excitations with strong intensity, comprised of characteristic coherent combinations of a few single-particle transitions with comparable weight. They give rise to stationary collective oscillations of the photo excited carrier density extending throughout the flake, and to a strong dipole and field enhancement. This behavior is robust with respect to width and length variations, thus ensuring tunability in a large frequency range. The implications for nanoantenna and other nanoplasmonic applications are discussed for realistic geometries. Our work shows that width modulation and edge functionalization [3-4] can be exploited to tune the optical spectra of such ribbons and to design all-graphene nano-junctions. We find that minimal width-modulations are sufficient to obtain confinement of both electrons and holes, thus forming optically active quantum dots with unique properties [7]. Moreover, electron affinities and ionization potentials of ribbons and flakes can be tuned by edge functionalization to form nanojunctions that allow for photoinduced charge separation [3,4]. Finally, we show that π-coupled nanoflakes with different widths or edge-functionalization can efficient systems presenting charge-transfer excitations.

References:
[1] J. Cai, P. Ruffieux, R. Jaafar, M. Bieri, T. Braun, S. Blankenburg, M. Muoth, A. P. Seitsonen, M. Saleh, X. Feng, K. Müllen, and R. Fasel, Nature 466 (2010) 470.
[2] C. Cocchi, D. Prezzi, A. Ruini, M. J. Caldas, and E. Molinari, J. Phys. Chem. C 116 (2012) 17328.
[3] C. Cocchi, A. Ruini, D. Prezzi, M. J. Caldas, and E. Molinari, J. Phys. Chem. C 115 (2011) 2969.
[4] C. Cocchi, D. Prezzi, A. Ruini, M. J. Caldas, and E. Molinari, J. Phys. Chem. Lett. 2 (2011) 1315.
[5] C. Cocchi, D. Prezzi, A. Ruini, E. Benassi, M. J. Caldas, S. Corni, and E. Molinari, J. Phys. Chem. Lett. 3 (2012) 924.
[6] D. Prezzi, D. Varsano, A. Ruini, A. Marini, and E. Molinari, Phys. Rev. B 77 (2008) 041404.
[7] D. Prezzi, D. Varsano, A. Ruini, and E. Molinari, Phys. Rev. B 84 (2011) 041404.



[P38] Studies on Ni@NiO core-shell nanoparticles: control of metal-oxide interface and tuning of exchange bias

S. D'Addato[1,2], M. C. Spadaro[1,2], P. Luches[1], V. Grillo[1], G. Paolicelli[1], S. Frabboni[1,2], S. Valeri[1,2], A. M. Ferretti[3], E. Capetti[3], and A. Ponti[3]

[1] CNR-NANO, S3 Research Centre, via G. Campi 213/a, Modena
[2] Dipartimento FIM, Università di Modena e Reggio Emilia, via G. Campi 213/a, Modena
[3] CNR-ISTM, via C. Golgi 19, 20133, Milano

Keywords: core-shell nanoparticles, exchange bias, Ni, nanomagnetism, High Resolution TEM.

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, encompassing (among others) medicine and diagnostic, photovoltaic, catalysis and magnetic recording. Particular efforts have been devoted to the application of the exchange bias effect (which is present in NP with ferromagnetic core and antiferromagnetic oxide shell) as a possible way for stabilizing the magnetic state of NP. 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 NiO shells prepared with different techniques: deposition in oxygen atmosphere, post-annealing in air, co-deposition of NP with Ni vapour in oxygen. 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 [1]. The samples were studied with in situ XPS, ex situ SEM, AFM and TEM, to obtain information about the NP chemical state, morphology and crystal structure. High quality HR-TEM and STEM-HAADF data allowed an in-deep analysis of the NP atomic structure, in both core and shell areas, while FC and ZFC magnetization curves and hysteresis cycles at T=5 K were recorded by a SQUID magnetometer. 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 correlation.

References:

[1] S. D'Addato, V. Grillo, S. Altieri, R. Tondi, S. Frabboni, and S. Valeri, J. Phys.: Cond. Matt. 3 (2011) 175003.

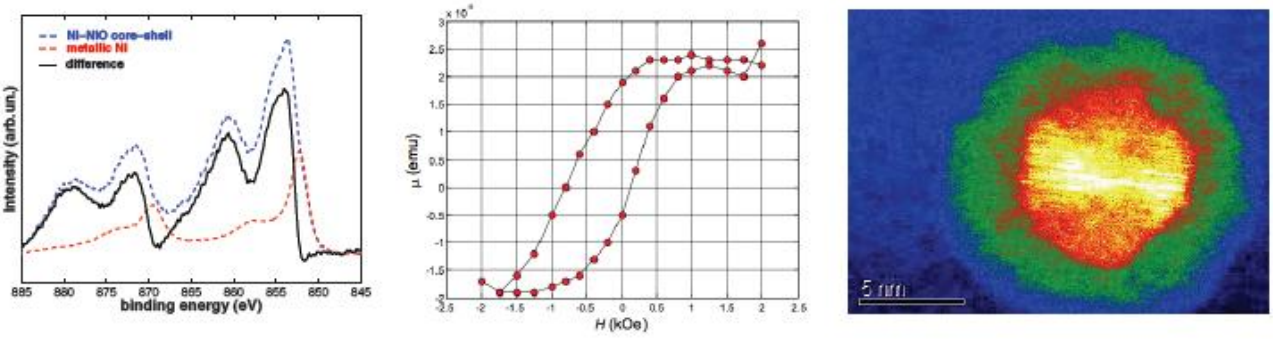


Fig. 1: Left: Background-subtracted Ni 2p XPS spectrum of Ni@NiO core-shell NP, plotted with metal and oxide (difference) components. Centre: Magnetic hysteresis loop measured on the same sample at T= 5 K. Right: STEM-HAADF image of Ni@NiO NP, showing icosahedral Ni core and NiO shell.

[P39] Theory of few interacting Fermi atoms in a one-dimensional trap: An exact approach

P. D'Amico and M. Rontani

CNR-NANO Research Center, Via Campi 213a, 41125 Modena, Italy

Keywords: cold atomic gases, few-body physics, one-dimensional confinement, exact diagonalization.

The physics of interacting cold Fermi atoms is attracting a great deal of attention due to the recent experimental realization of quasi-one-dimensional confinement of a few atoms with precise control on the atom number, starting from zero and proceeding up to ten through unit steps [1]. Indeed, the possibility to control the number of atoms as well as the interaction strength (both positive and negative) and the shape of the trap makes such systems ideal candidates as toy models of few-body physics. Fundamental properties such as energy spectra, state lifetimes, spin and space wave function symmetries can be investigated with high experimental accuracy, hence theoretical predictions may be tested [2]. The dimensionality of the confining traps appears to be a key issue, able to qualitatively change the fundamental physics of these ultraclean strongly interacting quantum systems. Theoretical investigations for three- and two-dimensional traps have been made [3-4] and a few theoretical works have focused on one-dimensional systems [5], but there is no systematic theory for this last case.

In this work we investigate systems made of three or more atoms confined in a purely one-dimensional harmonic trap interacting through a contact force. First, starting from the exact solution of the two-body problem we construct the exact three-body wave function through a variational approach that exploits the symmetries of the interacting system. By means of proper boundary conditions applied to the wave function we obtain feasible formulae for the eigenvalue problem that we solve with arbitrary numerical accuracy for both fermions and bosons.

In the case of fermionic atoms we use the obtained energy spectra as a benchmark for numerical calculations based on the configuration interaction (CI) method, as implemented in the home-made state-of-the-art code DonRodrigo. We observe good quantitative agreement for repulsive interaction and limited convergence for attractive interaction as the CI method needs an increasing orbital basis size with the increasing interaction strength to reach convergence, as shown in Fig. 1. Such convergence test is crucial to assess the accuracy of our CI calculations for larger numbers of atoms.

References:

[1] F. Serwane, G. Zuern, T. Lompe, T. B. Ottenstein, A. N. Wenze, and S. Jochim, Science 332 (2011) 336.

[2] M. Rontani, Phys. Rev. Lett. 108 (2012) 115302.

[3] M. Rontani *et al*., Phys. Rev. Lett. 102 (2009) 060401.

[4] X. Liu, H. Hu, and P. D. Drummond, Phys. Rev. A 82 (2010) 023619; Phys. Rev. B 82 (2010) 054524.

[5] J.-J. Wang, W. Li, S. Chen, Gao Xianlong, M. Rontani, and M. Polini, Phys. Rev. B 86 (2012) 075110.

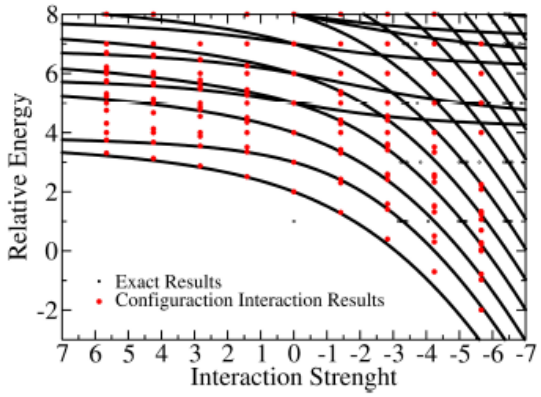


Fig. 1: LEEM image of graphene grown on SiC in an atmosphere of Ar (pressure close to 1bar). The surfaces are characterized by long (up to 50μm) terraces homogeneously covered by monolayer graphene (light gray). Only at the step edges the formation of bilayer and in some cases trilayer graphene is visible (darker regions), indicating that additional graphene layers nucleate predominantly at step edges.

[P40] All-Optical Polariton Transistor

M. De Giorgi[1,2], D. Ballarini[1,2], E. Cancellieri[3], E. Giacobino[4], A. Bramati[4], G.Gigli[1,2,5], and D. Sanvitto[1,2]

[1] NNL, Istituto Nanoscienze - CNR, Via Arnesano, 73100 Lecce, Italy
[2] Istituto Italiano di Tecnologia, IIT-Lecce, Via Barsanti, 73010 Lecce, Italy
[3] Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, Spain
[4] Laboratoire Kastler Brossel, École Normale Supérieure et CNRS, 75005 Paris, France
[5] Innovation Engineering Department, University of Salento, Via Arnesano, 73100 Lecce, Italy

Keywords: exciton polariton, transistor.

Optical technology has proved to be the best choice for the transmission of information at high data rate over long distances. However, the implementation of high-speed, low-energy, all-optical logics in semiconductors represents a formidable challenge due to the intrinsic difficulty of all-optical devices to satisfy the basic system requirements [1]. In particular, cascadability is difficult to obtain in optical systems, and it is assured only if the output of one stage is in the correct form to drive the input of the next stage. In this context, we demonstrate a scheme of all-optical transistor based on exciton polaritons in semiconductor microcavities, which exhibits full connectivity in the same chip plane.

Exciton-polaritons, which are composite particles resulting from the strong coupling between excitons and photons, have recently demonstrated huge non-linearities and unique propagation properties, being a very promising system for the realization of all-optical devices [2,3,4]. Here we demonstrate that polariton fluids moving in the plane of the microcavity can operate as input and output of an all-optical transistor. The control operation is performed by a polariton fluid of much lower intensity than the output, which is fed by an Address beam, showing amplification output/input of 12dB. Polariton propagation in the plane of the microcavity is used to control the switching of a second, spatially separated transistor, demonstrating the cascadability of the system. The characteristic times of the switching operation are of the order of the cavity lifetime, which is of about 10ps, while the total activation energy used for the transistor is lower than 1fJ. Moreover, the operation of the polariton transistor as an AND gate is shown, validating the connectivity of multiple transistors in the microcavity plane and opening the way to the implementation of polariton integrated circuits.

References:

[1] D. A. B. Miller, Nat Photon 4 (2010) 3-5.
[2] A. Amo, Nature Phys. 5 (2009) 805-810.
[3] T. C. H. Liew, A. V. Kavokin, and I. A. Shelykh, Phys. Rev. Lett. 101 (2008) 016402.
[4] D. Sanvitto *et al.*, Nat Photon 5 (2011) 610-614.

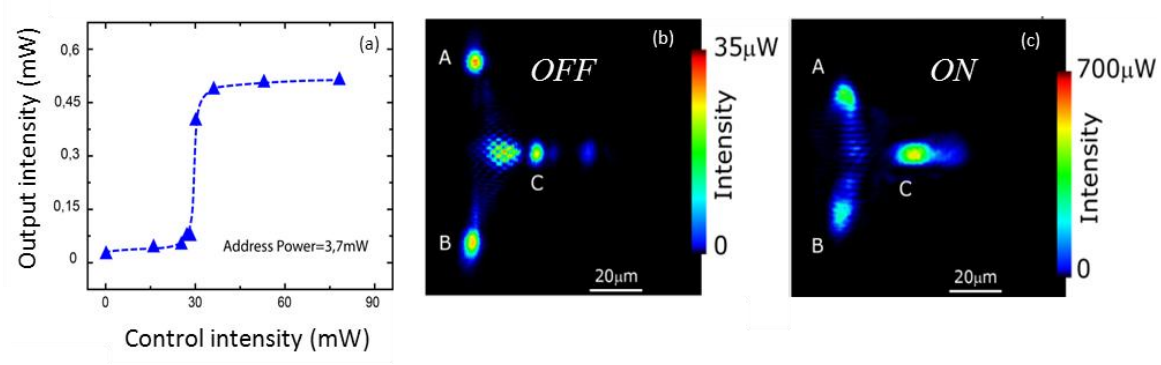


Fig. 1: (b) Output intensities against Control intensities, taken for an Address power of P=3.7mW. (b) Three transistors scheme (A,B and C, spatially separated by a distance of about 30 μm) in which C acts as AND logic gate with inputs A and B. When A, B and C are below threshold, as in (b), their output intensities are lower than 35 μW. Due to the increase of the intensities above threshold, the color scales in panels (c) is reduced by a factor 20 as compared with panel (b). (c) AND gate in the ON state, when both A and B are above threshold.

[P41] Anharmonic Oscillations in the formation of a polariton condensate

M. De Giorgi[1,2], D. Ballarini[2], F. Laussy[3], P. Cazzato[1,2], S. I. Tsintzos[4,5], P. G. Savvidis[4,5], G. Gigli[1,2,6], and D. Sanvitto[1,2]

[1] NNL, Istituto Nanoscienze - CNR, Via Arnesano, 73100 Lecce, Italy
[2] Istituto Italiano di Tecnologia, IIT-Lecce, Via Barsanti, 73010 Arnesano, Italy
[3] Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, Spain
[4] FORTH-IELS, PO Box 1385, 71110 Heraklion, Crete, Greece
[5] Department of Materials Science and Technology, University of Crete, 71003, Heraklion, Crete, Greece
[6] Innovation Engineering Department, Università del Salento, Via Arnesano, 73100 Lecce, Italy

In the past decade, microcavity polaritons have stimulated extensive research work due to their unique properties as non-equilibrium condensates and all related quantum phenomena. Recently, Josephson oscillations have been observed using two neighbouring defects, present in the random disorder, or by coupled micropillars molecule [1,2]. However, given to the non-equilibrium character of the condensate, the dynamical behaviour of polaritons is strongly conditioned by dissipation and pumping, which usually alter the standard superfluid description. Here we demonstrate that marked anharmonic oscillations, unrelated to Josephson effects, arise when condensation is happening in a confined region of a few microns squared. These oscillations are attributed to the interplay between slow exciton replenishing and fast stimulated condensate formation rate. Related phenomena are also observed in the form of "relaxation oscillations" in slow inversion solid state lasers [3].
In our experiments, an AlGaAs/AlAs microcavity containing 8 GaAs quantum wells kept at 10K is non-resonantly excited by a laser pulse of 100 fs in a micro-PL setup. Time resolved polariton photoluminescence is performed by using a streak camera coupled to a spectrometer, with 2ps time resolution. The microcavity sample we use show very non-uniform regions with defects of sizes varying between 1 to 10 um2 which work as natural traps for polariton condensation. In figure 1 three streak images show the dynamics of condensate formation at different powers. Increasing the exciton population, and so the pumping rate, we observe a clear oscillatory behaviour at the energy of the condensate. The oscillations together with their period are observed to shorten with polariton density while the population at early time gets blue shifted due to exciton interaction.

To study the real space dynamics of these oscillations we have acquired spatially resolved (resolution 0.7 μm) snap shots at different times and energies of the polariton condensate. Figure 2 shows three moments of the condensate formation which demonstrate the strong polariton localisation which moves back and forth between two adjacent points while its population oscillate between high and low emission condition. To account for the observation, a theoretical model which takes into account polariton losses, exciton-reservoir replenishement and decay as well as condensate stimulation, has been developed. We show that this oscillatory behaviour is always present in a polariton condensate when the dynamics of reservoir depletion is faster than the pumping rate.

References:
[1] K. G. Lagoudakis *et al.*, PRL 105 (2010) 120403.
[2] M. Abbarchi *et al.*, arXiv:1212.5467 (2012).
[3] Y. Lien *et al.*, J. Opt. Soc. Am. B 19 (2002) 1461-1466.

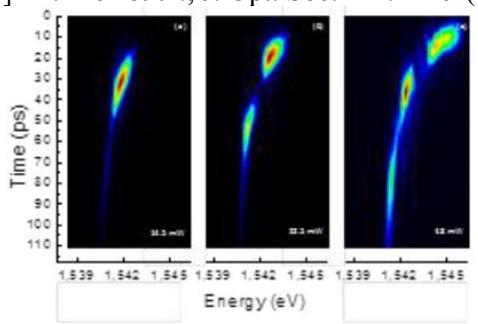


Fig.1(a) Time resolved photoluminescence at different excitation density

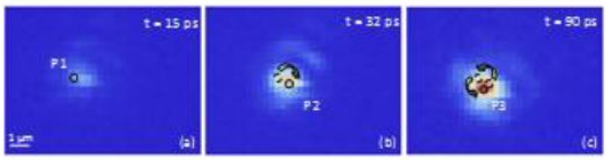


Fig.2(a) Real space images at different delay time

[P42] Non-empirical semilocal density functional based on the semiclassical atom theory

E. Fabiano[1], L. A. Constantin[2], and F. Della Sala[1,2]

[1] NNL - Nanoscience Institute of CNR, Lecce, Italy
[2] CBN@UNILE - Istituto Italiano di Tecnologia, Arnesano (Le), Italy

Keywords: density functional theory, exchange-correlation functional, non-interacting kinetic energy functional, generalized gradient approximation, semiclassical atom.

Density functional theory (DFT) is nowadays considered a fundamental tool for the prediction and interpretation of numerous properties in different fields, ranging from nanotechnology to life-science. However, the applicability and accuracy of DFT calculations for different problems strongly resides on the availability of efficient and accurate exchange-correlation (XC) functionals. The research of new XC functionals is thus a very active field, continuously demanding for improved accuracy, broader applicability, higher efficiency and reduced empiricism.

In this contribution we present our work in this field reporting on the development of a new semilocal XC functional, namely the APBE functional [1], which displays a remarkable accuracy for a broad range of problems in computational chemistry and physics.

The APBE functional is based on the well known ansatz of the Perdew-Burke-Ernzenhof (PBE) XC functional [2], which is the most used XC-functional. Therefore, APBE satisfies numerous important exact constraints of the exact XC energy functional. In addition, it is specifically designed to recover the Exchange asymptotic expansion of the semiclassical atom (i.e. an atom with an infinite number of electrons), which is remarkably accurate for the description of the exchange energy of all atoms in the periodic table.

As a result the APBE functional provides very accurate results for atomic and molecular properties, including atomization energies, barrier heights and structural properties [1,3]. Moreover, it is one of the most accurate semilocal approximations for non-covalent interactions (especially for hydrogen bonds). Finally, despite the APBE functional does not recover the exact second-order gradient expansion for the XC energy, it still performs well for metal clusters and solid-state systems [1,3].

To strengthen the importance of these results and highlight the merits of the non-empirical construction beyond the APBE functional, we perform also a detailed analysis of the APBE functional form [3]. This study shows that the non-empirical parameters characterizing the APBE functional are indeed the “best” possible choice to grant high accuracy on a large palette of properties of molecular and solid-state systems. This finding provides a clear evidence for the relevance of the semiclassical atom as a reference system in density functional theory [1]. Finally, we will show that the semiclassical atom theory can be also used to develop a non-empirical semilocal functional for the non-interacting kinetic energy [1,4]. Hence, we propose a new kinetic functional (APBEK) which provides an impressive accuracy for atoms, molecules, jellium clusters and surfaces, and frozen-density-embedding applications.

References:

[1] L. A. Constantin, E. Fabiano, and F. Della Sala, Phys. Rev. Lett. 106 (2011) 186406.
[2] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77 (1996) 3865.
[3] E. Fabiano, L. A. Constantin, and F. Della Sala, J. Chem. Theory Comput. 7 (2011) 3548.
[4] S. Laricchia, E. Fabiano, L. A. Constantin, and F. Della Sala, J. Chem. Theory Comput. 7 (2011) 2439.

[P43] Quantum synchronization of continuous variables systems

A. Mari[1], A. Farace[1], N. Didier[2], V. Giovannetti[1], and R. Fazio[1]

[1] NEST, CNR-Nano and Scuola Normale Superiore, Pisa, Italy
[2] Université de Sherbrooke and McGill University, Canada

Keywords: quantum synchronization, nano-mechanical resonators, quantum optomechanics.

In the 17th century, C. Huygens noticed that the oscillations of two pendulum clocks with a common support tend to synchronize. After this observation similar phenomena have been observed in many different contexts even outside the scientific range of physics, as in: neuron networks, chemical reactions, heart cells, fireflies, etc. [1]. The emergence of synchronization in so many different systems encouraged its theoretical investigation and description within the field of classical non-linear dynamical systems. Given the time evolution of two classical degrees of freedom undergoing limit cycles or chaotic evolution, like two pendula of positions $q_1(t)$, $q_2(t)$ and momenta $p_1(t)$, $p_2(t)$, standard definitions exist to determine whether their motion is synchronized: *complete synchronization* occurs when the two orbits in phase space are identical, i.e. $q_1(t)=q_2(t)$ and $p_1(t)=p_2(t)$; *phase synchronization* occurs when the orbits have a fixed phase shift, i.e. $\Phi_1(t)=\arctan(q_1(t)/p_1(t))= \Phi_2(t)+ \Phi_0$. The same approach cannot be straightforwardly extended to quantum systems. Quantum states are defined by wave functions (or density operators) and their time evolution cannot be described with classical phase space trajectories. The aim of this work is to develop a consistent and quantitative theory of synchronization for continuous variables systems evolving in the quantum regime. This should be considered in the global picture of the current research in this direction [2-7].

We introduce quantitative measures of *complete* and *phase synchronization* and study how classical and quantum noise affects the precision of such effects. We show that quantum mechanics imposes fundamental limits to these phenomena: perfect complete synchronization is impossible while high levels of phase synchronization imply that the quantum state of the system is non-classical (squeezed). We also clarify the difference between synchronization and entanglement. We finally analyze, via numerical simulations, the emergence of quantum synchronization in the specific experimental setting of coupled optomechanical systems [8,9] driven in the multi-stable regime.

Optomechanical systems look like macroscopic classical systems (e.g. springs, pendula, etc.) but at the same time they can be controlled by laser driving and brought in dynamical regimes where quantum effects are relevant. Such systems have all the properties (non-linear dynamics, limit cycles, etc.) which are necessary for the emergence of synchronization [2,10]. Since our task is extending the classical concept of synchronization to quantum mechanics, a pair of coupled optomechanical systems is a convenient toy-model where the previous theoretical investigation can be directly applied. Moreover, recent developments in nano-technology allow to realize optomechanical arrays composed of two or more coupled mechanical resonators controlled close to their quantum regime and indeed some first experimental evidences of synchronization have been found [6,7].

References:

[1] A. Pikovsky, M. Rosenblum and J. Kurths, Synchronization: A Universal Concept in Nonlinear Sciences, Cambridge University Press, New York (2001).
[2] M. Ludwig and F. Marquardt, arXiv:1208.0327.
[3] U. Akram and G. Milburn, AIP Conf. Proc. \textbf{1363}, 367 (2010).
[4] A. Tomadin, S. Diehl, M. D. Lukin, P. Rabl, and P. Zoller, Phys. Rev. A 86 (2012) 033821.
[5] G. L. Giorgi *et al.*, Phys. Rev. A 85 (2012) 052101.
[6] S. Shim, M. Imboden, and P. Mohanty, Science 316 (2007) 95.
[7] M. Zhang *et al.*, Phys. Rev. Lett. 109 (2012) 233906.
[8] F. Marquardt and S. M. Girvin, Physics 2 (2009) 40.
[9] M. Aspelmeyer, T. J. Kippenberg, and F. Marquardt, arXiv:1303.0733 (2013).
[10] G. Heinrich *et al.*, Phys. Rev. Lett. 107 (2011) 043603.

[P44] Molecular dynamics simulations in Graphene with empirical interatomic potentials

R. Farchioni[1,2], A. Rossi[1,3], and V. Tozzini[1,3]

[1] NEST - Istituto Nanoscienze - Cnr Pisa, Italy
[2] Dipartimento di Fisica, Università di Pisa, Italy
[3] Scuola Normale Superiore, Pisa, Italy

Keywords: Graphene, Empiric Potentials, Molecular Dynamics Simulations, Density Functional Theory.

In recent years, empirical potentials have been developed, in particular to model interatomic forces in covalent bonding of systems composed by Carbon and Silicon atoms. An important example is the Tersoff potential [1] which has the advantage of a simple functional form based on an attractive and a repulsive Morse-type potential, a many-body function and a cut-off function which restricts the action to the nearest neighbours, and of a low number of parameters. The Tersoff potential can be used to study dynamical properties for large systems over long time scales, and for this reason it has been implemented in the DL_POLY general purpose molecular-dynamics simulation code.

We illustrate the results of simulations for the study of the structural, mechanical and dynamical properties of a number of flat and rippled graphene layers, of SiC multilayers, and of their combination, emulating the epitaxially grown graphene sheets. We have evaluated the behaviour of the total energy and of the bond lenghts and compared the results with DFT calculations to test the applicability of the potentials on the systems studied. In our study, we have also used different sets of parameters which have been proposed in the literature.

References:
[1] J. Tersoff, Physical Review B 37 (1988) 6991.

[P45] BaY_2F_8 doped with Er^{3+}: A novel upconverter material for photovoltaic application.

A. Boccolini[1], R. Faoro[2], E. Favilla[2], S. Veronesi[2], and M. Tonelli[2]

[1] Dipartimento di Fisica dell'Università di Pisa, Largo B. Pontecorvo 3, 56127 Pisa, Italy
[2] NEST Istituto Nanoscienze-CNR and Dipartimento di Fisica dell'Università di Pisa, Largo B. Pontecorvo 3, 56127 Pisa, Italy

Keywords: fluoride crystals, photovoltaics (PVs), silicon solar cells, up-conversion (UC).

The reduction of losses mechanisms in conventional silicon solar cells is becoming an interesting task [1]. An increase of the upper limit in the energy conversion efficiency can be obtained considering a system made of a solar cell plus an upconverter.

According to the literature, the most efficient upconverter systems are based on fluoride crystals. Ordinary growth techniques makes high optical quality crystal samples feasible, obtaining materials less subjected to degradation, a striking feature for PV application.

Fluoride crystals (BaY_2F_8) doped with Er^{3+} ions with different doping level have been grown with an home-made Czochralski furnace. A spectroscopic characterization consisting in both absorption and fluorescence measurements were performed in order to investigate the upconversion mechanism occurring when the material is excited with a radiation at 1557 nm. The measured emission spectrum shows a photoluminescence mainly (more than 90%) distributed in the NIR region at $\simeq 1\ \mu$m. The spectral conversion due to the upconversion makes this material suitable for photovoltaic applications, especially if we combine it with a crystalline silicon solar cell.

Even if the employment of this kind of material doped with Rare Earths ions is well known for laser applications, it is, to our knowledge, a new host material for photovoltaic application. A device made of a single face silicon solar cell (designed for concentration systems) + upconverter material (PV-UC) was designed and his external quantum efficiency (EQE) at 1557 nm was measured. EQE values of 6.5% and 4.1% were reached under 8.5 W cm−2 power density illumination for the 30%Er^{3+} and 20%Er^{3+} samples, respectively. A comparison with previous works involving fluoride materials doped with erbium ions [2-3] shows that our results are encouraging and suggests that BYF is a promising host to be used as upconverter material for photovoltaic application.

References:

[1] C. Strümpel, M. McCann, G. Beaucarne, V. Arkhipov, A. Slaoui, V. Švrcek, C. del Cañizo, and I. Tobias, Solar Energy Materials and Solar Cells 91 (2007) 238.
[2] B. Richards and A. Shalav, Electron Devices, IEEE Transactions on 54 (2007) 2679.
[3] S. Fischer, J. C. Goldschmidt, P. Löper, G. H. Bauer, R. Brüggemann, K. Krämer, D. Biner, M. Hermle, and S. W. Glunz, Journal of Applied Physics 108 (2010) 044912.

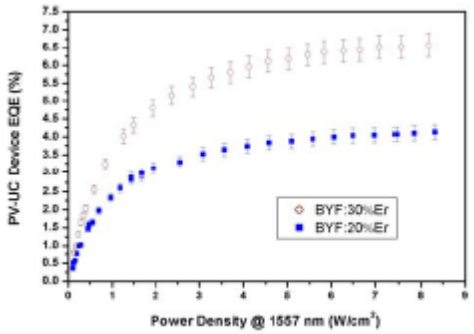


Fig. 1: Measured EQE for two samples (30% and 20% doping level) absorbing the same amount of incident power.

[P46] Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functionals

A. Ferretti[1], I. Dab[2], M. Cococcioni[3], and N. Marzari[4]

[1] Centro S3, CNR-Istituto Nanoscienze, 41125 Modena, Italy
[2] Université Paris-Est, CERMICS, 77455 Marne-la-Vallée Cedex 2, France
[3] Department of Chemical Engineering and Materials Science, University of Minnesota, USA
[4] THEOS Lab, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Keywords: DFT, functionals, Koopmans' theorem, spectroscopy.

Energy functionals which depend explicitly on the orbital densities (ODD), instead of the total charge density, appear when applying self-interaction corrections to density-functional theory. In these cases (e.g. the Perdew-Zunger [1] and the non-Koopmans [2] approaches) the total energy loses invariance under unitary rotations of the orbitals, and the minimization of the functionals leads to orbital-dependent Hamiltonians.

We show that it is possible to identify the orbital-dependency of densities and potentials with an effective and discretized frequency-dependency, in close analogy to the quasi-particle approximation of frequency-dependent self-energies and naturally oriented to interpret electronic spectroscopies [3]. Some of the existing ODD functionals are analyzed from this new perspective. Numerical results for the electronic structure of gas-phase molecules (within the Koopmans-corrected class of functionals) are computed and found in excellent agreement with photoemission (UPS) data [4].

References:

[1] J.-P. Perdew and A. Zunger, Phys. Rev. B 23 (1981) 5048.
[2] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, Phys. Rev. B 82 (2010) 115121.
[3] M. Gatti, V. Olevano, L. Reining, and I.-V. Tokatly, Phys. Rev. Lett. 99 (2007) 057401.
[4] I. Dabo, A. Ferretti, C.-H. Park, N. Poilvert, Y. Li, M. Cococcioni, and N. Marzari, Phys. Chem. Chem. Phys. 15 (2013) 685.

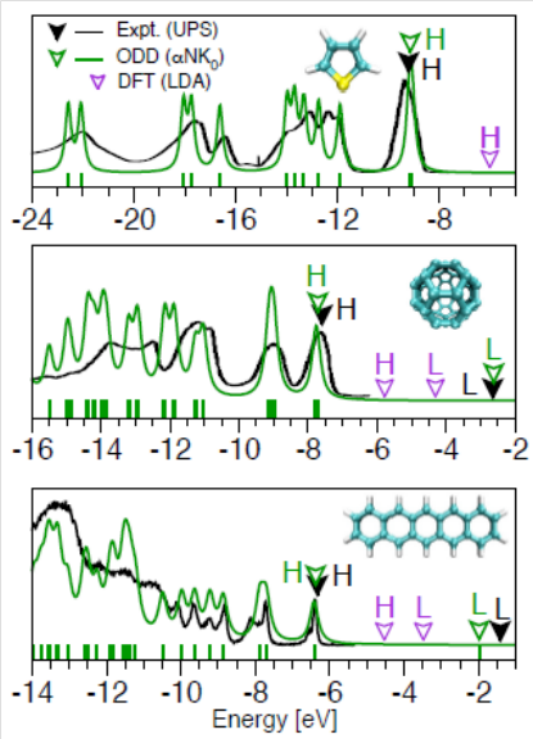


Fig. 1: ODD (KC) density of states compared to ultraviolet photoemission experiment (thick black line) for (a) thiophene, (b) C60, and (c) pentacene.
Filled (black) and empty triangles indicate respectively the experimental and theoretical (LDA, purple, and KC, green) HOMO, LUMO levels.

[P47] Wigner localization in a gate-defined graphene quantum dot

K. A. Guerrero Becerra[1,2] and M. Rontani[1]

[1] CNR-NANO Research Center S3, Via Campi 213a, 41125 Modena, Italy
[2] Università degli Studi di Modena e Reggio Emilia, Modena, Italy

Keywords: graphene, quantum dot, Wigner localization, exact diagonalization, few-body physics.

A fundamental and yet open issue concerning graphene is the role of electron-electron interaction. Since the density of states vanishes at the charge neutrality point, the long-range Coulomb interaction is unscreened, hence one would expect strong many-body effects. However, experiments show that electrons in bulk graphene (in the absence of the magnetic field) allegedly behave as non-interacting particles, except for small effects related to velocity renormalization and coupling with plasmons [1]. The fact that Coulomb and kinetic energies scale identically with the electron density rules out the formation of a Wigner crystal [2], the archetype of a strongly-interacting many-body state. Here we provide theoretical evidence that electrons may form a Wigner molecule -the finite-size counterpart of the Wigner solid- in a graphene quantum dot (QD).

We study a graphene QD where the confinement of Dirac fermions is due to the presence of an energy gap in the single-particle spectrum, induced by the interaction with an underlying substrate, in combination with a hard-wall circularly symmetric electrostatic potential that may be tuned by an external gate [3]. We solve the QD fully interacting Hamiltonian up to six electrons by means of exact diagonalization (ED). The single-particle basis set is obtained within the Dirac-Weyl two-component formalism for low-energy excitations in graphene. The ED in the many-electron space provides the few-body energy spectrum as well as the interacting wave functions from which we extract the charge density. In order to investigate different correlation regimes, we tune the key ratio of Coulomb interaction to confinement energy by varying both the QD radius and the static dielectric constant that mitigates the Coulomb potential.

Signatures of Wigner localization emerge from the analysis of both the few-body energy spectrum and the charge density radial profile. As shown in fig. 1, electrons are moved towards the outer QD region for increasing interaction strengths, which may be realized either by decreasing the dielectric constant [fig. 1a)] or by increasing the dot radius [fig. 1b)]. This trend is confirmed by the overlap of the spin-resolved densities at large interaction strength: indeed, in the Wigner limit, electrons localize in space so exchange interactions become negligible, hence spin degrees of freedom become irrelevant.

References:
[1] A. H. Castro Neto *et al.*, Rev. Mod. Phys. 81 (2009) 109.
[2] H. P. Dahal *et al.*, Phys. Rev. B 74 (2006) 233405.
[3] P. Recher *et al.*, Phys. Rev. B 79 (2009) 085407.

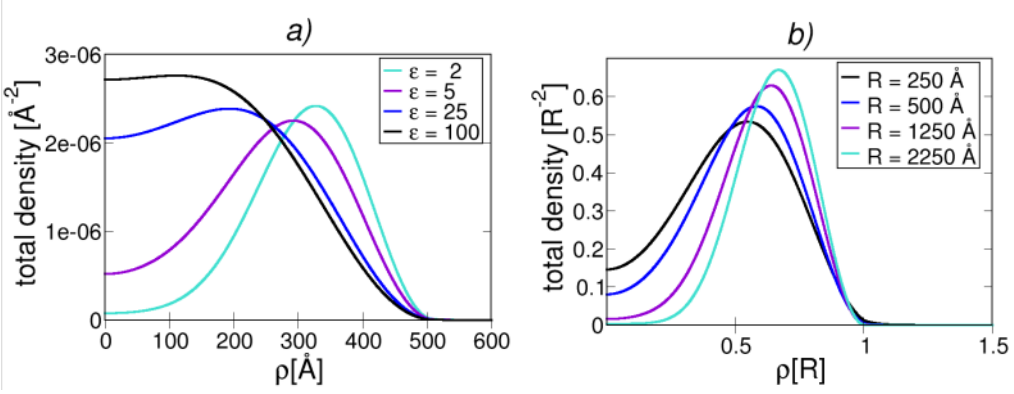


Fig. 1: Charge density of the three-electron ground state (A sublattice component) vs radial coordinate for different values of (a) the static dielectric constant ε (the QD radius is 50 nm) (b) the QD radius R (dielectric constant ε = 5).

[P48] Spin Transfer Torque for Excitons

K. L. Jensen[1,2], L. J. Sham[3], and M. Rontani[1]

[1] CNR-NANO Research Center S3, Via Campi 213A, 41125 Modena, Italy
[2] Università degli Studi di Modena e Reggio Emilia, Modena, Italy
[3] Department of Physics, University of California San Diego, La Jolla, California 92093-03

Keywords: Excitons, Spin Transfer Torque, Spin Transport through Interfaces, Quantum Scattering.

Spin-based interactions between a ferromagnet (FM) and a spin-polarized current can be used to switch the orientation of the magnetization within a thin ferromagnetic element. This phenomenon, known as spin-transfer torque (STT), which occurs because the transverse component of the spin current is absorbed across the interface, plays a crucial role in spintronics applications [1]. Since STT requires a spin current to flow, the spin carriers are usually taken to be electrons (or holes). In this work we will investigate the effect of STT induced by a flow of spin-polarized excitons though a thin ferromagnetic layer. The system considered for this study of STT is build on a one dimensional scattering model with mirror symmetry and consist of a thin ferromagnetic layer, sandwiched between two semiconductors (SC). The semiconductors are treated within a two-band model in the effective mass approximation. The thin ferromagnetic layer acts as a spin-dependent scattering center for the spin-polarized excitons which are created through irradiation by an external laser in a steady state regime.

By consider elastic scattering at equilibrium and matching the wave functions across the SC-FM junction, is it possible to find the probabilities coefficients for the transmitted and reflected states at the boundary [2]. The transmitted and reflected coefficients are then used to obtain the scattering matrix for the junction, which will be used to analyze the STT in two distinct cases: (i) a bias voltage is applied through the system [3], which tends to break the electron and hole components of the excitons (ii) an effective driving force for excitons is applied, as it is nowadays possible for indirect excitons in semiconductor bilayers.

This work is supported by EU-FP7 Marie Curie ITN INDEX and by US NSF ECCS-120258.

References:

[1] D. C. Ralph and M. D. Stiles, Journal of Magnetism and Magnetic Materials 320.7 (2008) 1190-1216.
[2] G. E. Blonder, M. Tinkham, and T. M. Klapwijk, Physical Review B 25.7 (1982) 4515.
[3] Y. Wang and L. J. Sham, Physical Review B 85.9 (2012) 092403.

[P49] Time-dependent Simulation of Exciton Dynamics in RTD Structures

M. Khurshudyan[1,2], A. Bertoni[2], and G. Goldoni[1,2]

[1] Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia, Modena, Italy
[2] Centro S3, Istituto Nanoscienze - CNR, Italy

Keywords: Indirect exciton, Fourier split-step approach, time dependent simulation, three-particle simulation.

Excitonic devices promise a leap forward in data-processing and optical systems, and new experimental achievements are being obtained for both applications. On one hand, an exciton-based integrated circuit that operates at 125 K (well above the liquid nitrogen temperature) has been realized [1] and an all-optical transistor based on the control of exciton fluxes has been demonstrated [2]. On the other hand, coherent radiation sources [3] and all-optical spin switches [4] have been realized. Moreover, a novel engineering of semiconductor structures based on two coupled 2DEG systems can be used to create new and improved active optical devices based on indirect excitons. Usually, the modelling of the above excitonic structures relies on balance equations or on the calculation of steady states through the solution of the electron-hole Schrödinger or Gross–Pitaevskii equations. However, the short-scale time evolution of single excitons, eventually charged, represents a key ingredient in understanding the dynamics and transient behavior of the aforementioned class of devices. Indeed, a time dependent simulation of the two- (neutral exciton) or three-particle (charged exciton) fully correlated dynamics is able to expose the paths followed by excitons in nanopatterned semiconductor structures. We will present preliminary results on single-exciton propagation in a quasi-1D semiconductor channel with either material modulation or electric field patterning along the propagation direction, forming an excitonic resonant tunneling diode (RTD) structure. Multi-mode split-gate channels will also be addressed, together with double channels where an electron and a hole localized in different layers form a weakly bound indirect exciton. Several material-modulation outlines will reproduce simple case studies, as single and double quantum wells and barriers. Three-particle simulations will specifically analyze autoionization states and trion dissociation in the above structures. Our method is based on a Fourier split-step approach [5]. In particular, the evolution operator is approximated by a second-order expansion and then applied iteratively to the initial exciton wave function consisting of a minimum indeterminacy wave packet in its center-of-mass coordinate and in its ground state in the electron-hole relative coordinate.

References:

[1] G. Grosso *et al.*, Nature Photonics 3 (2009) 577.
[2] Y. Y. Kuznetsova *et al.*, Optics Letters 35 (2010) 1587.
[3] S. Christopoulos *et al.*, Phys. Rev. Lett. 98 (2007) 126405.
[4] A. Amo *et al.*, Nature Photonics 4 (2010) 361.
[5] M. J. Ablowitz, B. Prinari, and A. D. Trubatch, Discrete and Continuous Nonlinear Schrödinger Systems, Cambridge University Press (2004).

[P50] Understanding properties and functions of reducible oxides

P. Luches[1], F. Pagliuca[1,2], F. Boscherini[3], V. Grillo[1], G. C. Gazzadi[1], and S. Valeri[1,2]

[1] S3, Insituto Nanoscienze – Consiglio Nazionale delle Ricerche, Modena, Italy
[2] Dip. di Scienze Fisiche Matematiche e Informatiche, Università di Modena e Reggio Emilia, Modena, Italy
[3] Dipartimento di Fisica, Università di Bologna, Italy

Keywords: cerium oxide, metal-oxide interaction, reducibility, epitaxial growth, spectroscopy.

Reducible oxides play a paramount role in many industrially and environmentally important applications, including catalysis, but also microelectronics, energy conversion and storage, sensor and fuel cells. The most outstanding property of these compounds is their capability to store, release and transport lattice oxygen, i.e. to act as oxygen reservoirs.

In order to understand and possibly optimize the material properties and functionalities, studies of model systems can be a convenient way of simplifying part of the complexity of real systems.

Cerium oxide has been identified as a reducible oxide prototype and studied in the form of epitaxial nanostructures grown by reactive MBE on a Pt(111) substrate. The low dimensional structures exhibit an atomically flat surface morphology and a high crystal quality [1]. The epitaxial structure of the layers has been analyzed by XAFS measurements on the Ce-L_3 edge [2] and by HR-TEM. The modifications of the properties of the system with thermal treatments in vacuum or O_2-rich atmosphere have been studied by XPS, STM and LEED.

The analysis of the obtained results has shown that the supported films are highly reducible, i.e. the oxidation state of the cations can be reversibly changed from +4 to +3. The maximum concentration of reduced cations depends on several factors, such as size, annealing time and temperature, and initial degree of oxidation. The proximity of the Pt surface can also play an important role. The reduction process is more relevant in the surface layers than in the deeper ones. The film surface shows remarkable changes after significant reduction, with the appearance of a different contrast in the STM images and of a reconstruction in the LEED patterns (Fig. 1). The reduction is always fully reversible, and the structure and morphology of the films can be brought back to the original ones.

The importance of the properties of the investigated material in the applications and the perspectives for their optimization will be discussed.

References:

[1] P. Luches, F. Pagliuca, and S. Valeri, J. Phys. Chem. C 115 (2011) 10718.
[2] P. Luches, F. Pagliuca, S. Valeri, and F. Boscherini, J. Phys. Chem. C 117 (2013) 1030.

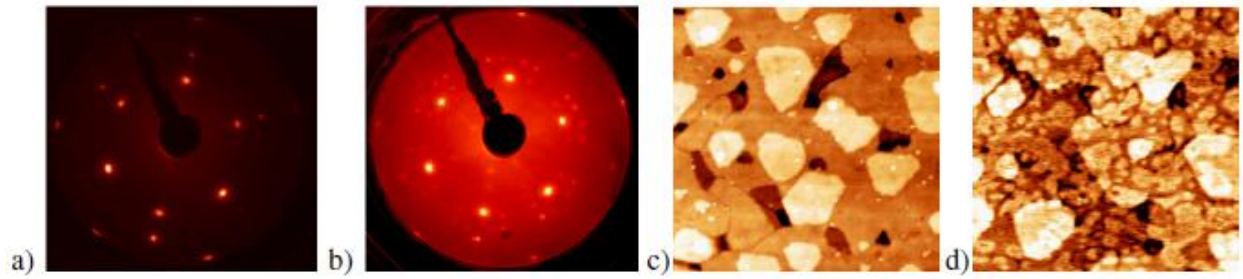


Fig. 1: LEED patterns of 2 ML CeO_2 on Pt(111) (a) before reduction and (b) after reduction, the latter showing the appearance of a long range surface reconstruction. STM images (size 125 nm × 125 nm) of 10 ML CeO_2 on Pt(111) (c) before reduction and (d) after reduction, evidencing the modification of surface topography.

[P51] Selective growth of InAs Quantum Dots on GaAs driven by As kinetics: experiment and theory

R. Magri[1], F. Arciprete[2], E. Placidi[3], M. Fanfoni[2], A. Balzarotti[2], and F. Patella[2]

[1] Dipartimento di Fisica, Università degli Studi di Modena e Reggio Emilia and Centro S3 CNR -Istituto Nanoscienze, Via Campi 213/A, 41100 Modena, Italy
[2] Dipartimento di Fisica, Università di Roma "Tor Vergata", Via della Ricerca Scientifica 1, 00133 Roma, Italy
[3] CNR - Istituto di Struttura della Materia, Via del Fosso del Cavaliere 100, 00133 Roma, Italy

Keywords: Quantum Dots, Molecular beam Epitaxy, Kinetic Modeling, Rate Equations.

A selective growth of InAs quantum dots (QDs) has been observed which is exclusively related to the As constituent. This experiment challenges the widespread belief that the As role in the InAs QDs growth is a minor one, being the QDs growth commonly described as dictated by the dynamics of cations assumed as the rate-limiting species. The selective growth is obtained by Molecular Beam Epitaxy at temperatures higher than 500°C and under an high As/In flux ratio, by changing and tuning the direction of the As flux on a rippled substrate. In these growth conditions the QDs become aligned along *only one* of the two mound slopes.

To explain the experiment we have developed a new kinetic model that incorporates many new features such as (i) a different dynamics for cations and anions; (ii) a distinction between the bulk and surface regions of the dot; (iii) a dot surface composition which comes to depend primarily on the growth conditions.

We find that the very small As flux gradient between the two mound slopes ($^{\Delta}F / F \sim (1\text{-}5)\%$) originates a cation current flow from one 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 cation adatom distribution between the two sides of the mound and activated by the relatively high temperatures.

Our findings shed a new light on the role of the molecular specie on the growth of compound semiconductor QDs and a comparable behavior is expected for the anions of other III-V and II-VI compound semiconductors as well.

References:

[1] F. Arciprete, E. Placidi, R. Magri, M. Fanfoni, A. Balzarotti, and F. Patella, ACS-Nano, in print.

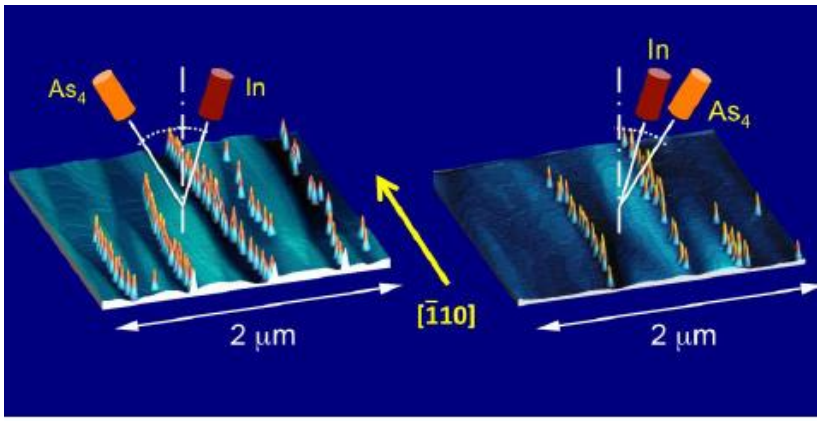


Fig. 1: AFM topographies showing the selective growth of InAs QDs as a function of the As flux direction.

[P52] THz imaging and non-destructive subwavelength biochemical assay/sensing with a QCL source

L. Masini[1,2,*], U. Siciliani de Cumis[2], J-H. Xu[2], S. Meucci[2], R. degl'Innocenti[2,3], F. Castellano[2], H. E. Beere[3], D. A. Ritchie[3], F. Beltram[1,2], M. S. Vitiello[2], M. Cecchini[2], and A. Tredicucci[2]

[1] Center for Nanotechnology Innovation @NEST, Istituto Italiano di Tecnologia, p.za S.Silvestro 12, 56127 Pisa, Italy
[2] NEST, Istituto Nanoscienze – CNR and Scuola Normal Superiore, p.za S.Silvestro 12, 56127 Pisa, Italy
[3] Cavendish Laboratory, University of Cambridge, J J Thomson Avenue, Cambridge CB3 0HE, UK
* luca.masini@sns.it

Our technologies focus on Terahertz (THz) Quantum Cascade Laser (QCL) for biological imaging and non-destructive assay/sensing of micro (subwavelenght) systems.

In particular we describe the implementation of a confocal microscopy system [1] based on a 2.9 THz QCL source. Lateral and axial resolutions better than 70 μm and 400 μm, respectively, are achieved, with a large contrast enhancement compared to the non-confocal arrangement. The capability of resolving overlapping objects lying on different longitudinal planes is also clearly demonstrated.

Furthermore we present our Lab-On-a-Chip technology for on-chip THz spectroscopy in a microfluidic environment (fig.1c). The system is based on a plasmonic metallic antenna that focalises the THz radiation produced from a 2.6 THz QCL source on a microfluidic channel of sub wavelength lateral dimension placed over the antenna layer (fig.1d). Collecting the transmitted radiation we can simultaneously detect the passage of sub wavelength objects inside the channel (preliminary tests were performed with polystyrene spheres) and analyze the THz response of the injected liquid/solution.

References:

[1] U. Siciliani de Cumis *et al.*, Optics Express 20 (2012) 21924.

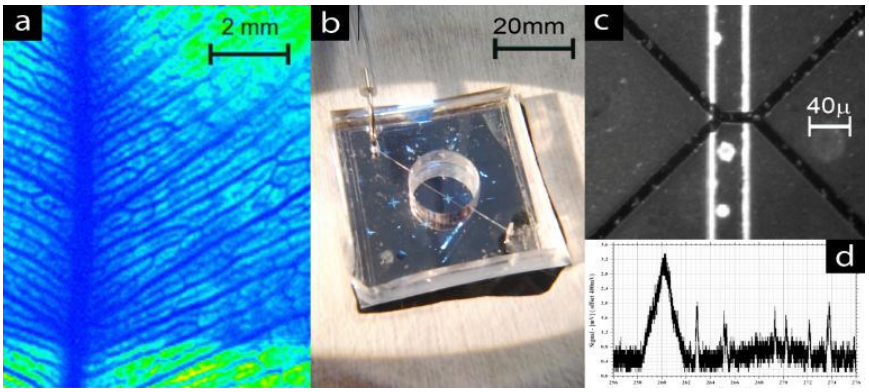


Fig. 1 THz imaging and non-destructive biological assay/sensing with a QCL source. (a) THz confocal image of the leaf 200x200 pixel. (b) Photograph of the microfluidic chip for THz On-Chip sub wave-length assay/sensing. (c) Microscope image of the microchannel aligned with the metallic plasmonic antenna with passing polystyrene spheres of various diameter. (d) Signal showing transmission peaks in correspondence of the passage of polystyrene spheres over the THz antenna.

[P53] Novel functional oxides for electronics and spintronic applications

A. G. Monteduro[1,2], C. Leo[2], S. Karmakar[1], Z. Ameera[2], A. P. Caricato[2], M. Martino[2], V. Tasco[1], R. Rinaldi[1,2], and G. Maruccio[1,2]

[1] NNL Istituto di Nanoscienze-CNR, Lecce, 73100, Italy
[2] Dipartimento di Matematica e Fisica "Ennio De Giorgi", Università del Salento, Lecce, Italy

Keywords: complex oxides, multiferroics, high-k materials, perovskites.

Complex transition metal oxides represent a vast class of materials with fascinating and interesting physical phenomena, such as high dielectric permittivities, ferroelectricity and multiferroicity. Their extreme sensitivity to structural distortions and crystal chemistry offers many routes to control these properties. Here we report our activity on multiferroic and high-k oxides, in particular $BiFeO_3$ (BFO) and Y_2CuTiO_6 (YCTO).

BFO is a promising multiferroic material for its high ordering temperatures far above room temperature [1] which make it suitable for the development of electrically controlled spin devices [2]. Our activity in Lecce ranges from material preparation to thin film deposition and characterization. Specifically, pure-phase BFO was prepared by solid state synthesis and structural characterization was carried out to confirm the absence of impurity phases. Dielectric measurements were then carried out, providing dielectric constant and dissipation factor respectively 61 and 0.1 at 100kHz. Magnetization measurements confirm the expected antiferromagnetic ordering and the absence of Fe-clusters in the sample. The ferroelectric response was measured using a home-made Sawyer-Tower circuit: spontaneous polarization, remnant polarization and coercive field were found to be $\approx 100 \mu C/cm^2$, 50 $\mu C/cm^2$ and 140kV/cm [4].

Bulk YCTO showed high dielectric constant (ε') and very small dielectric loss (tan δ) [3]. In resonators, antennas and transmitters, a high dielectric constant and a low dielectric loss are important to miniaturize the devices and reduce the bandwidth. Moreover, novel materials with improved dielectric properties are required to enhance the performance of CMOS field-effect transistors and to allow further miniaturization. However a quantitative analysis of the thin films is necessary for device applications. In our work we compared the dielectric properties of YCTO thin films prepared by PLD and characterized for their dielectric properties in comparison with SiO_2 and MgO. Bulk YCTO target were received from Prof. D.D. Sarma group. The dielectric constant of YCTO thin films was found to vary from 22 up to 100 at 100 kHz for the films deposited at 0.5 and 0.05 Pa oxygen pressure, respectively. This last value is about 25 times higher than for SiO_2 and 10 times higher than MgO [4].

References:

[1] J. Catalan and J. F. Scott, Adv. Mater. 21 (2009) 2463.
[2] T. Zhao *et al*., Nature materials 5 (2006) 823.
[3] D. Choudhury *et al.*, Phys. Rev. B 82 (2010) 134203.
[4] A. G. Monteduro *et al.*, in preparation.

[P54] AFM based friction analysis of few layer graphene

G. Paolicelli[1], M. Triphati[1,2], and S. Valeri[1,2]

[1] Centro S3, Istituto Nanoscienze CNR, Via Campi 213 Modena, Italy
[2] Dipartimento FIM, ,Università di Modena e Reggio Emilia, Via Campi 213 Modena, Italy

The exceptional properties of graphene range from large electron mobility, high thermal conductivity, optical transparency and elevated mechanical strength. In addition, graphene is a promising candidate as a thin solid lubricant [1] and as anti-wear coating agent due to its low friction coefficient and elastic characteristics. Graphene derives from graphite, one of the best and most utilized solid lubricant in mechanics, so this behavior appears reasonable. Nevertheless the lubricant properties of graphite often are attributed to its lamellar structure and to the low interaction between carbon planes along the stacking direction. Graphene properties, which shows comparable or lower friction coefficient respect to graphite, cannot be described by the mechanism of reduced interplane interaction.

Interesting and non intuitive experimental results has been obtained recently on both supported and epitaxially grown few layer graphene. Friction force measured by FFM set-up decreases with increasing graphene thickness. Single layer friction force is almost two times bigger than that recorded on 3-4 layer graphene. This behavior was attributed to the dependence of out-of-plane deformation on the number of layers onto a rigid substrate (SiO_2) [2] and to electron−phonon coupling for graphene grown epitaxially on SiC [3]. Theoretical simulations have produced contradictory results [4,5] that may depend by the effective binding strength of graphene sheet with its hosting surface. Here we will present our recent FFM results where we compare thickness dependent friction property of Si/SiO_2 supported graphene with respect to CVD grown graphene on polycrystalline Ni. This processes is emerging as one of the more relevant for large graphene sheet realization but it is well known the produce variable layer thickness graphene [6]. So from one side it is useful to analyze its friction properties for future technological applications but also it could be a benchmark to better understand thickness depend friction process in few layer graphene.

References:

[1] K. Kim *et al.*, ACS Nano 5 (2011) 5107.
[2] C. Lee *et al.*, Science 328 (2010) 76.
[3] T. Filleter *et al.*, Phys. Rev. Lett. 102 (2009) 086102.
[4] A. Smolyanitsky *et al.*, Phys. Rev. B 85 (2012) 035412.
[5] M. Reguzzoni *et al.*, Journal of Phys. Chem C 116 (2012) 21104.
[6] A. Reina *et al.*, Nano Lett. 9 (2009) 30.

[P55] A statistical mechanical model for cooperative conformational fluctuations: relaxation and plastic response in semicrystalline polymers

M. Pieruccini

C.N.R. Istituto Nanoscienze, via G. Campi 213/A, 41125 Modena, Italy

A recently developed statistical mechanical model [1] allows to highlight, from the direct analysis of relaxation data in semicrystalline polymers, the connection between the emergence of conformational constraints and the increasing average size of the cooperatively rearranging regions (CRR). The model is an extension of the Adam-Gibbs scheme of glass forming liquids, in the sense that the energy threshold ζ above which the thermodynamic fluctuations may drive conformational readjustment, is now envisaged as a fluctuating quantity itself, because it depends on the actual CRR conformation.

In the present contribution, the statistical mechanical approach to the relaxation data analysis will be briefly outlined. Examples from dynamical mechanical spectroscopy (DMS) and broadband dielectric spectroscopy (BDS) will be discussed in this framework, in order to point out:
1. The connection between the width of the relaxation spectrum and the height of the energy threshold ζ
2. The connection between CRR size, z, and chemical potential $\Delta\mu = z^{-1} \zeta$
3. The connection between CRR size and the density of states allowing for readjustment

As the model suggests, the presence of a stress field reduces the average height of the readjustment energy threshold and the CRR size as well. This is the basis on which the comparison between conformational relaxation features and results of microhardness measurements for poly(ethylene terephthalate) is discussed [2].

References:
[1] M. Pieruccini and T. A. Ezquerra, Eur. Phys. J. E 29 (2009) 163.
[2] M. Pieruccini, A. Flores, and F. J. Baltá-Calleja, Mech. Mat., submitted.

[P56] Electron-electron interactions in artificial graphene and other low-dimensional nanostructures

S. Pittalis[1], C. A. Rozzi[1], E. Rasanen[2], and G. Vignale[3]

[1] CNR - Istituto Nanoscienze, Centro S3, Modena, Italy
[2] Department of Physics, Tampere University of Technology, Tampere, Finland
[3] Department of Physics and Astronomy, University of Missouri-Columbia, MO, USA

Keywords: graphene, electron-electron interaction, low-dimensional systems, density functional theory.

In its original definition, artificial graphene is an engineered nanostructure that consists of identical potential wells (quantum dots) arranged in an adjustable honeycomb lattice in the two-dimensional electron gas [1]. As our ability to control the quality of artificial graphene samples improves, so grows the need for an accurate theory of its electronic properties, including the effects of electron-electron interactions. Here we determine those effects on the band structure and on the emergence of Dirac points by means of density functional theory [2]. Recent developments and future challenges for the evaluation of exchange-correlation effects in low-dimensional nanostructures are discussed [3].

References:

[1] M. Gibertini, A. Singha, V. Pellegrini, M. Polini, G. Vignale, A. Pinczuk, L. N. Pfeiffer, and K. W. West, Phys. Rev. B, 79 (2009) 241406(R).
[2] E. Rasanen, C. A. Rozzi, S. Pittalis, and G. Vignale, Phys. Rev. Lett. 108 (2012) 246803.
[3] S. Pittalis and E. Rasanen, Phys. Rev. B 82 (2010) 165123.

[P57] Quantum continuum mechanics: recent extensions and future applications

S. Pittalis[1], G. Vignale[2], I. V. Tokatly[3], and C. A. Rozzi[1]

[1] CNR - Istituto Nanoscienze, Centro S3, Modena, Italy
[2] Department of Physics and Astronomy, University of Missouri-Columbia, MO, USA
[3] IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Keywords: quantum continuum mechanics, quantum hydrodynamics, electron excitations, exchange-correlation kernels, time-dependent current density functional theory.

Classical continuum mechanics is a theory of the dynamics of classical liquids and solids in which the state of the body is described by a small set of collective fields, such as the displacement in elasticity theory; and density, velocity, and temperature in hydrodynamics. A similar description is possible for quantum many-electron systems, at all length scales. Its existence is guaranteed by the basic theorems of time-dependent current density functional theory (TD-CDFT). Here, we present an extension of quantum continuum mechanics [1,2] to systems in the presence of a strong magnetic field [3]. In order to obtain explicit equations of motion for the particle density and current, we consider the anti-adiabatic linear response regime. Implications for the development of approximate exchange-correlation kernels of TD-CDFT and future applications are outlined.

References:

[1] J. Tao, X. Gao, G. Vignale, and I. V. Tokatly, Phys. Rev. Lett. 103 (2009). 086401.
[2] X. Gao, J. Tao, G. Vignale, and I. V. Tokatly, Phys. Rev. B 81 (2010) 195106.
[3] S. Pittalis, G. Vignale, and I. V. Tokatly, Phys. Rev. B 84 (2011) 245118.

[P58] Frictional mechanisms in few-layer graphene

M. Reguzzoni[1,2], A. Fasolino[3], M. Sacchi[1,2], E. Molinari[1,2], and M. C. Righi[1]

[1] Istituto Nanoscienze, CNR - Consiglio Nazionale delle Ricerche, I-41125 Modena, Italy
[2] Dept of Physics, Informatics and Mathematics, University of Modena & Reggio, I-41125 Modena, Italy
[3] Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 Nijmegen, NL

Keywords: graphene, friction, nanotribology, atomistic simulations.

preserve relevant interactions (e.g. magnetic) between the sliding materials. Graphene -a revolutionary material for its known electronic and mechanical properties- has great potential also in this context as the thinnest solid lubricant. The fundamental mechanisms governing friction are however not yet clear, and important issues are still open e.g. concerning the role of multiple graphene layers [1].

We investigate the friction mechanisms in multilayer graphene films by calculating the potential energy surfaces (PES) from first-principles [2], and by simulating the motion of a model tip on the films by classical molecular dynamics [1].

From the ab-initio PES we derive an analytical expression the describes the interaction energy between two graphene layers vs their relative position. Thanks to its formal simplicity, the proposed model allows for an immediate interpretation of the interlayer binding and the potential corrugation. The latter plays a crucial role in determining the intrinsic resistance to interlayer sliding and controls the frictional behaviour under load (fig. 1). We show that the dominant mechanism in these p-bonded systems is the increase in Pauli repulsion with load, while the effect of van der Waals adhesion is negligible.

To understand the role of N-layer graphene films, we evaluate both the PES modifications as a function of N [3] and the onset of mechanisms of energy dissipation due to interlayer motions during finite temperature simulations [1]. We find that a sliding tip on a supported few-layer film induces both out-of-plane (fig. 2) and in-plane deformations, which increase with the number of layers in the film. We elucidate a new frictional mechanism connected with shear layer motions.

References:

[1] M. Reguzzoni, A. Fasolino, E. Molinari, and M. C. Righi, J. Phys. Chem. C 16 (2012) 21104, and references therein.
[2] M. Reguzzoni, A. Fasolino, E. Molinari, and M. C. Righi, Phys. Rev. B 86 (2012) 245424.
[3] M. C. Righi *et al*., to be published.

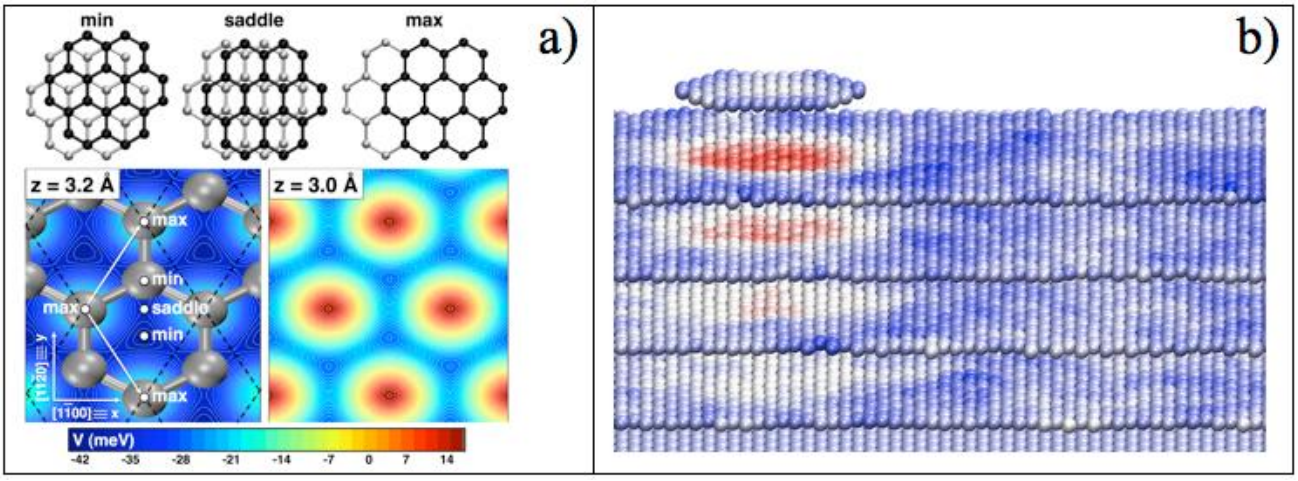


Fig. 1: PES function for bilayer graphene (a). Equilibrated structure of a 4-layer graphene film. The colour code indicates the deviation of the particle height from that of the layer center of mass. Blue corresponds to 0.4 Å and red to – 0.9 Å (b).

[P59] Real-time atomistic monitoring of diamond tribochemistry

G. Zilibotti[1,2], M. Ferrario[2], S. Corni[1], and M. C. Righi[1]

[1] Istituto Nanoscienze, CNR - Consiglio Nazionale delle Ricerche, I-41125 Modena, Italy
[2] Dept of Physics, Informatics and Mathematics, University of Modena & Reggio, I-41125 Modena, Italy

Keywords: diamond, solid lubricants, friction, tribochemistry, ab initio molecular dynamics.

Friction and wear are very common phenomena that impact many fields, from nanotechnologies to earthquakes, and are core to energy savings. Despite friction has been studied for centuries, our understanding of it is still unclear. The difficulty lies in the fact that this phenomenon is ultimately governed by atomic processes occurring at the interface between the two sliding materials.

One of the main challenges for modern tribology is, thus, answering the question: what processes are taking place at the buried sliding interface? A twofold task, which implies the development of new strategies for real-time, in-situ monitoring, and a new microscopic understanding of the physics and chemistry under the extreme conditions at such interface.

An important class of phenomena occurring at the buried interface, usually referred to as tribochemistry phenomena, is represented by the tribologically-induced chemical modifications of the surfaces interacting with lubricants or other molecules present in the environment surrounding the sliding media. These modifications can dramatically change the adhesion and friction of the materials in contact, therefore it is highly desirable understanding how they take place at the microscopic level. Our knowledge on the reaction kinetics and mechanisms at the open surface is not sufficient to this aim, since the tribological conditions can alter their rules. These conditions include the dissipation of frictional energy, molecular confinement, shear strains, high pressures.

Here we report the real-time atomistic description of the tribochemical reactions occurring at the interface between two diamond films in relative motion, by means of large scale ab initio molecular dynamics. Ultrahard, hydrogen-free carbon films are emerging as excellent solid lubricants, but their widespread application is limited by the enviromnental (e.g. humidity) dependence of their tribological properties. Our study unravels the dynamics of a mechanically-induced surface passivation by water, and reveals why this mechanism is fundamental to achieve low friction

References:

[1] G. Zilibotti, M. Ferrario, S. Corni, and M. C. Righi, submitted (2013).

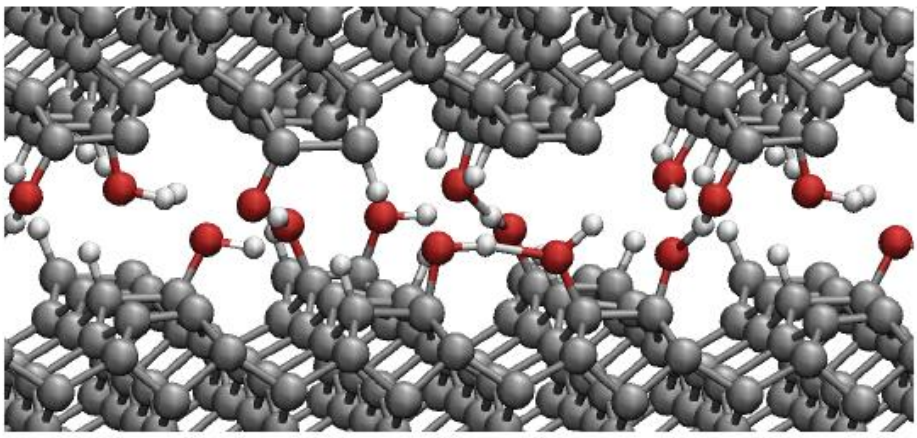


Fig. 1: Snapshot acquired during the *ab initio* molecular dynamics simulation of water confined at a clean diamond interface under pressure. The tribological conditions promote the dissociative adsorption of the water molecules with a consequent reduction of adhesion and friction.

[P60] New NMR approaches for the study or reorientational relaxation processes in organic solids

S. Sturniolo[1], M. Pieruccini[2], M. Corti[3], and A. Rigamonti[3]

[1] Rutherford Appleton Laboratory, Harwell Science Campus, Didcot, Oxfordshire, OX11 0QX, UK
[2] C.N.R. Istituto Nanoscienze, v. Campi 213/A, 41125, Modena, Italy
[3] Dipartimento di Fisica "A. Volta", v. Bassi 6, 27100, Pavia, Italy

The study of cooperative relaxation processes in polymers is fundamental for the understanding of many of their properties, most notably the glass transition. Nuclear Magnetic Resonance relaxometry provides a number of possible approaches to study molecular dynamics in solids, but most of them aren't suitable for the characterization of such relatively slow processes.

In this work a new approach to this analysis is presented. By relying on the geometric properties of dipolar interaction, a new model for the study of purely reorientational dynamics in solids containing proton pairs is developed [1]. The model is then applied to the study of alpha relaxation in Nitrile Butadiene Rubber [2] and poly(butadiene) and compared with previous results. Though there's still room for improvement, the new model proves a fast, consistent and reliable way of interpreting NMR dipolar signals in presence of motions with a single fitting parameter. The technique requires only the use of common NMR equipment and a very quick fitting step. The software developed for the purpose of performing these fits, EDDIE [3], is also presented. EDDIE has been released to the public as open source and is available for download to anyone who has an interest in it.

References:
[1] S. Sturniolo and M. Pieruccini, J. Mag. Res. 223 (2012) 138-147.
[2] S. Sturniolo, M. Pieruccini, M. Corti, and A. Rigamonti, Solid State Nucl. Mag. Res. (2013) [Epub ahead of print].
[3] https://sites.google.com/site/eddienmr/home.

[P61] Theory of graphene plasma-wave Terahertz photodetectors

A. Tomadin and M. Polini

NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy

Keywords: plasmonics, graphene, photodetection.

In a well-known Letter, Dyakonov and Shur [1] proposed a novel mechanism for detecting radiation by means of a simple field-effect transistor (FET). Recent experimental work [2] has demonstrated that this mechanism is active also in the case of the 2D massless Dirac fermion (MDF) fluid in a graphene FET. In this poster we present a theory of plasma-wave-assisted photodetection, which takes into account fundamental differences between massive 2D electron gases, considered by Dyakonov and Shur, and 2D MDF fluids. The theory we describe [3] relies on the fact that when electron-electron interactions are strong enough, there is a range of temperatures and sample purity [1,4] where thermodynamic equilibrium is established on a length scale which is much smaller than all other length scales over which momentum conservation is violated (e.g. electron-impurity and electron-phonon mean free paths). In this regime, the transport properties of the 2D MDF fluid in the FET channel can be described by hydrodynamics, a theory that relies only on the conservation of macroscopic quantities (charge, momentum, and energy). We demonstrate that the non-linearities that are peculiar to graphene hydrodynamics enhance the photodetector response [3] with respect to conventional 2D parabolic-band electron liquids. Our theory clearly shows that graphene is an ideal candidate to achieve the so-called "resonant" regime, where detection of THz radiation is resonantly enhanced by weakly-damped plasma waves confined under the FET gate.

References:

[1] M. Dyakonov and M. Shur, Phys. Rev. Lett. 71 (1993) 2465.
[2] L. Vicarelli, M. S. Vitiello, D. Coquillat, A. Lombardo, A. C. Ferrari, W. Knap, M. Polini, V. Pellegrini, and A. Tredicucci, Nature Mater. 11 (2012) 865.
[3] A. Tomadin and M. Polini, to be submitted.
[4] A. V. Andreev, S. A. Kivelson, and B. Spivak, Phys. Rev. Lett. 106 (2011) 256804.

[P62] A Multi-Scale - approach to graphene hydrogenation

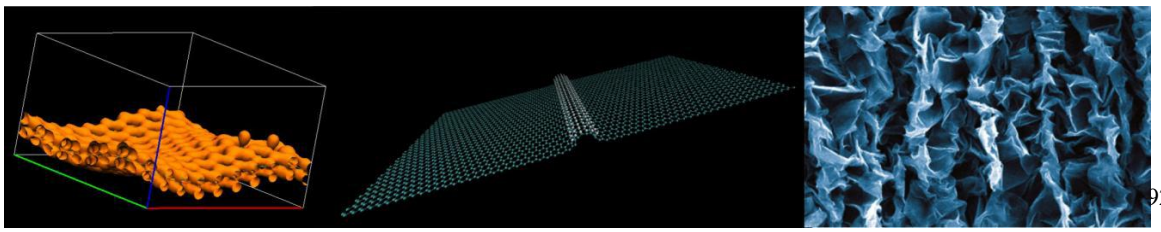
V. Tozzini[1,2], A. Rossi[1,2], R. Farchioni[1,3], and N. Pugno[4,5]

[1] NEST - Istituto Nanoscienze - Cnr Pisa, Italy
[2] Scuola Normale Superiore, Pisa, Italy
[3] Dipartimento di Fisica, Università di Pisa, Italy
[4] Laboratory of Bio-Inspired and Graphene Nanomechanics, Dipartimento di Ingegneria Civile, Ambientale e Meccanica, Università di Trento, Italy
[5] Fondazione Bruno Kessler, Centre for Materials and Microsystems, Trento, Italy

Keywords: Graphene, Molecular Dynamics Simulations, Density Functional Theory, Continuum approach.

Graphene[1] is a conductor, while its completely hydrogenated counterpart "graphane", is an insulator. Consequently, partially hydrogenated graphene is a semiconductor[2], whose electronic and transport properties can be tuned controlling the quantity and conformation of adsorbed hydrogen. The interest in hydrogenated graphene is also related to the fact that it has been recently proposed as a high capacity medium for hydrogen storage[3]. Its mechanical properties are equally noticeable: its flexibility and resistance to strain allow it to form ripples with various geometries and topologies.
Theoretical and experimental work [4] indicate that reactivity towards H is enhanced on convexities and decreased in concavities, opening the possibility of exploiting the curvature to control graphene hydrogenation. The relationship between curvature and H binding energy was quantified by means of DFT calculations on a sheet with nano-sized ripples[5]. Both H-storage and nano-electronics could take advantage of this effect: ripples could be used to guide H adsorption/release with specifically designed decorations; inversion of curvature can be used to release H as shown by Car-Parrinello simulations[5].
However, creation and manipulation of ripples is realistically feasible on the scale of 10-100nm, 1-2 orders of magnitude larger than those addressable with DFT. The times necessary to reach equilibrium in hydrogenation are orders of magnitude larger than those accessible to Car-Parrinello simulation.
To the aim of increasing the space and time scales reachable in silico, we adopted a multi-scale approach. Based on DFT calculations, we propose an empirical atomistic force field for graphene-graphane, including the dependence of chemical and deformation energy on the curvature. With this, we examined the structural, mechanical and dynamical properties of a number of structures with different patterns of ripples and hydrogenation on the scale of tens or hundreds of nanometers. This force field is also compatible with available ones for SiC, so that simulations of epitaxially grown graphene are addressable. The structures obtained with this approach are then used for single structure electronic structure and transport properties calculations.
On the other hand, we address the problem with a continuum approach [6-9], based on elasticity, contact mechanics and geometry, incorporating in the model energetic and structural information from the two previous description levels. With this approach, one can access statistically relevant information of hydrogenation of macroscopic graphene structures.

References:
[1] A. K. Geim and K. S. Novoselov, Nat. Mat 6 (2007) 183.
[2] V. Tozzini and V. Pellegrini, PRB 81 (2010) 113404.
[3] V. Tozzini and V. Pellegrini, PCCP 15 (2013) 80.
[4] S. Goler *et al.*, submitted.
[5] V. Tozzini and V. Pellegrini, JPCC 115 (2011) 25523.
[6] J. Zang, Q. Wang, Q. Tu, S. Ryu, N. Pugno, M. Buehler, and X. Zhao, Nat. Mat (2013).
[7] N. Pugno, A. Astron. 82 (2013) 221.
[8] N. Pugno, J. Mech. Phys. Solid. 58 (2010) 1397.
[9] X. Shi, Y. Cheng, N. Pugno, and H. Gao, Small 6 (2010) 739.



[P63] Andreev levels spectroscopy in topological SNS junctions

S. Valentini, F. Taddei, V. Giovannetti, and R. Fazio

NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, I-56126 Pisa, Italy

Keywords: Majorana fermions, Quantum transport, Andreev reflection, Josephson effect.

The emergence of Majorana excitations in solid state systems is an extraordinary phenomenon not only per se (a Majorana particle is its own antiparticle [1]), but also for possible applications in topological quantum computation. The latter would not require any quantum error correction since Majorana excitations are immune to local noise due to their nonlocal topological nature [2][3].

The presence of Majorana excitations has been predicted in nanowires with strong spin-orbit Rashba interaction, in presence of a Zeeman field and proximity coupled to an s-wave superconductor. When the magnetic field is large enough, a quantum phase transition is induced and the superconducting wire is brought into a topological phase. Majorana fermions then emerge at the ends of the wire as bound states at zero energy [4][5].

In this work the effects of Majorana Fermions in quasi-1D Superconductor-Normal-Superconductor (SNS) heterostructures are investigated. A single nanowire is proximity coupled to s-wave superconductors in two different regions, leaving a normal one in the middle to form an SNS junction.

Effects due to the presence of the Majorana modes are investigated by studying the local density of states in the junction region and the tunneling current flowing through a probe attached to the weak link. Numerical calculations within a tight-binding model have been conducted and demonstrate that the differences between results for the trivial and topological phases can be used as "smoking-gun" detectors for the topological phase.

References:

[1] E. Majorana, Nuovo Cimento 14 (1937) 171.
[2] M. Leijnse and K. Flensberg, Semicond. Sci. Technol. 27 (2012) 124003.
[3] J. Alicea, Rep. Prog. Phys. 75 (2012) 076501.
[4] R. M. Lutchyn, J. D. Sau, and S. Das Sarma, Phys. Rev. Lett. 105 (2010) 077001.
[5] Y. Oreg, G. Refael, and F. von Oppen, Phys. Rev. Lett. 105 (2010) 177002.

[P64] Topological regulation of activation barriers on fractal substrates

A.Vezzani[1], R. Burioni[2], and F. Corberi[3]

[1] Centro S3, CNR-Istituto di Nanoscienze, Via Campi 213A, 41125 Modena, Italy
[2] Dipartimento di Fisica e Scienza della Terra, and INFN, Gruppo Collegato di Parma, Università di Parma, Parco Area delle Scienze 7/A, I-423100 Parma, Italy
[3] Dipartimento di Fisica "E. R. Caianiello" and INFN, Gruppo Collegato di Salerno, and CNISM, Unità di Salerno, Università di Salerno, via Ponte don Melillo, 84084 Fisciano (SA), Italy

Keywords: non-equilibrium statistical physics, coarsening.

We study phase-ordering dynamics of a ferromagnetic Ising system on fractal graphs. We describe this coarsening process using a dynamical scaling approach, inspired by renormalization group ideas. In such approach the system dynamics is determined by the scaling length L(t) that is the typical size of the growing ordered domains. On homogeneous lattices L(t) grows diffusively with time while on inhomogeneous systems the dynamics is typically slowed down by the presence of free energy barriers and activated processes. On the fractal structures considered in this work the effects of such barriers can be analytically estimated. In particular, we evidence the existence of two classes of inhomogeneous substrates, on finitely ramified graphs the free energy barriers encountered by domains walls grow logarithmically with L(t) while they increase as a power-law on infinitely ramified structures. This produces different asymptotic growth laws (power-laws vs logarithmic) and different dependence of the crossover length on the model parameters. Our theoretical picture agrees very well with extensive numerical simulations.

References:
[1] R. Burioni, F. Corberi, and A. Vezzani, Phys. Rev. E 87 (2013) 032160.

[P65] Frontiers in germanium-based photonics

M. Virgilio and G. Grosso

Dipartimento di Fisica E. Fermi, Università di Pisa, Largo Pontecorvo 3, I-56127 Pisa, Italy
NEST, Istituto Nanoscienze-CNR, Piazza San Silvestro 12, I-56127 Pisa, Italy

Keywords: Silicon Photonics.

We present the fundamental aspects and expectations of germanium-based photonics which is a fast growing research field aimed at the development and integration of optical functionalities in the mainstream silicon technology.

We demonstrate that appropriate strategies in the design of experimental conditions and sample preparation offer the possibility of circumventing the well-known limitations of group IV indirect-gap materials as interband light emitters.

In particular, we show that the theoretical and numerical tools developed in our group are able to provide the necessary information on electronic levels, band parameters, band alignment, effective mass values, etc., needed for the quantum design of bulk and nanostructured germanium systems considering the most complete range of doping conditions, lattice strain values, injection charge densities and temperature.

[P66] Exciton Build-up from Polymer Precursors to Graphene Nanoribbons

S. D. Wang[1], A. Ferretti[1], D. Prezzi[1], A. Ruini[1,2], and E. Molinari[1,2]

[1] Centro S3, CNR-Istituto Nanoscienze, Modena, Italy
[2] Dipartimento di Scienze Fisiche, Informatiche e Matematiche, UNIMORE, Italy

Keywords: quasiparticle energies, excitons, graphene nanoribbons.

Recent advancements in production techniques have allowed the bottom-up fabrication of atomically precise graphene nanoribbons (GNRs) [1], finally enabling the first experimental investigations of the properties of this exciting class of materials (see e.g. [2]). The ribbon topology, width and edge periphery are dictated by precursor monomers designed on purpose, which couple into linear polyphenylenes via surface-assisted synthesis and are subsequently transformed by cyclodehydrogenation.

Here we investigate from first-principles the optical properties of GNRs and of their corresponding molecular and polymer precursors. We consider graphene nanoribbons with different topologies, i.e. armchair (N=7) and chevron-like [(6_A,9_A) CGNRs], with and without nitrogen edge-doping. The quasiparticle band structure is obtained within the *GW* scheme; excitonic effects are included in the calculation of optical excitations and absorption spectra through the solution of the Bethe-Salpeter equation.

Our results on the spectral evolution from molecular/polymer precursors to nanoribbons are in excellent agreement with recent cutting-edge optical measurements [3]. Moreover, the analysis of the composition of the optical excitations and of the exciton wavefunctions of the different systems allows us to characterize the build-up of quasi-1D excitons in graphene nanoribbons.

References:

[1] J. Cai *et al*., Nature 466 (2010) 470.
[2] P. Ruffieux, J. Cai, N. C. Plumb, L. Patthey, D. Prezzi, A. Ferretti, E. Molinari, X. Feng, K. Müllen, C. A. Pignedoli, and R. Fasel, ACS Nano 6 (2012) 6930.
[3] P. Ruffiex *et al.*, unpublished work.

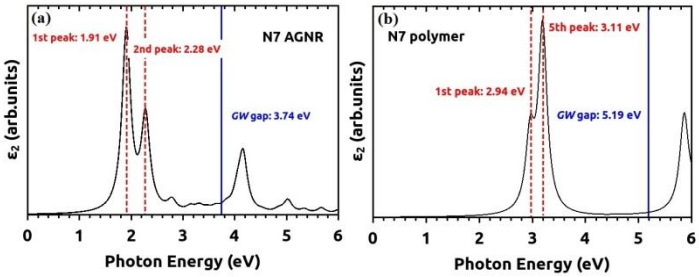


Fig. 1: Optical absorption spectra of (a) N=7 armchair GNR and (b) its polymer precursor. The dashed lines (red) and solid lines (line) denote peak positons and *GW* gap values, respectively.

[P67] When microfluidics meets chemistry

V. Arima[1], A. Zizzari[1], A. Zacheo[1,2], M. Bianco[1], I. Viola[1], E. Perrone[1], L. Marra[1], and R. Rinaldi[1,2]

[1] National Nanotechnology Laboratory (NNL) - CNR-Istituto Nanoscienze, U.O.S. Lecce, Via per Arnesano 16, 73100 Lecce, Italy
[2] Università del Salento, Dipartimento di Matematica e Fisica "E. De Giorgi", ex Collegio Fiorini Campus extraurbano, via per Arnesano, 73100, Lecce, Italy

Keywords: Microfluidics, organic chemistry, microreactors, radiochemistry, surfactants.

In the last decade new generation of chemists are exploiting microfluidics as innovative tool for chemical synthesis as well as for the study of chemical interactions at microscale.

Continuous-flow microreactors are nowadays applied to several fields of synthetic chemistry, and are of great appealing especially in radiochemistry and catalysis since with reduced volume of solvents, chemical reactions are less wasteful, more safety and are carried out significantly faster than those in batch, with increases in yield and selectivity. [1]

Additionally, thanks to the fluid confinement, microfluidics allows to accurately exploit chemical interactions between molecules and solid or liquid interfaces at micro/nanoscale.

In this work we will describe three applications of microreactors to the synthesis and purification of chemicals developed in collaboration with other European groups. We will focus on the fabrication of microfluidic-based networks for the synthesis of radiopharmaceuticals and on the advantages of the microfluidic approach in comparison with traditional vessel production [2]. Then we will demonstrate the possibility to perform a process of solvent exchange in a microfluidic environment to enrich a water/acetonitrile mixture in water [3]. A third application we will report on is the synthesis of biaryl compounds in a multichannel micro reactor embodying a silica supported nickel catalyst (Ni/SiO_2) [4].

Then we will move to three different studies of chemical interactions in confined environments. Firstly we will focus on the fluid dynamics of several solvents in fluorinated-coated polydimetyl siloxane (PDMS) microchannels [5] and on their modeling in a capillary-driven system. Then microchannel arrays will be used to investigate the propellant effect of some molecules embodied in microcapsules; the molecule-induced turbulence effects in a capillary flow model will be explained and quantified [6]. Finally a droplet microfluidic network able to produce fluorosolvent droplets in water will be described and the role of a protein as surfactant demonstrated [7].

References:

[1] B. P. Mason, K. E. Price, J. L. Steinbacher, A. R. Bogdan, and D. T. McQuade, Chem. Rev. 107 (2007) 2300.
[2] V. Arima, G. Pascali, O. Lade, H. Kretschmer, I. Bernsdorf, V. Hammond, P. Watts, F. De Leonardis, M. Tarn, N. Pamme, P. Dittrich, B. Cvetkovic, N. Vasovic, R. Duane, A. Jaksic, A. Zacheo, A. Zizzari, L. Marra, E. Perrone, P. Salvadori, and R. Rinaldi, Lab on a Chip, accepted for publication.
[3] B. Z. Cvetković, O. Lade, L. Marra, V. Arima, R. Rinaldi, and P. S. Dittrich, RSC Adv. 2 (2012) 11117.
[4] L. Marra, V. Fusillo, C. Wiles, A. Zizzari, P. Watts, R. Rinaldi, and V. Arima, Sci. Adv. Mat. (SAM), accepted for publication.
[5] M. Bianco, I. Viola, M. Cezza, F. Pietracaprina, G. Gigli, R. Rinaldi, and V. Arima, Microfluid. Nanofluid. 13 (2012) 399-409.
[6] L. L. Del Mercato, V. Arima, I. Viola, M. Bianco, A. Zizzari, R. Miglietta *et al*., in preparation.
[7] R. Milani, E. Monogioudi, M. Baldrighi, G. Cavallo, V. Arima, L. Marra, A. Zizzari, R. Rinaldi, M. Linder, G. Resnati, and P. Metrangolo, Chemical Science, submitted.

[P68] 2π and 4π Josephson current in superconductor-2d topological insulator-superconductor junction with interactions

S. Barbarino[1], F. Taddei[1], M. Sassetti[2], and R. Fazio[1]

[1] NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, I-56126 Pisa, Italy
[2] Dipartimento di Fisica, Università di Genova and CNR-SPIN, I-14146 Genova, Italy

Keywords: topological insulators, Josephson effect, Luttinger liquid.

Two-dimensional topological insulators (TI) are a new phase of matter which admit one-dimensional helical edge states whose existence was theoretically conjectured by Bernevig, Hughes and Zhang in 2006 for CdTe/HgTe/CdTe quantum-wells [1]. Since their prediction the scientific community has devoted great efforts in studying the electrical transport properties of these helical edge states where electrons have spin direction and momentum locked each other.

In 2008 for the first time, Fu and Kane considered a Josephson junction [2] where such topological insulators are coupled to s-wave superconductors (S-TI-S). In particular, they focused on the short junction-regime where the length of the weak link is much shorter than the BCS coherence length, and showed the existence of a 4π periodic Josephson current if the fermion parity is conserved. More recently, Beenakker et al.[3] studied the same system in the long junction regime showing that the 4πcritical Josephson current is doubled with respect to the 2π periodic critical current.

Our research project is devoted to study how the 2π and 4π periodic Josephson currents are affected by the Coulomb interaction. We focused on the long junction-regime where the helical edge states can be described as Luttinger liquids and can be exactly studied, even in presence of short-range two-body interactions, using the bosonization technique.

For transparent interfaces, where only perfect Andreev reflection occurs at the superconductor-topological insulator boundaries, the Josephson current is only affected by the back-scattering term induced by the Coulomb interaction and no significant corrections arise with respect to the non interacting case. However, if a strong point-like magnetic barrier is present in the weak link, the situation changes abruptly. The Josephson current is now strongly affected by the Coulomb interaction and it exhibits interesting power laws depending on its strength both in the low and high temperature regimes. Surprisingly, if a magnetic barrier in present the 4π periodic critical current is halved with respect to the 2π one, unlike the transparent regime.

Furthermore, a phase-shift of Josephson current can be induced by changing the direction of the magnetization of the barrier. These results can be easily generalized if there are many point-like magnetic barriers or even if an extended magnetic domain is present.

References:

[1] B. A. Bernevig, T. L. Hughes, and S. C. Zhang, Science 314 (2006) 1757.
[2] L. Fu and C. L. Kane, Phys. Rev. B 79 (2008) 161408(R).
[3] C. W. J. Beenakker, D. I. Pikulin, T. Hyart, H. Schomerus, and J. P. Dahlhaus, Phys. Rev. Lett. 110 (2013) 017003.

[P69] Polymer nanostructures: got to work into device platforms

A. Camposeo[1,2], L. Persano[1,2], F. Di Benedetto[1], P. Del Carro[1], and D. Pisignano[1,2,3]

[1] National Nanotechnology Laboratory of Istituto Nanoscienze-CNR, via Arnesano, 73100 Lecce, Italy
[2] Center for Biomolecular Nanotechnologies @ UNILE, Istituto Italiano di Tecnologia Via Barsanti, 73010 Arnesano (LE), Italy
[3] Dipartimento di Matematica e Fisica "Ennio De Giorgi", Università del Salento via Arnesano, 73100 Lecce, Italy

Keywords: nanocomposites, nanostructures, microfluidics.

Polymer and nanocomposite micro- and nanostructures are widely exploited in different fields; properly designing and combining their constituents is a direct and effective way to obtain new materials with tailored or improved properties. However, nanopatterning and interfacing nanostructures with devices at macro-scale remain challenging. Here we present a few model technologies that we developed, concerning the realization of electro-optical devices including electrically tunable lasers based on organic nanostructures, the use of polymer and composite nanostructures in nanophotonic devices, the fabrication of novel device-embeddable polymer fibrous nanostructures by three-dimensional lithographies and elastomeric polymeric microspheres employed as a direct-writing tool for the continuous delivery of molecular materials. Advantages include superior control on particles dispersion, size and positioning, highly favorable film-forming and flow properties, and controllable light-emission of patterned polymer–nanoparticle composites, fibers etc.

Acknowledgments. The financial support from the FIRB Contract RBFR08DJZI "Futuro in Ricerca" is acknowledged.

References:
[1] A. Camposeo *et al.*, Journal of Materials Chemistry 22 (2012) 9787.
[2] S. C. Laza *et al.*, Advanced Materials 24 (2012) 1304.
[3] A. Camposeo *et al.*, Adv. Mater. 24 (2012) OP221.
[4] A. Polini *et al.*, Scientific Reports 2 (2012) 607.
[5] F. Di Benedetto *et al.*, Soft Matter 9 (2013) 2206.

[P70] Functional polymer nanofibers for nanophotonics, nanoelectronics and tissue engineering

A. Camposeo[1,2], L. Persano[1,2], M. Moffa[2], V. Fasano[2], and D. Pisignano[1,2,3]

[1] National Nanotechnology Laboratory of Istituto Nanoscienze-CNR, via Arnesano, 73100 Lecce, Italy
[2] Center for Biomolecular Nanotechnologies @ UNILE, Istituto Italiano di Tecnologia Via Barsanti, 73010 Arnesano (LE), Italy
[3] Dipartimento di Matematica e Fisica "Ennio De Giorgi", Università del Salento via Arnesano, 73100 Lecce, Italy

Keywords: polymer nanofibers, electrospinning.

Functional polymer nanofibers are novel one-dimensional nanostructures, exhibiting smart physico-chemical properties, with applications ranging from textiles to sensing and filtrating elements, tissue engineering and regenerative medicine, nanoelectronics and optoelectronics. Technologies for producing polymer nanofibers are rapidly evolving from the production of inert nanofibers materials to more specialized, functional and multi-functional nanofibers. The nanostructure capabilities range from conduction properties to light-sensing, from promoted cellular differentiation to enhanced mechanical and anisotropy properties. Here results and perspectives of our research on functional polymer nanofibers are presented, focusing on complementary applications of electrospun nanofibers. Demonstrators include photo- and field-effect transistors, smart controllable surfaces, polarized light-emitters, lasers and bioactive scaffolds.

The financial support from the FIRB Contracts RBFR08DJZI "Futuro in Ricerca" and RBNE08BNL7 "Merit" is acknowledged.

References:
[1] A. Polini *et al.*, Soft Matter 6 (2010) 1668.
[2] D. Tu *et al.*, Nanoscale 2 (2010) 2217.
[3] D. Tu *et al.*, Adv. Funct. Mater. 21 (2011) 1140.
[4] D. Tu *et al.*, Appl. Phys. Lett. 98 (2011) 023307.
[5] A. Polini *et al.*, Plos One 6 (2011) e26211.
[6] M. Moffa *et al.*, Soft Matter (2013) in press.

[P71] Visualizing Cellular Nuclear Pore Viscosity in CHO cells

R. Castagna[1], F. Cardarelli[2], A. Battisti[1], B. Storti[1], and R. Bizzarri[1,3]

[1] NEST, Istituto Nanoscienze-CNR, Scuola Normale Superiore di Pisa, 56127 Pisa, Italy
[2] Center for Innovation Technology@NEST, Istituto Italiano di Tecnologia, 56127 Pisa, Italy
[3] Istituto di Biofisica - CNR, 56124 Pisa, Italy

Keywords: nano-imaging, fluorescence anisotropy, viscosity at nanoscale.

The constant demand for nano-scaled systems to be used in nano-bio-imaging and nano-diagnostics brings our research to explore different approaches: on one side, the development of fluorescence microscopy methods functional to probe the nanoenvironment of selected cell organelles, on the other side the development of new systems for nanoimaging, by using nonlinear and fluorescent optical materials. Concerning the first approach, we have been focusing on the measurement of viscosity at the level of nuclear pores. This investigation has been carried out by a methodology that involves the measure of fluorescence anisotropy (static anisotropy). In more details, we measured and compared the fluorescence anisotropies of the cytoplasm, of the nuclear pore district, and of the nucleus of the cell. High values of fluorescence anisotropy correspond to high values of medium viscosity, due to steric hindrance exerted by the medium upon the free molecular rotation. The used method implies simultaneous observation of the perpendicular and parallel polarization components through separate channels. For our experiments we used: (a) Enhanced-Green Fluorescent Protein (EGFP), a fluorescent protein that diffuses isotropically in the cell; (b) POM-Cherry, a fluorescent protein targeted to bind to nucleoporins, a class of protein whose the nuclear pore is enriched.

Cell fluorescence was measured using a Leica TCS SP5 SMD inverted confocal microscope (Leica Microsystems AG) interfaced with an Ar laser for excitation at $\lambda = 488$ nm and 561 nm. In short, we measured the fluorescence anisotropy of passively diffusing EGFP in Hamster Chinese Ovary cells across a line starting from cytoplasm, ending in the nucleoplasm, and crossing the nuclear envelope as highlighted by the POM-Cherry (Fig. 1).

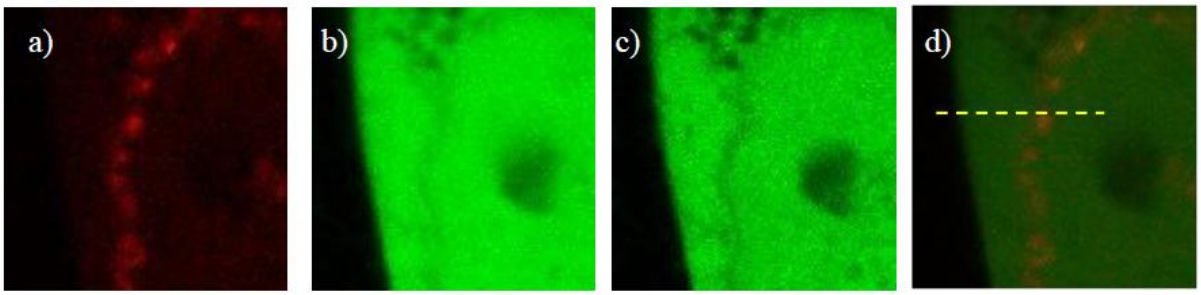


Figure 1: a) fluorescent emission of POM identify porins and trace the nucleus membrane (excitation wavelength $\lambda = 561$ nm); b) detection of 0° polarization laser-light component (excitation wavelength $\lambda = 488$ nm); c) 90° polarized light component (excitation wavelength $\lambda = 488$ nm). d) Superimposition of the pictures a) and b). Yellow dashed line: scanned region.

The scanned line (128 pixel) was repetitively acquired (512 lines) in order to detect eventual variations of the anisotropy in time due to physiological internal mobility of the cell compartments and components. In this manner we determine matrices corresponding to the different polarization component detected (Figs. 3b and 3c).

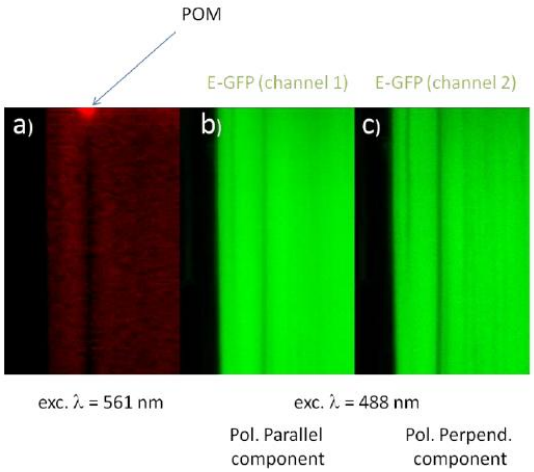


Fig. 2: a)-c) matrices obtained from scanning the region identified in Figure 1d) by yellow dashed line. As it is evident in the figure a) POM bleaches after few scans: however POM location is well identifiable. b) matrix related to the 0° pol.; matrix related to 90° pol.

Preliminary data indicates that, at nuclear pore level, anisotropy is significantly different from that detectable in cytoplasm and nucleoplasm. The significance of our findings resides in the fact that they represent the first optical detection and measurement of the viscosity medium into one single nuclear pore of a cell.

References:

[1] J. R. Lackowitz, Principles of Fluorescence Spectroscopy, Springer, 2 Ed. (1999).

[P72] Integrated polymeric waveguide components for THz quantum cascade laser outcoupling

F. Castellano and M. Vitiello

CNR Istituto Nanoscienze, NEST, Piazza S. Silvestro 12, 56127 Pisa

Keywords: THz components, quantum cascade laser, frequency tuning.

THz quantum cascade lasers are actively being developed with the goal of using them in THz spectroscopic systems[1], which require power semiconductor sources capable of single mode continuous tuning over a large bandwidth. The most promising technology to realize THz QCLs is the double metal waveguide process, consisting of a metallic parallel plate waveguide filled with the optically active material. This geometry provides the highest cavity field confinement and thus allows to reach the highest operating temperatures (200 K), but it usually causes highly multimodal emission of the laser and poses intrinsic limitations on the quality of the emitted beam, that is highly diffracted by the subwavelength sized emission facet.
In addition, the large wave impedance mismatch between the inside of the cavity (~ 10 ohm) and free space (377 ohm) makes it extremely hard to modify the laser spectrum from the outside (i. e. with optics) and obtain frequency control of the emission over a large bandwidth. For this reason, reported tuning efforts of double metal THz QCLs always point in the direction of changing the effective refractive index of the lasing modes, thus changing the emission frequency by changing an internal property of the cavity[2]

We recently developed a novel approach based on the use of onchip components to couple the laser emission out of the low impedance laser cavity, into higher impedance waveguides that can be more easily coupled to the outside to achieve spectral control.
The validity of our approach is backed by FEM simulations that show that it is possible to achieve almost 100% coupling over a large (> 500 GHz) bandwidth by using grating couplers patterned in the common wall of stacked metallic waveguides. While this geometry is well established in the microwave domain, its scaling into the THz range poses many technological challenges, mainly coming from the difficulty of finding suitable materials and processes for the fabrication of the required components. THz transparent moldable polymers [3] exhibit a refractive index that is intermediate between the one of GaAs and that of air, and can be cast into the desired shape by molding and imprinting at temperatures that are compatible with the laser process. These two features make these materials a good platform for the development of onchip THz components to be coupled with double metal QCLs. We have simulated and designed the the devices (directional couplers, horns, waveguides) and we are developing the techniques and tools that will allow us to fabricate them and integrate them in a QCL process, experimenting with different polymeric materials.

References:
[1] S. Kumar, IEEE Journal of , 17, 1 (2011) 38.
[2] M. S. Vitiello and A. Tredicucci, IEEE Trans. Terahertz Sci. Tech, 1 (2011) 76.
[3] P. D. Cunningham *et al.*, J. Appl. Phys. 109 (2011) 043505.

[P73] Microwave-assisted synthesis of TiO_2 nanocrystals, with dimension and shape control

C. Carlucci[1], G. Antico[1], and G. Ciccarella[1,2]

[1] Istituto Nanoscienze – CNR ,NANO, Via Arnesano, 73100 Lecce, Italy.
[2] Dipartimento di Ingegneria dell'Innovazione, Università del Salento, Via Monteroni, 73100, Lecce, Italy

Keywords: Microwave, TiO_2 nanocrystals.

Titanium dioxide, TiO_2, is a well studied and widely used material for many photocatalytic and photoelectrochemical applications. In photocatalysis, it has been used for decomposition of water and degradation of organic pollutants in air as well as in aqueous media, while in photoelectrochemistry, it has found use in dye sensitized solar cell (DSSC) applications thanks to its electrical and electronic properties its high catalytic activity and excellent stability in many solvents over a wide pH range. Many efforts have been made to modify the electronic properties of TiO_2 in order to extend its optical absorption edge into visible light and enhance its photocatalytic activity.

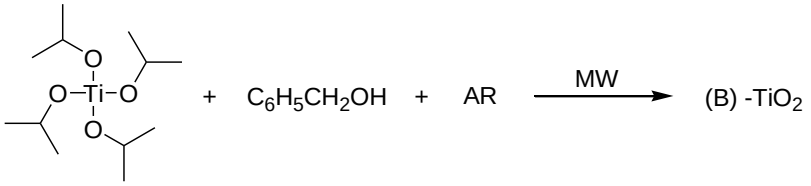
An efficient method to synthesize anatase TiO_2 nanorods by hydrolysis of titanium tetraisopropoxide (TTIP) in benzyl alcohol has been developed [1], using acetic or oleic acid as additive reagents. The different shaped TiO_2 nanocrystals were obtained tuning the TTIP-acetic acid or TTIP-oleic acid ratio and were characterized in detail. The novelty of the present approach relies on the shape controlled synthesis of anatase TiO_2 nanocrystals via microwave-solvothermal method.

A simple synthesis was applied and tested to prepare boron-doped titanium dioxide [TiO_2(B)] nanocrystals using titanium tetra-isopropoxide (TTIP) together with boric acid and benzyl alcohol as reaction solvent. The changes in the TTIP:H_3BO_3 molar ratio allowed to set up a scalable synthetic protocol with a significant B-dopant control. In particular, this approach does not need the use of surfactants and a final calcination step [2].

Furthermore a microwave-assisted method to synthesize B-doped TiO_2 nanorods by hydrolysis of titanium tetraisopropoxide (TTIP) in benzyl alcohol, together with boric acid and in the presence of oleic acid as additive reagents, has been developed. Chemical modification of TTIP by oleic acid is proven to be a rational strategy to tune the shape of the Anatase TiO_2 nanocrystals [3].

The different nanocrystals were characterized in detail by X-ray diffractometry (XRD), low and high resolution Transmission Electron Microscopy (TEM and HRTEM), micro Raman spectroscopy, Inductively Coupled Plasma-Atomic Emission Spectroscopy (ICP-AES), ^{11}B cross-polarized magic angle spinning nuclear magnetic resonance (^{11}B CP-MAS NMR), X-ray photoelectron spectroscopy (XPS), microphotoluminescence and UV-vis absorption. The photocatalytic activity of TTIP-acetic acid and TTIP-oleic acid nanocrystals was also evaluated.

References:
[1] G. Ciccarella, R. Cingolani, L. De Marco, G. Gigli, G. Melcarne, F. Martina, F. Matteucci, and J. Spadavecchia, PCT Int. Appl. WO 2009/101640 A1.
[2] H. Xu, R. A. Picca, L. De Marco, C. Carlucci, A. Scrascia, P. Papadia, B. F. Scremin, E. Carlino, C. Giannini, C. Malitesta, M. Mazzeo, G. Gigli, and G. Ciccarella, European Journal of Inorganic Chemistry 1 (2013) 364-374.
[3] J. Joo, S. G. Kwon, T. Yu, M. Cho, J. Lee, J. Yoon, and T. Hyeon, Journal of Physical Chemistry B 109 (2005) 15297-15302.



AR = CH_3COOH, $C_{17}H_{33}COOH$, H_3BO_3

[P74] Second-harmonic generation in strained silicon waveguides

E. Degoli[1], E. Luppi[2], V. Véniard[3], and S. Ossicini[1]

[1] Istituto di Nanoscienze-CNR-S3 and Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, via Amendola 2 Pad. Morselli, I-42122 Reggio Emilia, Italy
[2] Laboratoire de Chimie Théorique - UMR 7616, Université Pierre et Marie Curie – CNRS, 4 place Jussieu, 75005 Paris, France
[3] Laboratoire des Solides Irradiés, Ecole Polytechnique, Route de Saclay, F-91128 Palaiseau and European Theoretical Spectroscopy Facility (ETSF), France

Keywords: Non-linear optics, Strained Silicon, ab-initio calculations.

Silicon photonics is a relatively recent research field that aims to substitute electrons with photons as the carriers of information in devices such as planar lightwave circuits. The technology marries the device electronic performance of traditional semiconductor materials with the speed and bandwidth offered by light. Although in the linear regime a silicon photonic circuit can efficiently guide, modulate, and detect IR light, in the nonlinear (i.e., ultrafast, ultrahigh capacity) regime the situation is more complex. In particular, nonlinear second-order optical phenomena are needed to generate, convert, and modulate light at the desired speeds inside complex networks of silicon wires.

In silicon only third-order optical nonlinearities are present owing to its crystalline inversion symmetry. Introducing a second-order nonlinearity into silicon photonics by proper material engineering would be highly desirable. It would enable devices for wideband wavelength conversion operating at relatively low optical powers.

Through this work [1] we have unambiguously shown, both theoretically and experimentally, that silicon can be efficiently stressed to become a good second-order nonlinear crystal: this is the first observation of bulk second-order nonlinearity in silicon.

In particular, a sizeable second-order nonlinearity at optical wavelengths has been induced in a silicon waveguide by using a stressing silicon nitride overlayer. We carried out second-harmonic-generation experiments and first-principle calculations, which both yield large values of strain-induced bulk second-order nonlinear susceptibility, up to 40 pmV^{-1} at 2,300 nm. We envisage that nonlinear strained silicon could provide a competing platform for a new class of integrated light sources spanning the near- to mid-infrared spectrum from 1.2 to 10 μm.

References:

[1] M. Cazzanelli, F. Bianco, E. Borga, G. Pucker, M. Ghulinyan, E. Degoli, E. Luppi, V. Véniard, S. Ossicini, D. Modotto, S. Wabnitz, R. Pierobon, and L. Pavesi, Nature Materials 11 (2012) 148.

[P75] Layer-by-Layer Carrier Vessels for Sensing and Drug Delivery

L. L. del Mercato[1], M. Ferraro[1], R. Miglietta[1], A. Quarta[1], T. Pellegrino[1], and R. Rinaldi[1,2]

[1] NNL, Istituto Nanoscienze-CNR, Lecce, Italy
[2] Scuola Superiore ISUFI, Università del Salento, Lecce, Italy

Keywords: Layer-by-Layer, ion sensing, optical read-out, drug delivery, cells.

Layer-by-Layer (LbL) is a highly versatile technique utilized for preparing well-defined multilayer films onto charged surfaces [1]. Applying the classical LbL assembly onto colloidal particles results in production of core-shell particles which have great applications as carriers for local diagnosis and treatment inside the human body [2].

Herein, the design and preparation of LbL micro- and nanocontainers in relation to their use as intracellular optical reporters and drug carriers are presented. In particular, an innovative methodology for assembling quantum-dots barcoded sensors for multiplexed sensing of protons, sodium and potassium ions is described [3]. In addition, recent data on the use of pH-sensitive capsules for monitoring pH changes that occurs in cells in which the functionality of the V-ATPase proton pump have been altered are shown [4]. Finally, we present a new concept of stimuli-responsive carriers based on the LbL assembly of biodegradable drug-loaded multilayer walls around the external surface of magnetic nanobeads [5].

The reported examples demonstrate that LbL-based nano- and microcarriers are promising systems for drug delivery and real-time sensing of biologically relevant molecules inside living cells in a non-invasive way.

References:

[1] G. Decher, Science 277 (1997) 122.
[2] L. L. del Mercato, P. Rivera-Gil, A. Z. Abbasi, M. Ochs, C. Ganas, I. Zins, C. Sönnichsen, and W. J. Parak, Nanoscale 2 (2010) 458.
[3] L. L. del Mercato, A. Z. Abbasi, M. Ochs, and W. J. Parak, ACS Nano 5 (2011) 9668.
[4] L. L. del Mercato, M. Ferraro, M. De Luca, C. Bucci, and R. Rinaldi, in preparation.
[5] S. R. Deka, A. Quarta, R. Di Corato, A. Riedinger, R. Cingolani, and T. Pellegrino, Nanoscale 3 (2011) 619.

[P76] Anisotropy-graded exchange-coupled composite media obtained by ion-irradiated L10 FePt figure

A. di Bona[1], P. Luches[1], G. C. Gazzadi[1], F. Albertini[2], F. Casoli[2], P. Lupo[2], L. Nasi[2], S. D'Addato[1,3], and S. Valeri[1,3]

[1] Consiglio Nazionale delle Ricerche – Istituto Nanoscienze, Centro S3, Italia
[2] Consiglio Nazionale delle Ricerche – Istituto Materiali per Elettronica e Magnetismo, Italia
[3] Università degli Studi di Modena e Reggio Emilia, Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Italia.

Keywords: FePt, graded media; exchange coupled composite media, high density recording, thin magnetic films.

The effect of Ar^+ irradiation on chemically ordered FePt thin films has been investigated. Epitaxial $L1_0$ FePt films with high uniaxial perpendicular anisotropy and high coercivity have been grown on MgO(001) by RF sputtering. Ar^+ ion irradiation at 5 keV and low doses ($< 10^{15}$ ions/cm^2) is found to be effective in turning the chemically ordered, magnetically hard, $L1_0$ phase into the cubic A1, magnetically soft phase [1,2]. Due to the limited penetration depth of the ions, a thin, magnetically soft layer builds up at the surface of the film. This results in an exchange-coupled, anisotropy-graded, composite media with perpendicular anisotropy and domain wall assisted switching. The spatial distribution of the chemical order parameter has been determined by high resolution transmission electron microscopy. Irradiation at different angles allow the control of the anisotropy depth profile via the chemical disorder of the material, and therefore the magnetic switching of the system. A model for the depth distribution of the chemical order parameter, based on Monte Carlo calculations, is proposed. Ion erosion (sputtering) of the film has been observed at doses significantly higher than that needed for the magnetic transition to occur. The magnetic properties and coupling regimes of the resulting exchange coupled systems are discussed.

References:

[1] B. D. Terris, D. Weller, L. Folks, J. E. E. Baglin, A. J. Kellock, H. Rothuizen, and P. Vettiger, J. Appl. Phys. 87 (2000) 7004.
[2] F. Albertini, L. Nasi, F. Casoli, S. Fabbrici, P. Luches, G. C. Gazzadi, A. di Bona, P. Vavassori, S. Valeri, and S. F. Contri, J. Appl. Phys. 104 (2008) 053907.

[P77] Nanomachining and in-situ characterization of cantilever microbeams by Dual Beam FIB-SEM

G. C. Gazzadi[1], G. Bursi[2], A. Fornieri[2], and S. Frabboni[1,2]

[1] CNR – NANO – S3, Modena, Italy.
[2] Dipartimento di Fisica, Università di Modena e Reggio Emilia, Modena, Italy.

Keywords: FIB nanomachining, mass-sensing cantilevers.

Cantilever microbeams are used as mass-sensing devices in a wide range of applications and environments [1], and extensive research is devoted to enhance their mass sensitivity (S_M), for example by scaling down the dimensions [2]. Focused ion beam (FIB) technology is a valuable tool to accomplish this task thanks to the direct nanomachining approach [3], and, combined with scanning electron microscope (SEM) in Dual Beam systems, also offers the possibility of in-situ characterization of the fabricated structures.

In a first experiment we compare static and dynamic characterizations of FIB-machined Si microcantilevers. Starting from cantilever dimensions of 200 x 37 x 3 μm^3 (length (L) x width (w) x thickness (t)), L is reduced by 10μm-steps, and static characterization is performed at each step using a force sensor attached to a nanomanipulator. From deflection vs. force data, following Hooke's law, the elastic constant (K) is derived. Dynamic characterization is performed by mounting the sample on a piezoelectric holder and by imaging the cantilever oscillation while piezo frequency is swept around the expected resonance value (f_0), as shown in Fig.1(a). The K values obtained from static (10.6 ± 1.5 N/m) and dynamic (10.7 ± 0.6 N/m) measurements are in remarkable agreement.

In a second experiment a novel nanofabrication geometry is adopted to increase SM, leaving the cantilever dimensions unchanged: a latticework structure is fabricated by milling an array of holes into the lateral face of the cantilever. Since $S_M = f_0/2m$ and $f_0=(1/2\pi)(k/m)^{1/2}$, a reduction of the oscillating mass (m) that preserves the structural rigidity leads to an increase of both f_0 and S_M. With respect to dimensional reduction, this geometry offers a larger cross section for mass capture because of the larger exposed area, and an easier operation in standard optical detection setups, where nanosized cantilevers are difficult to measure. Latticework structure is designed by finite-elements (FE) calculations varying the size and shape of the holes, and the length of the latticework. The maximum increase in f_0 (+56%) and S_M (+153%) is predicted for rectangular holes with a basis/height ratio of 3.31, and for latticework extension of 55% the cantilever length. Eleven rectangular holes are milled through the cantilever side by FIB, and the fabricated latticework is shown in Fig. 1b, along with the resonance frequency measured before and after FIB nanomachining. The original structure has f_0 = 183.5 kHz, while the latticework structure has f_0 = 258.6 kHz, corresponding to an increase of 41%. This result demonstrates the validity of the latticework geometry though the f_0 increase is lower than expected.

References:
[1] P. S. Waggoner and H. G. Craighead, Lab Chip 7 (2007) 1238.
[2] M. Li, H. X. Tang and M. L. Roukes, Nature Nanotech. 2 (2007) 114.
[3] N. V. Lavrik and P. G. Datskos, Appl. Phys. Lett. 82 (2003) 2697.

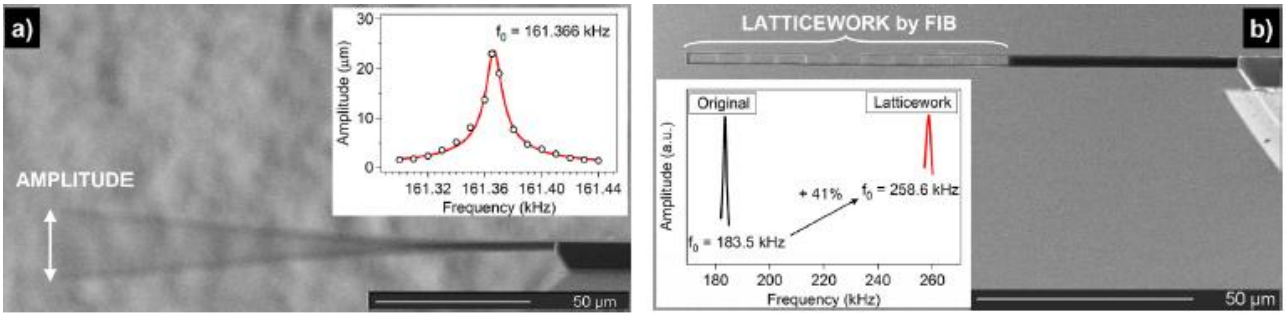


Fig 1. (a) Dynamic characterization by piezo-driven oscillation and, in the inset, oscillation amplitude vs frequency curve. (b) Latticework-cantilever by FIB nanofabrication and, in the inset, resonance frequency curves of the original and the lattice-worked cantilevers.

[P78] Coplanar microwave resonators for electron spin resonance spectroscopy of molecular magnets

A. Ghirri[1], S. Ferrari[2], and M. Affronte[1,2]

[1] Istituto Nanoscienze - CNR, Centro S3, via Campi 213/a, Modena, Italy
[2] Dipartimento di Fisica, Università di Modena e Reggio Emilia, via Campi 213/a, Modena, Italy

Keywords: molecular nanomagnets, microwave resonators, electron spin resonance.

Resonating microstrip circuits can provide an efficient way to realize localized electromagnetic fields at microwave frequency and circuit quantum electrodynamics experiments with few photons. These devices can also be optimized to perform electron paramagnetic resonance experiments with high sensitivity and improved power handling [1,2].
Magnetic samples, such as microcrystals or films, are placed in close proximity to the region where the magnetic component of the electromagnetic field is maximized and the detection of the spin transitions is performed by measuring the transmission parameters of the resonant circuit by means of a vector network analyzer. Resonance conditions are met by varying the microwave frequency and the applied magnetic field.
Here we report the fabrication of Al/A_2O_3 coplanar microstrips with resonant frequency in the X band (10 GHz). These devices are installed on a low-temperature measurement set-up (base temperature 300 mK) with triaxial magnetic field up to 9 T. We show the preliminary results obtained with organic 2,2-diphenyl-1-picrylhydrazyl (DPPH) radicals and antiferromagnetic molecular wheels.

References:

[1] P. Bushev, A. K. Feofanov, H. Rotzinger, I. Protopopov, J. H. Cole, C. M. Wilson, G. Fischer, A. Lukashenko, and A. V. Ustinov, Phys. Rev. B 84 (2011) 060501(R).
[2] C. Clauss, D. Bothner, D. Koelle, R. Kleiner, L. Bogani, M. Scheffler, and M. Dressel, arXiv:1209.5061v1 (2012).

[P79] Quantitative analysis in STEM and HRTEM: toward atom by atom analysis

V. Grillo[1,2], G. Bertoni[2], E. Rotunno[2], and S. D'Addato[1]

[1] CNR-Istituto Nanoscienze, Centro S3, Via G Campi 213/a, I-41125 Modena, Italy
[2] CNR-IMEM, Parco delle Scienze 37a, I-43100 Parma, Italy

Keywords: Electron microscopy, STEM-HAADF, Exit wave reconstruction.

The characterization to atomic scale of nanostructures on the nanoscale is one of the leading forces driving the development of quantitative (S) TEM techniques.

Thanks to the use of the parallel computing simulations we have developed quantitative methods for the quantitative interpretation of the intensity in STEM HAADF[1]. A technique with a high chemical sensitivity capable of counting single atoms in a structure. We propose here to extend the analysis in order to be able to retrieve 3D information by a systematic change of a few relevant experimental parameters.

At the same time we are working on the use of simulation to make also high resolution TEM more quantitative. For this we use Exit wave reconstruction algorithms (EWR) to retrieve the complex wavefunction at the exit of the sample removing aberrations due to the lenses.

An appropriate analysis of such kind of EWR images has similar potentiality as HAADF but we are exploring the limits of interpretability.

Fig. 1 shows a collection of recent results with both technique: a,b are experiment and simulation of HAADF images of core shell ZnSe/ZnS and CdSe/CdS nanorods [2]. Fig 1c,d are HREM experiment and atom counting in ZnSe/ZnS. Fig 1e,f are simulation of and HAADF image of an InGaN layer and a 3D analysis of In distribution. Fig1g,h are HRTEM experiment, simulation and model for a multitwinned icosahedral FePt nanoparticles [3]. All elaborations are based on STEM_CELL code produced by the author V.G. (http://tems3. nano.cnr.it/).

References:
[1] V. Grillo, E. Carlino, and F. Glas, Phys. Rev. B 77 (2008) 054103.
[2] G. Bertoni, V. Grillo, R. Brescia *et al.*, ACS Nano 6 (2012) 6453.
[3] S. D'Addato, V. Grillo, and S. Altieri, J-Phys.: Cond mat 23 (2011) 175003-7.

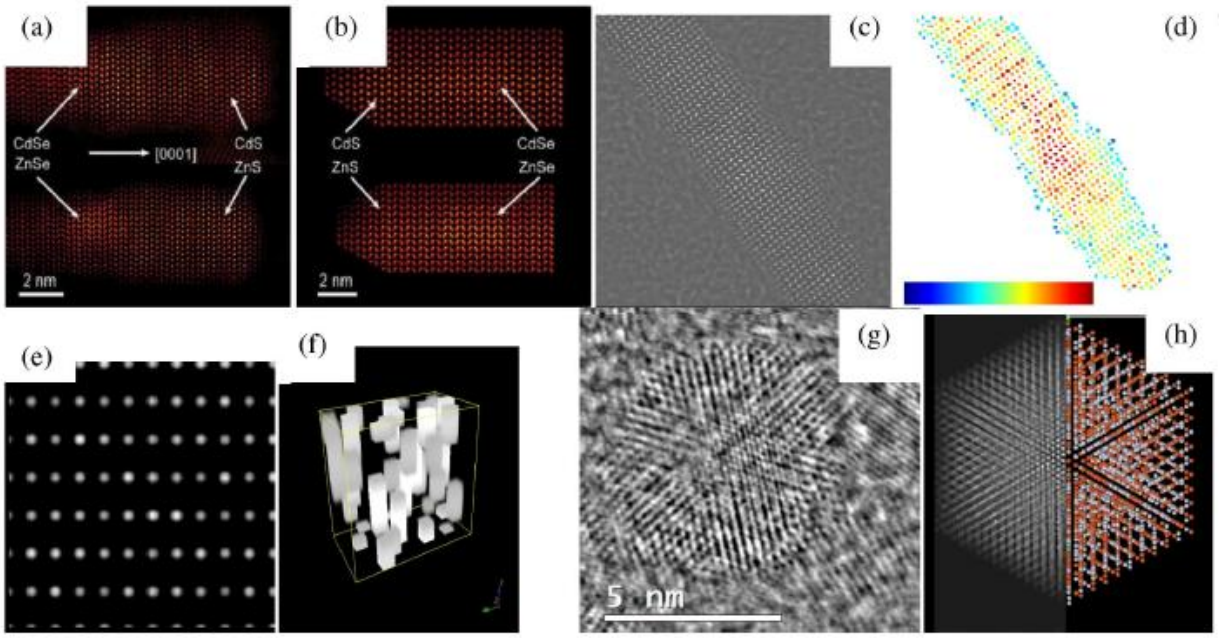


Fig. 1a,b are experiment and simulation of HAADF images of core shell ZnSe/ZnS and CdSe/CdS nanorods. Fig 1c,d are HREM experiment and atom counting in ZnSe/ZnS. Fig 1e,f are simulation of and HAADF image of InGaAn/GaN and a 3D analysis of composition. Fig. 1g,h are HRTEM experiment, simulation and model for a multitwinned icosahedral FePt nanoparticles.

[P80] Combination of multi-layered coatings and micro-texturing strategies

E. Gualtieri[1], A. Ballestrazzi[2], A. Rota[1], A. Spagni[2], and S. Valeri[2,3]

[1] Centre InterMech-MO.RE, University of Modena & Reggio Emilia, Italy
[2] Dept. of Physical, Informatics and Mathematical Sciences, University of Modena & Reggio Emilia, Italy
[3] CNR-NANOSCIENZE Institute, Modena, Italy

Keywords: Physical Vapour Deposition, hard coating, self-lubricant, friction, wear.

Nitrogen-based coatings (e.g.: TiN, CrN) are suitable ceramics for protective purposes with superior mechanical performances like high hardness, low wear rate, corrosion and oxidation resistance. On the other hand, they do not completely solve tribological issues, since they exhibit relatively high coefficients of friction (CoF) mainly against steel.

For this major reason, "intelligent" strategies for a proper functionalization are often required. Remarkable studies proved that adding a third ingredient like a softer metal [1] (Ag, W, Mo, Cu) or a transition metal dichalcogenide [2] (MoS_2, WS_2), by means of doping approaches or multi-layering designs, can provide self-lubricating properties. However, as a matter of fact, this kind of material engineering solution implies a decrease of abrasive wear resistance. To overcome this further limit, surface micro-texturing strategies have been widely studied as well, revealing a promising effectiveness in terms of gradual release of solid lubricant during sliding contact, that reflects the reduction of CoF and the increasing of the lifetime of tribological systems [3-7].

We report on TiN-based coatings deposited by PVD magnetron sputtering technique on $20MnCr^5$ steel in a mixed Ar^+N^2 atmosphere, and capped with a MoS2-based self lubricating top-layer. Two different strategies (see Fig. 1) were exploited in order to texture such multi-layered coatings: A) mechanical polishing of the substrates that induced controlled surface coating roughness by means of randomly distributed sequences of micro-asperities and micro-valleys; B) Laser Surface Texturing method (LST) that allowed to cover the surface with geometrically ordered patterns of micro-sized dimples. Tribological characterization of such multi-layered engineered coatings was carried out through ball-on-disk tribometer. Friction tests point out that micro-texturing strategies are able to improve the durability of such multi-layered coatings, due to the presence of micro-cavities acting as "solid lubricant reservoirs" in different modes. The correlation between friction behaviours and wear mechanisms has finally been discussed.

References:

[1] S. H. Yao *et al.*, Surface and Coatings Technology 201 (2006) 2520
[2] R. Gilmore *et al.*, Surface and Coatings Technology 108–109 (1998) 345
[3] A. A. Voevodin *et al.*, Wear 261 (2006) 1285.
[4] L. Rapoport *et al.*, Surface & Coatings Technology 202 (2008) 3332.
[5] P. Basnyat *et al.*, Surface & Coatings Technology 203 (2008) 73.
[6] J. E. Krzanowski, Surface & Coating Technology 204 (2009) 955.
[7] C. G. Guleryuz and J.E. Krzanowski, Surface & Coating Technology 204 (2010) 2392

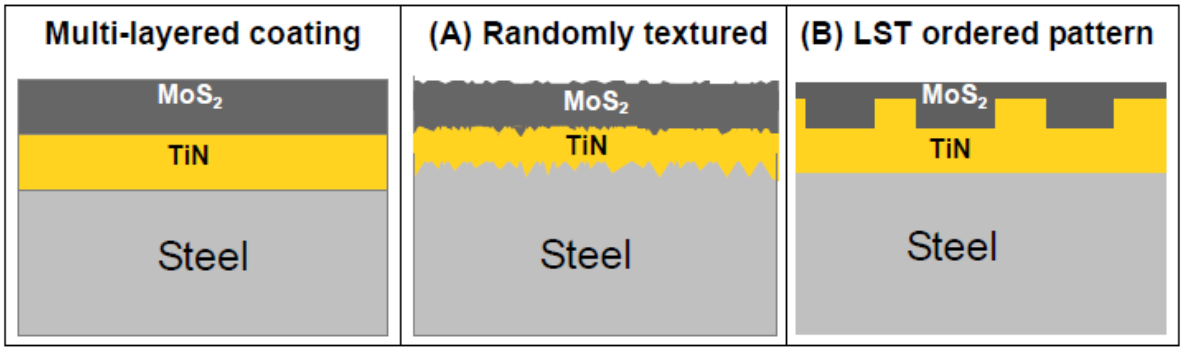


Fig. 1: Schematic representation: multi-layered coating design (MoS2/TiN/20MnCr5 Steel) and microtexturing strategies.

[P81] CAT microscopy: a novel tool for 3D cell investigation

M. F. Cascione[1], V. Vergaro[1], N. Denora[2], M. Franco[2], R. Rinaldi[1], and S. Leporatti[1]

[1] NNL-Istituto Nanoscienze CNR, Lecce, Italy
[2] Pharmaco-Chemistry Department, University of Bari, Italy

Keywords: Confocal Microscopy, Atomic Force Microscopy, TIRF, Colocalization, Citomechanics.

CAT (Confocal-AFM-TIRF) microscopy [1] is a combination of an advanced scanning probe microscope (Bioscope Catalyst, Bruker Inc. USA), a confocal microscope (LSM 700, Zeiss GERMANY), and a total internal reflection fluorescence microscope (Laser TIRF 3, Zeiss GERMANY). Devices are mounted on an inverted microscope. AFM allows elasticity and topographical single cell membrane characterization, confocal microscopy permits volume cell investigation whereas TIRF gives information about cell-substrate interface. Their combined use provides a topographic and spectroscopic imaging, and nano-scale adhesion forces and elastic forces mapping of the sample. Therefore the simultaneous combination of all three microscopies gives rise to a complete three-dimensional point of view.

By using CAT microscopy we have explored morphological and cytomechanical modifications of cancer cells. In particular we have investigated the effects of ROC-inhibitor (Y-27632) on three different cancer cell lines (MCF-7, MDA-361, SKOV-3) by nanoindentation [2]. ROC inhibitor induced re-arrangement of the actin fibers into the cytoskeleton as visualized by confocal images [1,2]. As further proof of concept, by CAT microscopy we have also investigated the internalization of dendrimers into mitochondrial structures and their targeted colocalization inside cellular compartments [3]. These experiments demonstrate that CAT microscopy is a novel powerful tool for cancer cell and targeted drug delivery investigation.

References:

[1] M. Cascione, Master thesis in Physics, Università del Salento, A.A. 2010-2011.
[2] S. Leporatti *et al.*, Nanotechnology 20(5) (2009) 1-6.
[3] N. Denora *et al.*, (2013) manuscript in preparation.

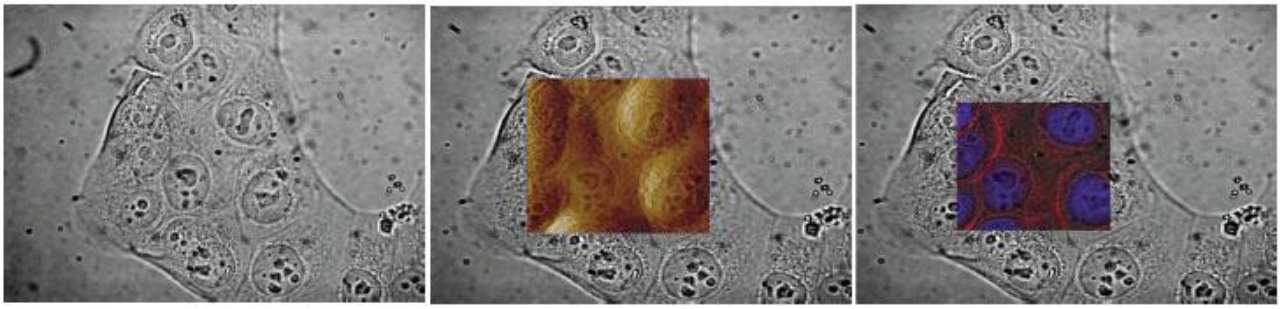


Fig. 1: (a) Transmission image of MCF-7 cells; (b) point by point overlapping of transmission and AFM, and (c) of transmission and confocal image by MIRO Nanoscope Software (Bruker, Inc.).

[P82] Nanotechnology for Cancer Therapy

V. Vergaro[1], Y. M. Lvov[2], and S. Leporatti[1]

[1] NNL-Istituto Nanoscienze CNR, Via Arnesano 16, 73100 Lecce, Italy
[2] Institute for Micromanufacturing (IfM) of Lousiana Tech University, Ruston, Lousiana LA, USA

Keywords: Nanotechnology, Nanocarriers, Nanocapsules, Nanotubes, Nanocolloids, Scanning Force Microscopy.

Cancer is one of the most studied pathologies in research laboratories all over the world, however it remains nowadays one of the principal causes of death. The novel opportunities offered by nanotechnologies have attracted great attention in cancer research. In particular, there is strong interest in the development of novel materials and tools based on biocompatible polymers for targeted drug delivery. The promising features of pharmaceutical drug delivery with intravenous administration are their small size, biodegradability, high content of a drug in a final preparation, prolonged circulation in the blood, and the ability to target required areas. These features are usually not met in a single multifunctional carrier. For these reasons we have compared efficacy of different carrier types (some combined with natural compounds), having complementary properties for pharmaceutical delivery in cancer therapy. Drug nano-colloids encapsulated by combination of layer-by-layer (LbL) techniques and ultra-sonication, hollow polyelectrolyte capsules [1, 2] and drug-loaded clay nanotubes [3,4] have been investigated for uptaking by cancer cells. In this seminar I will also overview our most recent investigations of neoplastic cells morpho-mechanical changes induced by cargo-loaded carriers by a combination of high resolution optical and scanning force microscopy techniques. Future development in direction of personalized (nano)medicine and novel instrumental improvements towards a more detailed 3D investigation of (cancer) cell components and complexity will be finally outlined.

References:

[1] V. Vergaro, F. Scarlino, C. Bellomo, R. Rinaldi, D. Vergara, M. Maffia, F. Baldassarre, G. Giannelli, X. C. Zhang, Y. M. Lvov, and S. Leporatti, Adv Drug Del Rev 63 (2011) 847-863.
[2] D. Vergara, C. Bellomo, X. Zhang, V. Vergaro, A. Tinelli, V. Lorusso, R. Rinaldi, Y. M. Lvov, S. Leporatti, and M. Maffia, Nanomedicine: NBM 8 (2012) 891–899.
[3] V. Vergaro, E. Abdullayev, Y. M. Lvov, A. Zeitoun, R. Cingolani, R. Rinaldi, and S. Leporatti, Biomacromolecules 11 (2010) 820.
[4] V. Vergaro, Y. M. Lvov, and S. Leporatti, Macromolec. Biosci. 12 (2012) 1265-1271.

[P83] Developing of solid state laser source for metrological application

D. Parisi[1], G. Bolognesi[3] and M. Tonelli[1,2]

[1] NEST Istituto Nanoscienze—CNR piazza S. Silvestro 12, 56127 Pisa, Italy
[2] Dipartimento di Fisica Università di Pisa, Largo B. Pontecorvo 3, 56127 Pisa, Italy
[3] Istituto Nazionale di Ricerca Metrologica INRIM Strada delle Cacce 91, 10135 Torino, Italy

Keywords: Metrology, Solid state laser, Yellow emission, Yb clock, laser.

In this work we grew a BaY_2F_8 crystal doping with Dy^{3+} and Tb^{3+} using Czhocharlsky technique. In particular, we studied the manifolds transition of Dy^{3+} ($^4F_{9/2} \rightarrow {}^6H_{13/2}$) at around 578 nm. The choice of codoping with Tb^{3+} is due to optimise the population in the laser levels, using several energy transfer process between the rare earth ions. During the work a comparison with BaY_2F_8:Dy^{3+} was made in order to understand the effects of codoping in the optoelectronics properties of material.

The 578 nm is an important wavelength which correspond to the transition in the optical clock with Yb ($1S_0 \rightarrow 3P_0$). Moreover this kind of laser source is very attractive in the research of optical clocks, because it allows to miniaturise the clock and open towards new transportable optical clocks or space clocks scenario.

At first we carried out the spectroscopic analysis at room temperature (absorption and emission) of the yellow transition, by the excitation of the upper level with a commercial high power blue diode laser at 454 nm. We reported the results of the doped and codoped material to highlight the difference in the two cases. Secondly we made the lifetime experiments at room temperature for the $^4F_{9/2}$ and $^6H_{13/2}$ in both samples. We studied and reported the effects of the energy migrations from $^6H_{13/2}$ Dysprosium level to the $^7F_4$ and $^7F_5$ Terbium levels. Using the spectroscopic data we investigated the transition parameters: the emission and absorption cross section.

After the spectroscopic characterisation we built a “L” cavity to investigate the laser efficiency and to study the spectral properties of the emission. This kind of laser source, at best of our knowledge, is the first direct solid state laser in the yellow region.

References:

[1] S. R. Bowman *et al.*, Optics Express 20 (12) (2012).
[2] M. Takamoto, F.-L. Hong, R. Higashi, and H. Katori, Nature 435 (2005) 321.

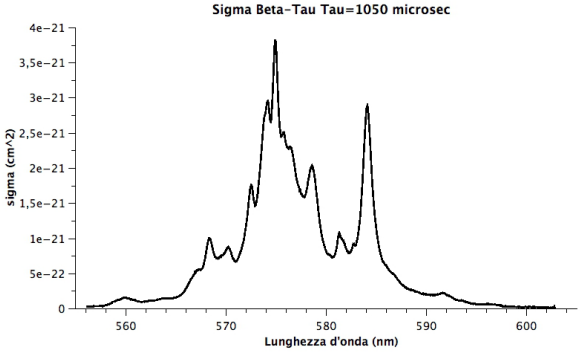


Fig. 1: Here is reported the emission cross section of $^4F_{9/2} \rightarrow {}^6H_{13/2}$ transition of the BaY_2F_8:Dy^{3+},Tb^{3+}.

[P84] Novel laser materials and efficient laser emissions in the 2 micron region

D. Parisi[1], S. Veronesi[1], Y. Z. Zhang[2], G. Bolognesi[2], and M. Tonelli[1,2]

[1] NEST Istituto Nanoscienze– CNR piazza S. Silvestro12, 56127 Pisa, Italy
[2] Dipartimento di Fisica Università di Pisa, Largo B. Pontecorvo 3, 56127 Pisa, Italy

Keywords: Single crystal, laser materials, solid state laser, Mid-IR

Mid-infrared (Mid-IR) solid-state lasers emitting in the eye-safe 2 μm spectral region have attracted more and more attention in recent years, because of their huge potential for applications in medicine, LIDAR systems, security, and high resolution spectroscopy for atmospheric pollution monitoring. The holmium 5I7 metastable level has a very long lifetime (typically around 14 ms) and a strong emission cross section, offering very good characteristics for generating high pulse energies when operating the laser in Q-switched mode [2]. Fluoride materials are particularly suitable to develop lasers operating in the Mid-IR because of their low phonon energy (300-500 cm^{-1}) with respect to oxides (800-1000 cm^{-1}) that decreases the detrimental effect of non radiative transition which could quench the upper laser level. We report on two topics: the first laser emission of a fluoride crystal grown by micro–Pulling Down (μ-PD) method in the 2 μm wavelength range and on a novel laser material that has been used as laser media for the first time in this wavelength region.
Regarding the μ-PD sample, we have performed a spectroscopic investigation and achieved an efficient Ho:$LiLuF_4$ laser in-band pumped at 1938 nm. The Ho:$LiLuF_4$ laser yielded a maximum output power of 7.1W with a slope efficiency of 41% and a threshold around 5W, at lasing wavelength of 2054.2 nm [3]. The other sample allows the first observation to our knowledge of room-temperature continuous-wave laser operation on the $^5I_7 \rightarrow {}^5I_8$ transition of Ho^{3+} ions in a KY_3F_{10} single crystal. Using a Tm-doped silica fiber laser operating at 1938 nm as a pump source, a maximum laser power of 1.8 W was obtained at a wavelength of ~2040nm for 27 W of absorbed pump power with a slope efficiency of 19.1% with respect to absorbed power. At low cavity output coupling, the lasing wavelength shifted to 2060.5 nm. The beam propagation factor (M2) was measured to be <1.06 at the maximum output power, confirming fundamental transverse-mode (TEM00) operation. Performing a Caird analysis, we determined resonator round-trip losses and intrinsic slope efficiency of 30% and 43.8%, respectively [4].

References:
[1] B. M. Walsh, Laser Phys. 19 (2009) 855.
[2] P. A. Budni, C. R. Ibach, S. D. Setzler, E. J. Gustafson, R. T. Castro, and E. P. Chicklis, Opt. Lett. 28 (2003) 1016.
[3] S. Veronesi, Y. Zhang, M. Tonelli, and M. Schellhorn, Opt. Express 20 (2012) 18723.
[4] M. Schellohorn, D. Parisi, S. Veronesi, G. Bolognesi, and M. Tonelli, Opt Lett. 38 (2013) 504.

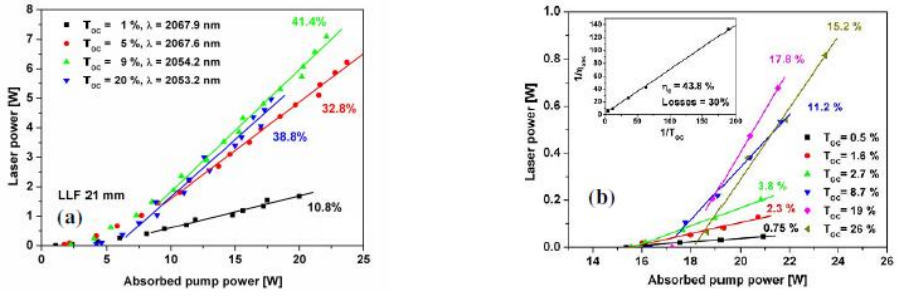


Fig. 1: a) slope efficiency of Ho:LLF single crystal fiber grown by μ-PD method; b) slope efficiency of a sample of Ho:KY_3F_{10} single crystal grwn by Czochralski method.

[P85] Nanocomposite And Fibers: In-Situ Synthesis And Nanopatterning

L. Persano[1], A. Camposeo[1], F. Di Benedetto[1], and D. Pisignano[1,2]

[1] National Nanotechnology Laboratory of Istituto Nanoscienze-CNR, via Arnesano, 73100 Lecce, Italy
[2] Dipartimento di Matematica e Fisica "Ennio De Giorgi", Università del Salento via Arnesano, 73100 Lecce, Italy

Keywords: nanocrystals, nanocomposites, nanofibers, polymer.

Nanocomposite systems mainly consist of polymers embedding inorganic nanoparticles. These materials are widely exploited in different fields, since by properly combining their constituents, new materials with tailored or improved physical properties can be designed. Among different fillers, light-emitting nanocrystals are largely used due to their size-dependent optical properties and thermal stability. In particular, organic-inorganic nanocomposites, which combine the peculiar properties of nanocrystals with the ease of processing and structural flexibility of organic compounds are widely used as active material in light emitting diodes, lasers, solar cells and opto-mechanical devices. However, nanopatterning light-emitting organic-inorganic composites [1] and shaping them to obtain fluorescent nanostructures and fibers remain an important challenge in order to employ these systems in optoelectronic devices. In fact, a general problem for nanopatterning composites lies in the often disfavored plastic behavior and flow conditions of these nanomaterials. In particular, in situ synthesis in which inorganic nanoparticles are directly generated inside a polymer matrix by thermal, chemical, or optical decomposition of suitable molecular precursors, offer a superior control on particles dispersion and can be strategic to pattern nanocomposite materials. This approach allows the exploitation of highly favorable film-forming and flow conditions of polymer solutions, allowing the achievement of light-emitting nanocrystals only after the composite films have been deposited and eventually patterned or shaped in fiber form. Here we review our work on light-emitting patterned polymer–nanoparticle composites and fibers obtained by the smart combination of complementary nanofabrication approaches including nanoimprinting [2] and multi-photon lithography,[3] electron beam-writing and electrospinning.[4,5].

Acknowledgement: The authors gratefully acknowledge the support from the Italian Ministry of Education, University and Research (MIUR) through the FIRB project RBFR08DJZI "Futuro in Ricerca".

References:

[1] L. Persano *et al.*, Advanced Functional Materials 18 (2008) 2692.
[2] L. Persano *et al.*, Advanced Materials 24 (2012) 5320–5326.
[3] A. Camposeo *et al*., Journal of Materials Chemistry 22 (2012) 9787.
[4] L. Persano *et al*., Macromol. Mater. Eng. (2013) DOI: 10.1002/mame.201200290.
[5] A. Camposeo *et al*., Macromol. Mater. Eng. (2012) DOI: 10.1002/mame.201200277.

[P86] Multipurpose biochips - Toward on-chip medicine

E. Primiceri, M. S. Chiriacò, A. G. Monteduro, F. De Feo, R. Rinaldi, and G. Maruccio

NNL, Istituto Nanoscienze-CNR, Lecce, Italy
Dipartimento di Matematica e Fisica "Ennio De Giorgi", Università del Salento, Lecce, Italy

Keywords: lab-on-a-chip, microfluidics, biosensors, electrochemistry.

Recently the development of lab-on-chip devices attracted large interest for detection of specific analytes/markers, cellular studies and drug screening. In this respect, electrochemical impedance spectroscopy is a powerful tool.

Here the development of a multipurpose biochip with integrated microfluidic components is described. Specifically, the layout consists of various sensing areas, each one including an array of transducers (gold interdigited electrodes), while microfluidic channels are used for the delivery of functionalization and sample solutions into the chambers. Such biochips are first demonstrated to be suitable for viability assays, cytotoxicity tests and migration assays on cell populations [1]. Then other applications are discussed concerning the ultrasensitive (pM) detection of biorecognition events in flow immunoassays, such as in the case of cholera toxin in solution or cancer biomarkers in sierra [2].

Our recent publications demonstrate that these biochips are very suitable for clinical analysis, being faster and more reproducible than traditional techniques. In particular our attention was so far focused mainly on cancer diseases. For example, by means of appositely developed biochips, we assessed the presence of autoantibodies against Ser-419-phosphorylated ENOA in sera originating from patients with pancreatic ductal adenocarcinoma (PDAC) [3]. Biochip results are in agreement with those from traditional techniques, such as ELISA and Western Blot, but measurements are much more sensitive and specific increasing the possibility of PDAC diagnosis. Similar chips also allowed to evaluate the free-to-total PSA ratio useful for screening of prostate cancer risk [4]. On a different approach, these biochips were modified to enable automatic tests to quantify the invasive potential of cell lines by detecting the migratory activity of hepatocellular carcinoma (HCC) cells as a function of microenvironment [5]. Presently, we are pursuing the integration of monolithic valves for fluid handling using thermo-responsive hydrogels [6].

References:

[1] E. Primiceri *et al.*, Biosensors and Bioelectronics 25 (2010) 2711.
[2] M. S. Chiriacò *et al.*, Lab on a Chip 11 (2011) 658.
[3] M. S. Chiriacò *et al.*, Lab on a Chip 13 (2013) 730.
[4] M. S. Chiriacò *et al.*, submitted to PNAS.
[5] E. Primiceri *et al.*, Lab on a Chip 11 (2011) 4081.
[6] A. G. Monteduro *et al.*, in preparation.

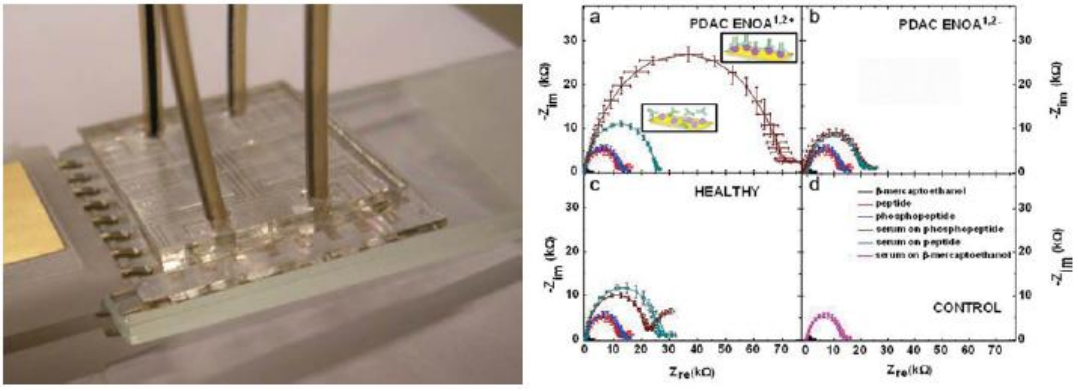


Fig. 1: (left) Multipurpose biochip with microfluidic and electrochemical components. (right) Impedance Nyquist spectra from PDAC ENOA1,2+ sera, ENOA1,2- sera, healthy sera and control samples.

[P87] Targeting Cancer with inorganic nanoparticles: from surface engineering to in vitro and in vivo studies

A. Quarta[1], M. Figini[2], G. Nano[3], C. Cesta[3], J. Granja[4], S. Canevari[2], and T. Pellegrino[1]

[1] Istituto Nanoscienze CNR, Lecce, Italy
[2] Istituto Nazionale dei Tumori, Milano, Italy
[3] Dompe Spa, L'Aquila, Italy
[4] Universidad de Santiago de Compostela, Spain

Keywords: inorganic nanoparticle, cancer, antibody, targeting.

Inorganic nanoparticles have raised enormous attention in the biomedical field thanks to the size-tunability of their physical properties and to the possibility to engineer their surface with a variety of biomolecules [1-2] and drugs. Thanks to these features, nanocrystals of semiconductor materials and metal oxide, like iron oxides, have been proposed as advanced diagnostic methods and innovative therapeutic approaches to several human diseases, like cancer. A clear definition of the interactions of these materials with living systems is fundamental prior to their use on humans.

In this regard we have developed both fluorescent and magnetic nanoparticles for targeting, imaging and treating ovarian cancer, which is one of the most aggressive types of female tumors. For the targeting study the surface of the nanocrystals was engineered with human Fab fragments against the α-isoform of the folate receptor which is over-expressed on the membrane of the ovarian cancer cells. In vitro and in vivo studies have been performed in order to assess the targeting ability of the nanobioconjugate.

Furthermore a therapeutic approach to the same type of malignancy is under development through the binding of a chemotherapeutic drug to the surface of the magnetic nanoparticles. Preliminary results will be presented.

References:

[1] A. Quarta, A. Curcio, H. Kakwere, and T. Pellegrino, Nanoscale 4 (11) (2012) 3319-3334.
[2] A. Quarta, A. Ragusa, S. Deka, C. Tortiglione, A. Tino, R. Cingolani, and T. Pellegrino, Langmuir, 25 (21) (2009) 12614-12622.

[P88] Single-photon transfer in ultrastrongly coupled three-cavity arrays

D. Rossini[1], R. Fazio[1], S. Felicetti[2], G. Romero[2], and E. Solano[2,3]

[1] NEST, Scuola Normale Superiore and Istituto di Nanoscienze - CNR, Pisa, Italy
[2] Departamento de Química Física, Universidad del País Vasco UPV/EHU, Bilbao, Spain
[2] IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Keywords: Light-matter interaction, cavity QED, photon blockade, quantum simulators.

Light-matter interaction is one of the most fundamental processes in nature, and its progress has allowed the development of impressive architectures where fundamentals of quantum mechanics can be tested [1]. In particular, arrays of coupled QED cavities have been devised as promising candidates for simulating strongly interacting models and performing quantum computation [2]. The possibility to implement different geometries enables one to engineer quantum networks for distributed quantum information processing. These lattice models have proved useful to describe the scattering of a single-photon interacting with a qubit in a one-dimensional waveguide [3].

In this work we study, by means of analytical and numerical exact techniques, the photon transfer along a linear array of three coupled cavities where the central one contains an interacting two-level system in the strong and ultrastrong coupling regimes. We find that an inhomogeneously coupled array forbids a complete single-photon transfer between the external cavities when the central one performs a Jaynes-Cummings dynamics. This is not the case in the ultrastrong coupling regime, where the system also exhibits singularities in the photon transfer time as a function of the cavity-qubit coupling strength. Our model can be implemented within the state-of-the-art circuit quantum electrodynamics technology, and represents a building block for studying excitation and state transfer through scalable cavity arrays.

References:

[1] J. M. Raimond, R. Brune, and S. Haroche, Rev. Mod. Phys. 73 (2001) 565.
[2] A. A. Houck, H. E. Tureci, and J. Koch, Nature Phys. 8 (2012) 292.
[3] P. Longo, P. Schmitteckert, and K. Busch, J. Opt. A: Pure Appl. Opt. 11(2009) 114009; Phys. Rev. Lett. 104 (2010) 023602.

[P89] FIB patterning-induced hydrophobicity on Si(001)

A. Rota[1,2], M. Tripathi[2,3] G. C. Gazzadi[3], and S. Valeri[1,2,3]

[1] Centro Interdipartimentale per la Ricerca Applicata e i Servizi nel settore della Meccanica Avanzata e della Motoristica - Università di Modena e Reggio Emilia, Via Vignolese 905/b, 41125 Modena, Italy
[2] Dip. di Scienze Fisiche, Informatiche e Matematiche, Univ. Modena e Reggio Emilia, Modena, Italy
[3] CNR-Istituto di Nanoscienze, Centro S3, Via Campi 213/A – 41125 Modena, Italy

Keywords: hydrophobicity, patterning, adhesion, friction.

The unexpected physical and chemical properties observed at the nano-scale induced the development of novel technologies in many fields. Following this trend, also in the case of tribology novel phenomena occurs when contact size and load are in the nano-regime. These new effects are related to adhesion, which dominates on gravity and inertia at the nano-scale. Surface patterning has been demonstrated to be able to modify adhesion and coefficient of friction (CoF) of the surface, depending on the dimensionality of the texture [1-4]. Most of these findings relate these effects to the lower contact area of the patterned surface, but a satisfactorily understanding of the occurring phenomena is still lacking.

The present study aims to better define the borderline between nano-tribology and micro/macro-tribology, and which is the role played by the nano-structures in modifying the hydrophobic/hydrophilic properties of surfaces. The system under investigation is the Si(001) covered by its native oxide, which is the base material of MEMS and NEMS. The surface was patterned by FIB to obtain parallel and equally spaced nano-grooves, 50nm wide and some nm deep, with variable pitch of 125, 250, 500 and 1000nm. Adhesion and CoF have been measured by friction force microscopy in air and in high vacuum, in order to identify the effect of water capillary on tribology.

Both adhesion and CoF are lower on the patterns, related to a hydrophobic character induced by the nano-structures on the surface [5]. These reductions depend on the separation among the grooves, becoming negligible as the pitch approaches the micro-scale. The analysis of Trace-Minus-Retrace profiles reveals the presence of low-friction regions which surround each nano-structures. The superposition of these regions becomes very effective for 125 and 250nm-pitch [6]. The tests in humidity-free ambient have not evidenced detectable difference in adhesion and CoF between the patterns and the flat area, confirming that the nano-structures inhibit the capillary formation.

The present research was funded by Centro Interdipartimentale per la Ricerca Applicata e i Servizi nel settore della Meccanica Avanzata e della Motoristica - INTERMECH MO.RE., located at the Faculty of Engineering “Enzo Ferrari”, University of Modena and Reggio Emilia, and by Regione Emilia Romagna, Italy.

References:

[1] Y. Wang, L. Wang, Q. Xue, N. Yuan, J. Ding, Colloids and Surfaces A: Physicochem. Eng. Aspects 372 (2010) 139.
[2] W. Zhao, L. Wang and Q. Xue, Appl. Mat. Interf. 2 3 (2010) 788.
[3] D.-C. Pham, K. Na, S. Piao, I.-J. Cho, K.-Y. Jhang, and E.-S. Yoon, Nanotechnology 22 (2011) 395303.
[4] D.-C. Pham, K. Na, S. Piao, S. Yang, J. Kim, and E.-S. Yoon, Surface Engineering 27 4 (2011) 286.
[5] D. Marchetto, A. Rota, L. Calabri, G. C. Gazzadi, C. Menozzi, and S. Valeri, Wear 268 (2010) 488.
[6] A. Rota, M. Tripathi, G. C. Gazzadi, and S. Valeri, Langmuir in press.

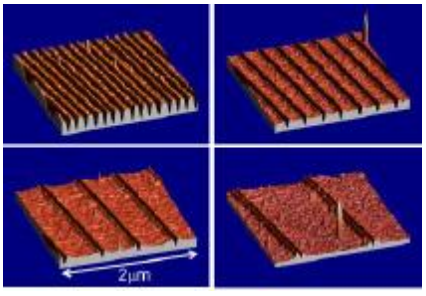


Fig. 1: AFM 3D-images of 125, 250, 500 and 1000nm-pitch patterns.

[P90] Electron gas in modulation-doped GaAs/AlxGa1-xAs nanowire radial heterojunctions

M. Royo[1], A. Bertoni[1], and G. Goldoni[1,2]

[1] CNR-NANO S3, Institute for Nanoscience, Via Campi 213/a, 41125 Modena, Italy
[2] Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia, Italy

Keywords: multi-shell nanowire, modulation doping, Quantum Hall regime, magnetoconductance.

Multi-shell semiconductor nanowires (NWs) are attracting much interest due to their possible application as light harvesting devices, nanophotonic sources, and nanoscale FETs with novel geometries [1].These radial heterostructures have the potential to host axially symmetric high-mobility electron gases, similar to traditional planar 2DEGs formed in modulation doped GaAs/AlGaAs heterojunctions, but with a different topology.

In this contribution we shall discuss the nature and formation of electronic states, both at zero field [2] and in the Quantum Hall regime [3], in modulation doped NW heterojunctions. Calculations have been conducted within a 3D Schrödinger-Poison approach on symmetry compliant grids, including the self-consistent field of the static donors and the free carriers at a mean-field level. This allows to treat explicitly the compositional profiles in complex core-multi-shell GaAs/AlGaAs NWs with experimentally relevant dimensions.

We show that, contrary to planar heterojunctions, conduction electrons do not form a uniform 2D electron gas (2DEG) localized at the GaAs/AlGaAs interface, but rather show a transition between anisotropic cylindrical distribution deep in the GaAs core (low density regime), and a set of six tunnel-coupled quasi-1D channels at the corners of the hexagonal interface (high density regime, see, e.g., Fig. 1(a)). In the presence of a transverse magnetic field the energy subbands deviate from the zero-field parabolic dispersion, and can be described in terms of Landau levels and edge states, similarly to planar 2DEGs, only in the low density regime. In the high density regime the subbands develop complex dispersions, with local minima at finite values of the in-wire momentum, which bring about an anisotropic magnetoconductance with regions of negative and anisotropic magnetoresistance (see, e.g., Fig. 1(b)), these being possible clear signatures of the inhomogeneous localization of the electron gas.

References:
[1] C. M. Lieber and Z. L.Wang, MRS Bulletin 32 (2007) 99.
[2] A. Bertoni, M. Royo, F. Mahawish, and G. Goldoni, Phys. Rev. B 84 (2011) 205323.
[3] M. Royo, A. Bertoni, and G. Goldoni, Phys. Rev. B 87 (2013) 115316.

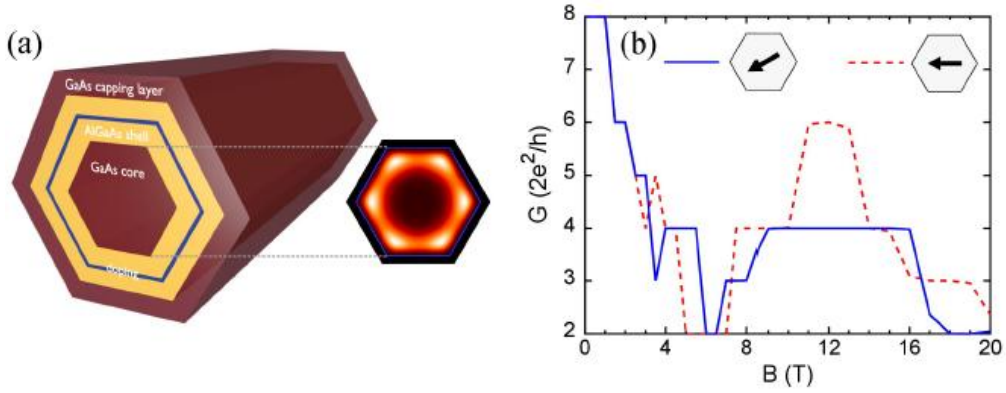


Fig. 1: a) Schematics of a modulation-doped radial heterojunction in a core-shell NW, and electron gas distribution in the high-density regime. b) Magnetoconductance of a NW in the high-density regime for a magnetic field applied in the two most relevant directions illustrated in the insets.

[P91] Controlled focused ion beam deposition of platinum chiral nanostructures

M. Esposito[1], V. Tasco[1], A. Campa[1], I. Tarantini[1], A. Benedetti[2], C. Sibilia[2], and A. Passaseo[1]

[1] National Nanotechnology Laboratory, CNR-Nano, Lecce I-73100, Italy
[2] Università di Roma La Sapienza- Dip. SBAI-Via Scarpa 16 00161 Roma, Italy

Keywords: 3D chirality, dichroism, focused ion beam induced deposition, metamaterials.

Metamaterials(MMs), i.e. artificial materials with electromagnetic properties not available in nature, are currently subject of intense investigation due to their intriguing potential applications such as cloaking or superlensing. Among them, chiral structures[1] can be used to realize MMs with negative refractive index or enhanced circular polarization sensitivity. Considerable efforts have been made to realize chiral MMs in both three dimensional and planar configurations by using two-dimensional electron beam lithography and ultra violet lithography, but with operation far from the optical visible range, due to the achievable sizes in the micrometer range.

In this work, we discuss the design and fabrication of metallic (platinum) 3D spirals able to operate as polarization sensitive filter with a wide resonance in the visible range. The required nanometer sizes have been obtained by a scanning procedure applied to Focused Ion Beam Induced Deposition (FIBID). In order to test the complex interaction of the incident ion-beam with the substrate surface charge during the nanostructure growth, substrates with different electrical conductivity have been considered, in particular silicon and epitaxial gallium nitride-based samples, including structures with a two dimensional electron gas confined at about 20 nm from the surface.

The helical structure has been modelized in order to obtain MMs sensitive to the light polarization state by using "Lumerical" code. According to numerical results, the radius and the pitch of the helix are the fundamental features driving the optical spectral response. Calculations highlight that such objects, if properly scaled in size down to the nanometer range, can exhibit widely resonant behavior in the visible range, with a strong asymmetry between the short wavelength and long wavelength region response to circular polarization state of incoming light. The nanoscale control of the single metallic spring has been accurately obtained by implementing a calibrated scanning procedure applied to FIBID allowing the reduced influence of proximity and charge effects on the helical structures, as a function of substrate conductivity. The growth of such nanostructures is controlled by the interaction of the ion beam with the substrate surface and with the ongoing metallic structure. Proximity and charge effects must be taken into account and compensated for during the spiral formation process. A high control is obtained by a dose compensation procedure to be applied along the axial direction of the structure. By this procedure, we obtained platinum helix structures with core diameter of 80 nm, ring diameter of about 280 nm and vertical pitch of 200 nm (Fig.1-a). The calculated transmission spectra, related to the fabricated structure (Fig.1-b) show the expected wavelength-dependent polarization sensitivity, with a wide geometric resonance centered at about 830 nm for left circular polarization of the incident field and high field confinement on the top of the structures.

References:

[1] V. K. Valev, J. J. Baumberg, C. Sibilia, and T. Verbiest, Adv. Mater. (2013) doi: 10.1002/adma.201205178.

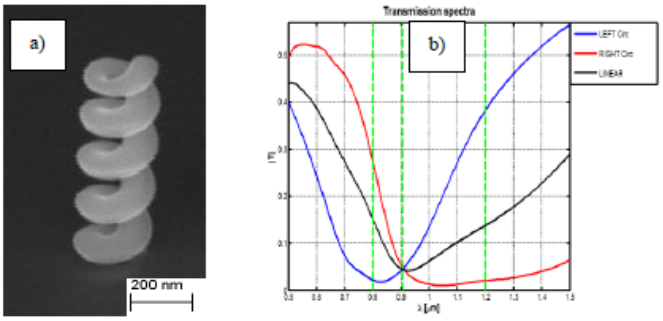


Fig. 1: Scanning electron microscope image (a) of the realized Pt nanostructure obtained by FIBID and related calculated transmission spectra (b) for left circular, right circular and linear polarization states of the incident field.

[P92] Piezoelectric AlN devices for vibrational energy harvesting

M. T. Todaro[1,2], F.Guido[2], A. Qualtieri[2], S. Petroni[2], and M. De Vittorio[1,2,3]

[1] National Nanotechnology Laboratory, Istituto Nanoscienze-CNR, 73100, Lecce, Italy
[2] Center for Biomolecular Nanotechnologies, Istituto Italiano di Tecnologia, 73010 Arnesano (LE), Italy
[3] Dipartimento di Ingegneria dell'Innovazione, Università del Salento, 73100, Lecce, Italy

Keywords: energy harvesting, piezoelectrics, aluminium nitride.

There is an increasing research effort in the development of energy sources for powering micro devices such as small wireless sensor networks, portable electronics, biomedical implants and environmental condition monitoring systems. Power harvested from mechanical vibration represents a very promising energy source as low level vibrations occur in many environments like commercial and industrial buildings.

Among the transduction mechanisms, the attention is mostly focused on piezoelectricty due to the ability of piezoelectric materials to directly convert vibration energy into electric energy. Additionally piezoelectric transducers based on thin film piezoelectric materials can be easily designed and fabricated by exploiting MEMS technologies as a potential low cost manufacturing method making them well suited for miniaturization and integration in a system. AlN is a promising piezoelectric material for harvesters, due to its interesting properties including good piezoelectric coefficients, good electromechanical coupling coefficients, low permittivity and high Young's modulus. Moreover AlN thin films can be grown by low temperature techniques, such as sputtering deposition, making them fully compatible with standard silicon Integrated Circuits. Despite this, so far a few works reported on AlN-based energy harvesters [1] and AlN thin film technology applied to micro power generators is not yet fully exploited.

This work reports on the design, fabrication and analysis of piezoelectric thin film AlN-based devices for vibrational energy harvesting resonating in a range spanning from 200 Hz to 2 KHz.

An array of devices with different geometries has been designed by multi-physics FEM simulations in order to maximize output power at values of tens of μW. The piezoelectric harvesters consist of a 40 μm-thick silicon cantilever beam ended with a proof mass shaped into the silicon substrate. On top of this, a piezoelectric AlN thin film embedded into two Molybdenum electrodes is deposited by DC magnetron sputtering. Devices have been realized by conventional micromachining techniques (see Figure 1). Electromechanical measurements have been carried out by means of an ad-hoc workbench comprised of an electromagnetic shaker for vibration generation and a lock-in amplifier measuring the voltage generated by the excited devices. The cantilever deflections and the resonance frequencies have also been evaluated by laser Doppler vibrometry. Preliminary analysis carried out on a 6.5 mm-long and 5.2 mm-wide cantilever with a 170 μm-thick silicon beam have shown a maximum displacement of 4.5 μm at the first resonance frequency of 1.495 KHz under 1g acceleration. Under the same working conditions the measured peak-peak root mean square open circuit voltage was of 39 mV while the device provided an output power of 0.54 nW under an optimal load of 120 KΩ. FEM simulations of such device showed good agreement with the experimental findings.

References:

[1] R. Elfrink, D. Hohlfeld, Y. van Andel, and R. van Schaijk, J. Micromech. Microeng. 19 (2009) 094005.

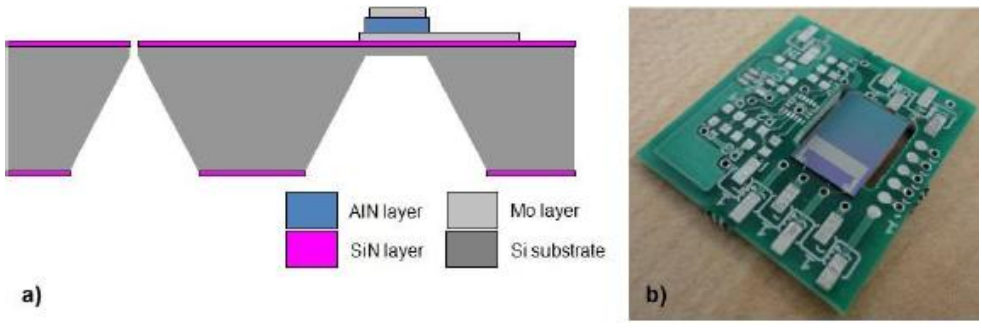


Fig. 1: a) Cross-section scheme of the energy harvester; b) a fabricated device mounted on a PCB board.

[P93] Fluoride based passively Q-Switching lasers emitting at 1.9 µm

S. Veronesi[1], D. Parisi[1], R. Faoro[1], and M. Tonelli[1,2]

[1] NEST Istituto Nanoscienze– CNR piazza S. Silvestro12, 56127 Pisa, Italy
[2] Dipartimento di Fisica Università di Pisa, Largo B. Pontecorvo 3, 56127 Pisa, Italy

Keywords: Single cristal, laser materials, solid state laser, passive QS, Mid-IR.

Solid-state lasers operating in the 2 µm eye-safe spectral range are of interest for applications in spectroscopy, laser ranging, photo-medicine, optical communications, and metrology. Q-switched lasers in this wavelength range are especially important for pumping nanosecond Optical Para metric Oscillators for efficient conversion into the mid-IR. The Tm^{3+} (Tm)-ion, emitting on the $^3F_4 \rightarrow {}^3H_6$ transition , is promising for power scaling of such lasers because its absorption band, at around 800 nm, matches the emission of AlGaAs laser diodes de-signed for Nd^{3+}-ion pumping. Passive Q-switching (PQS) of such diode-pumped solid-state lasers (DPSSL) by a saturable absorber (SA) is a common technique to generate short and high peak power pulses, mainly due to the simplicity and low cost of the cavity design. We report on the Passive Q-Switching (PQS) of 3 different fluoride hosts $LiYF_4$, $LiLuF_4$ and BaY_2F_8 doped with Tm^{3+}.

Stable passive Q-switching of a Tm: $LiYF_4$ laser is obtained using polycrystalline Cr^{2+}:ZnS as a saturable absorber. The achieved maximum pulse energy of 0.9 mJ and peak power of 65 kW for a pulse duration of ~ 14 ns represent substantial improvement and highest values for a passively Q-switched diode-pumped Tm laser operating at about 1 .9 µm [2].

Moreover we demonstrate efficient passively Q -switched Tm:$LiLuF_4$ laser operation near 1.9 µm. The CW slope efficiency reached 54.8% with respect to absorbed power. Stable passive Q-switching with Cr^{2+}:ZnS saturable absorbers resulted in minimum pulse duration of 7.6 ns and maximum pulse energy and peak power of 1.26 mJ and 166 kW, respectively[3].

Finally we report on passive Q-switching of a Tm-doped BaY_2F_8 laser using Cr^{2+}:ZnS saturable absorber achieving single pulse energies as high as 0.72 mJ, peak power exceeding 17 kW and pulse duration of 40 ns[4].

References:
[1] A. Godard, C.R. Phys. 8 (2007) 1100.
[2] R. Faoro, M. Kadankov, D. Parisi, S. Veronesi, M. Tonelli, V. Petrov, U. Griebner, M. Segura, and X. Mateos, Opt. Lett. 37 (2012) 1517-1519.
[3] H. Yu, V. Petrov, U. Griebner, D. Parisi, S. Veronesi, and M. Tonelli, Opt. Lett. 37 (2012) 2544-2546.
[4] X. Mateos, S. Veronesi, H. Yu, V. Petrov, D. Parisi, U. Griebner, and M. Tonelli, CLEO (2013) oral communication.

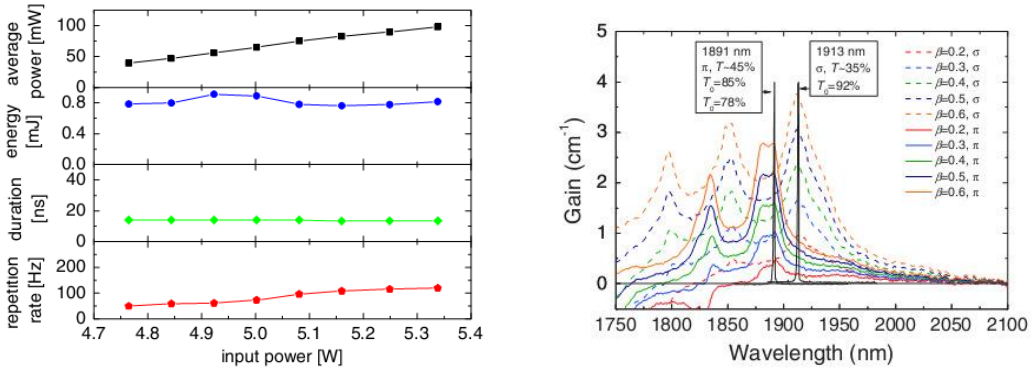


Fig. 1: a) PQS characteristics of the Tm:YLF laser; b) gain curve and laser output spectra in PQS regime with different SAs.

[P94] Confined self-assembly: a route for novel random lasers

I. Viola[1], N. Ghofraniha[2], A. Zacheo[1,3], F. Di Maria[4], G. Barbarella[4], V. Arima[1], C. Conti[2], and G. Gigli[2,3,5]

[1] National Nanotechnology Laboratory, CNR-Institute Nanoscience, UOS Lecce, Italy
[2] CNR-Institute for Physical Chemical Processes, UOS Rome Kerberos,and Dip. Di Fisica, Università La Sapienza, 00185, Rome, Italy
[3] Dip. di Matematica e Fisica "Ennio de Giorgi", Università del Salento, Lecce, Italy
[4] CNR-Istituto per la Sintesi Organica e la Fotoreattività, Bologna, Italy
[5] Italian Institute of Technology (IIT), Centre for Biomolecular Nanotechnologies, Lecce, Italy

Keywords: Self-assembly, Oligo-Thiophene, Nano-photonics, Nano-lithography, Random laser.

Recent developments in the field of micro and nanophotonics have shown that it is possible to make use of the intrinsic disorder in photonic materials to create useful optical structures [1].

It is well-known that functional properties of macromolecular materials strongly depend on their shape, size and chemistry, making them useful in a broad range of fields. Fundamental properties, including self-assembly, supra-molecular organization, diffusion and elasticity, can be effectively tailored [2].

In this work we will report promising methods for the fabrication of random lasers (RL) with different size and shape, based on active molecular systems in which defects, supra-molecular aggregates, confined structures or external beads behave as scattering centers, without involving any external feedback. However, due to the intrinsically randomness of the scattering centers, conventional methods for the fabrication of random lasers do not allow for a careful control of the device geometrical parameters, and in turn of the lasing properties. The development of different types of bottom-up lithographic approaches will be selectively proposed as function of application and materials used such as surface-tension-driven lithography and microfluidics.

We will focus on four different approaches for the realization of novel types of RLs by modulating supra-molecular organization of thiophenes and photonic materials under energetic [3,4] and geometric constrains [5] or by tuning the elasticity of polymeric materials [6]. The effects of confinement will be coupled with mode locking techniques.

References:

[1] D.S. Wiersma, Nature Photonics 7 (2013) 188.
[2] J.M. Lehn, Science 295 (2002) 2400.
[3] N. Ghofraniha, I. Viola, F. Di Maria, G. Barbarella, C. Conti, and G. Gigli, Laser & Photon. Rev. 7 (2013) DOI 10.1002/lpor.201200105.
[4] I. Viola, N. Ghofraniha, F. Di Maria, G. Barbarella, C. Conti, and G. Gigli, in preparation.
[5] I. Viola, N. Ghofraniha, A. Zacheo, V. Arima, C. Conti, and G. Gigli, in preparation.
[6] I. Viola, A. Zacheo, V. Arima, R. Rinaldi, G. Gigli, *et al.*, Appl. Surf. Sci. 258 (2012) 8032.

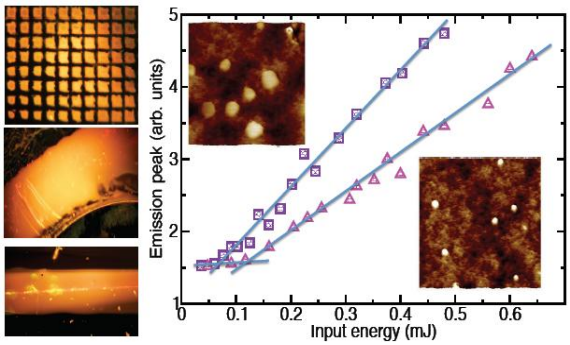


Fig. 1: (left) Optical images in true color of the random laser samples fabricated by modulating supra-molecular organization of thiophene-based fluorophore by soft lithography approaches. (right) Peak emission intensities of samples prepared at different conditions; insets: correspondent AFM zooms.

[P95] Self-assembly at all scales: reporting cellular events

I. Viola[1], G. Meli[2], F. Paoletti[2], I. E. Palamà[1], G. Barbarella[3], A. Cattaneo[2], and G. Gigli[1,4]

[1] National Nanotechnology Laboratory, CNR-Institute Nanoscience, UOS Lecce, Italy
[2] European Brain Research Institute (EBRI), Rome and Scuola Normale Superiore, Pisa, Italy
[3] CNR-Istituto per la Sintesi Organica e la Fotoreattività, Bologna, Italy
[4] Dip. di Matematica e Fisica "Ennio de Giorgi", Università del Salento and Italian Institute of Technology (IIT), Centre for Biomolecular Nanotechnologies, Lecce, Italy

Keywords: self-assembly, hierarchical structures, collagen, tissue engineering, Alzheimer's disease.

In Nature, hierarchical assembly at multiple scale-order of a limited numbers of building blocks gives rise to a wide range of structures, properties and functionalities. In such cases conformation functionality and diversity appear to be related to the sequence information of the building blocks. The controlled encoding of materials at molecular level, combining nature's molecular tools with synthetic constructs, is emerging as strategic technology [1]. The conceptual guideline for the design of new materials is that different spatiotemporal composition of existing molecules could lead to a physiochemical modulation up to the macroscale.[2] Anyway, the control over the assembly and functionality of synthetic nanostructures and efficient materials for new applications are still open challenges.

In this work will be reported studies of the assembly-functionality interaction involving different types of proteins. The two projects focus on a functional material setting and a biochemical one, respectively, For a tissue engineering field, a suitably designed synthetic semiconducting fluorophore is spontaneously incorporated by living fibroblasts of human and murine derivation thus physiologically generating fluorescent and conductive microfibers. The microfibers, mainly made of type-I collagen, are secreted intracellularly and subsequently extruded into the ECM without adverse effects on cell viability and proliferation activity. We demonstrated that - similar to nature, in which functional materials are generated by combining diverse compositions of existing matter - fluorophore physico-chemical instructions (optical, electrical, mechanical properties) are periodically fixed at the structural level, during the hierarchical assembly of the fluorescent microfibres, thus generating innovative biocompatible smart materials [3,4].

From a biochemical point of view, the aim was to study mechanisms of interactions in different types of misfolded proteins as functional biomarkers for Alzheimer's disease (AD). An ultrasensitive detection of functional conformation and kinetics of interaction of principal AD biomarkers is realized under crowding physiological conditions by a combination of microfluidic approach with scanning probe and confocal microscopy. The supramolecular aggregation and interactions have been selectively tuned and the conformation has been correlated to biochemical functionalities. All the approaches are also directed to the investigation of antigen-antibody interactions and dynamical processes of accumulation for the more toxic forms [5].

References:

[1] M. J. Buehler, Nature Nanotech. 5 (2010) 172.
[2] G. M. Whitesides, B. Grzybowski, Science 295 (2002) 2418.
[3] I. E. Palamà, F. Di Maria, I. Viola, E. Fabiano, G. Gigli, C. Bettini, G. Barbarella, J. Am. Chem. Soc. 133 (2011) 17777.
[4] I. Viola, I. E. Palamà, A. Coluccia, M Biasiucci, F. Di Maria, G. Barbarella, G. Gigli, *et al.*, Integr. Biol, submitted to.
[5] G. Meli, R. Ghidoni, I. Viola, G. Gigli, L. Benussi, A. Cattaneo *et al.*, submitted paper.

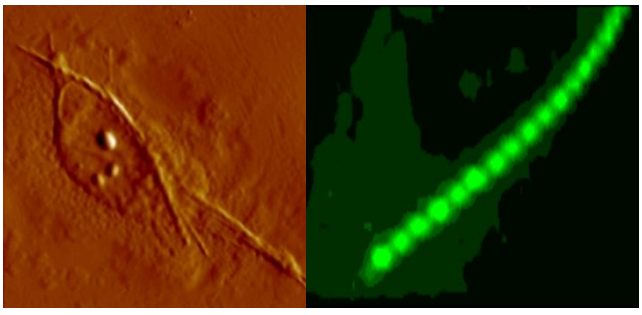


Fig. 1. Morphological and confocal characterizations of microfibres production.

[P96] The NANOLAB Project : bringing the big ideas of nanoscience to school labs

A. Lisotti[1,2,3], V. De Renzi[2,3], and G. Goldoni[2,3]

[1] PhD School in Physics and Nanoscience, University of Modena and Reggio E., Italy
[2] Department of Physics,Informatics and Mathematics, University of Modena and Reggio E. Modena , Italy
[3] CNR-Institute for Nanoscience S3, Modena, Italy

Keywords: nanoscience, nanomaterials, high school, undergraduates, modern physics.

The growing role of the nano-perspective in contemporary technologies naturally calls for the inclusion of nanoscience in high school curricula. In addition to rising student consciousness about such a pervasive topic and to the huge technological interest, which naturally appeals to students, nanosciences are a natural playground to introduce modern physics in a hands-on interdisciplinary way. Indeed, owing to the fact that nano-systems set themselves between the intrinsically quantum scale of atoms and the classical macroscopic scale, they easily couple to several controllable external fields (temperature, pressure, visible light, electrostatic fields, etc). This, for example, opens the possibility to expose intrinsically quantum phenomena in school laboratories by simple experiments with electrical conduction, elasticity, friction, etc. which openly challenge the 'classical' view by counterintuitive results.

NANOLAB is an open project aiming at including nano-inspired hands-on activities in high schools[1] [2] to upgrade Nano outreach, from simple understanding to actual engagement, and final embedding into classroom practice. Some of the proposed activities are actually being used also at undergraduate level.

NANOLAB consists of simple, cheap, robust and safe experimental protocols, currently covering four areas of nanoscience (nanoparticles, nano-friction, smart metals, conductive polymers), each conveying one of the key ideas of nanoscale: ‘size matters’, ‘the new hierarchy in forces’, ‘structure and function’, ‘quantum mechanics at work’. Within each area, different integrated hands-on activities and levels of sophistication are offered, from manual to digital data collection and elaboration, including use of pupils’ own mobile devices (cell and smart phones, tablets) which turn out to be powerful, low-cost, sensitive multi-purpose lab tools, with an added impact on student motivation and active involvement. The experimental protocols, including videoguides, students' sheets, and large sets of supporting materials for teachers, focused on the new physics behind the phenomena, are published under Creative Commons license in an open website To give teachers adequate support and provide solid background knowledge a first coaching course was held in autumn 2011 in Modena and a new one will be run at national level in September 2013 aiming at growing in a networking community of both teachers and researchers.

References:

[1] NANOLAB is on-line at http://www.nanolab.unimore.it .
[2] A. Lisotti, V. De Renzi, C. A. Rozzi, E. Villa, F. Albertini, and G. Goldoni, Physics Education accepted.

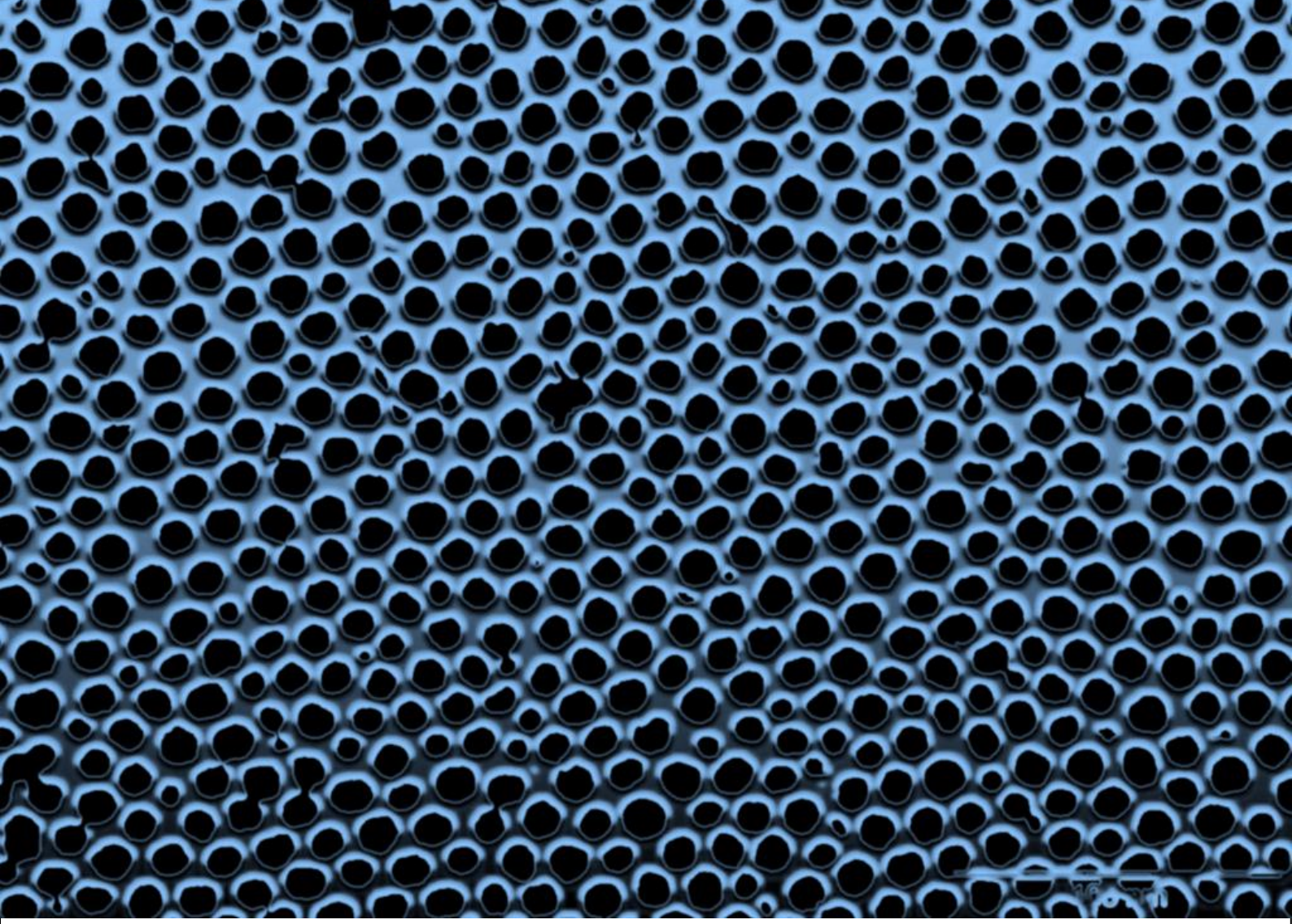
Fig.1. All the materials can be downloaded from NANOLAB website.

LIST OF CNR NANO AUTHORS

LIST OF PARTICIPANTS

Marco Affronte	MO
Andrea Alessandrini	MO
Valentina Arima	LE
Paolo Arosio	MO
Simone Barbarino	PI
Valerio Bellini	MO
Luca Bellucci	MO
Enrico Benassi	MO
Stefania Benedetti	MO
Andrea Bertoni	MO
Roberto Biagi	MO
Monica Bianco	LE
Ranieri Bizzarri	PI
Lorenzo Bordonali	MO
Carlo Augusto Bortolotti	MO
Giorgia Brancolini	MO
Arrigo Calzolari	MO
Andrea Camposeo	LE
Andrea Candini	MO
Matteo Carrega	PI
Oliver Carrillo	MO
Riccardo Castagna	PI
Fabrizio Castellano	PI
Alessandra Catellani	MO
Marco Cecchini	PI
Giovanni Checcucci	PI
Ciro Cecconi	MO
Giuseppe Ciccarella	LE
Silvia Colella	LE
Stefano Corni	MO
Valdis Corradini	MO
Massimo Cuscunà	LE
Sergio D'Addato	MO
Pino D'Amico	MO
Milena De Giorgi	LE
Valentina De Renzi	MO
Massimo De Vittorio	LE
Elena Degoli	MO
Loretta Laureana del Mercato	LE
Umberto del Pennino	MO
Alain Delgado Gran	MO
Alessandro di Bona	MO
Rosa Di Felice	MO
Eduardo Fabiano	LE
Paolo Facci	MO
Alessandro Farace	PI
Riccardo Farchioni	PI
Elena Favilla	PI
Rosario Fazio	PI
Andrea Ferretti	MO
Stefano Frabboni	MO
Anna Garbesi	MO
Gian Carlo Gazzadi	MO
Francesco Ghetti	PI
Alberto Ghirri	MO
Francesco Giazotto	PI
Giuseppe Gigli	LE
Guido Goldoni	MO
Vincenzo Grillo	MO
Giuseppe Grosso	PI
Karina Andrea Guerrero Becerra	MO
Stefan Heun	PI
Karsten Leding Jensen	MO
Martiros Khurshudyan	MO
Silvia Landi	PI
Alessandro Lascialfari	MO
Stefano Leporatti	LE
Giacomo Levita	MO
Annamaria Lisotti	MO
Paola Luches	MO
Rita Magri	MO
Vincenzo Maiorano	LE
Ivan Marri	MO
Giuseppe Maruccio	LE
Luca Masini	PI
Elisa Molinari	MO
Anna Grazia Monteduro	LE
Umberto Muscatello	MO
Riccardo Nifosì	PI
Tomas Orlando	MO
Stefano Ossicini	MO
Ilaria Elena Palamà	LE
Guido Paolicelli	MO
Daniela Parisi	PI
Adriana Grazia Passaseo	LE
Vittorio Pellegrini	PI
Luana Persano	LE
Marco Pieruccini	MO
Silvio Pipolo	MO
Dario Pisignano	LE
Stefano Pittalis	MO
Marco Polini	PI

Deborah Prezzi	MO
Elisabetta Primiceri	LE
Alessandra Quarta	LE
Gian Michele Ratto	PI
Maria Clelia Righi	MO
Rosaria Rinaldi	LE
Stefano Roddaro	PI
Massimo Rontani	MO
Marta Rosa	MO
Davide Rossini	PI
Alberto Rota	MO
Miguel Royo Valls	MO
Carlo Andrea Rozzi	MO
Alice Ruini	MO
Daniele Sanvitto	LE
Antonella Sgarbossa	PI
Ilaria Siloi	MO
Lucia Sorba	PI
Maria Chiara Spadaro	MO
Wenming Sun	MO
Fabio Taddei	PI
Vittorianna Tasco	LE
Maria Teresa Todaro	LE
Andrea Tomadin	PI
Ilaria Tonazzini	PI
Mauro Tonelli	PI
Valentina Tozzini	PI
Alessandro Tredicucci	PI
Manoj Tripathi	MO
Filippo Troiani	MO
Ilaria Valenti	MO
Stefano Valentini	PI
Sergio Valeri	MO
Daniele Varsano	MO
Stefano Veronesi	PI
Alessandro Vezzani	MO
Ilenia Viola	LE
Michele Virgilio	PI
Miriam Vitiello	PI
Shudong Wang	MO
Laura Zanetti Polzi	MO
Giampaolo Zuccheri	MO



Modena
10-11 | 06 | 2013