Italian National Conference on the Physics of Matter

Catania, September 30 – October 4, 2019

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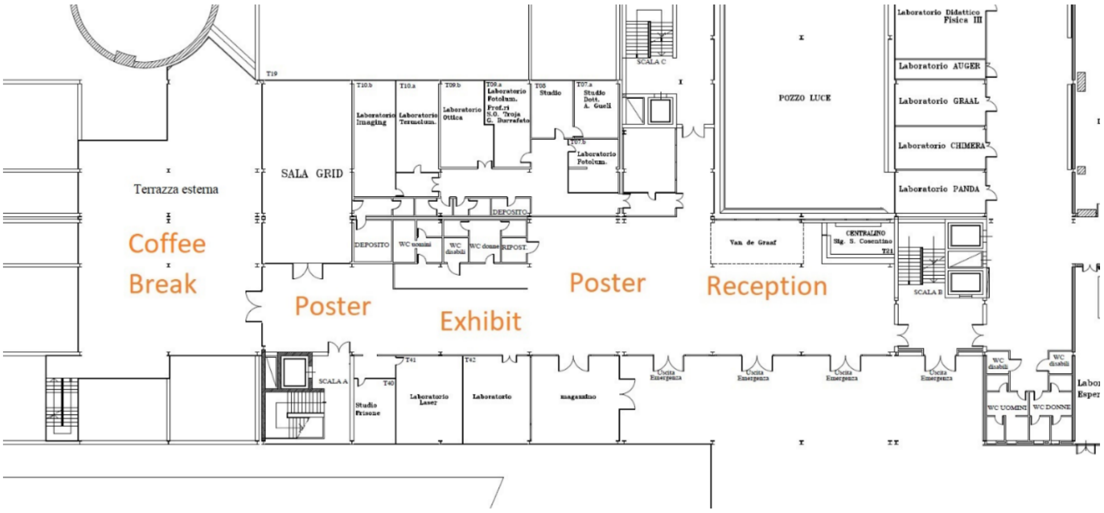
	Sunday 29	Monday 30	Tuesday 01	Wednesday 02	Thursday 03	Friday 04
9:00			Julia Yeomans	Kai Kaila	Dirk Van der Marel	Jukka Pekola
9:30						
10:00			Coffee break	Coffee break	Coffee break	Coffee break
10:30		Registration	Parallel sessions	Parallel sessions	Parallel sessions	Parallel sessions
11.00						
11.30		Opening				
12.00		Amos Maritan				
12.30						
13.00		Lunch	Lunch	Lunch	Lunch	Good bye party
13.30						
14.00		Ian Robinson	Christian Schonenberger	Riccardo Betti	Stefan Maier	
14.30						
15.00		Parallel sessions	Parallel sessions	Special session on the italian research infrastructures	Parallel sessions	
15.30						
16.00						
16.30						
17.00						
17.30		Coffee break and poster session	Ursula Keller	Stefan Goedeker	David Quere	
18.00	Welcome party and visit to the Monastero dei Benedettini					
18.30			Coffee break and poster session		Coffee break and poster session	
19.00						
19.30						
20.00				Social dinner		
20.30						

Conference site

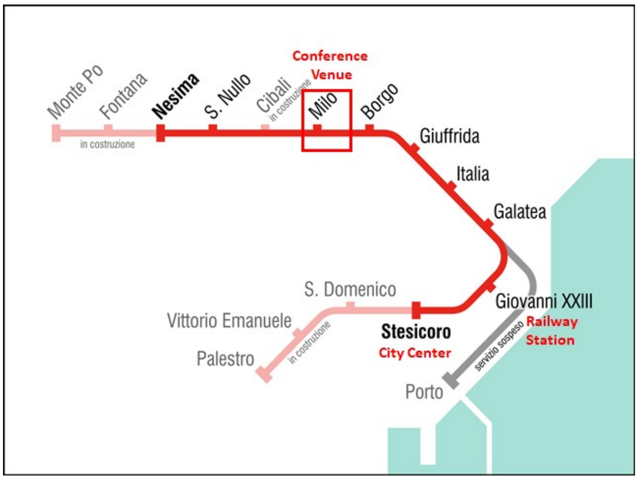
All the activities will take place at the Physics Department of the University of Catania located in Via Santa Sofia 64, and in the nearby Department of Mathematics and Informatics.

In the entrance hall of the Physics Department, along with the registration desk it will be located the tables of the exhibitors, the panels for the poster session and it is where the coffee break will be served.



It will be possible to have lunch in a reserved area in the Physics Department. The cost of lunch is not included in the registration fee and can be payed directly to the caterer that will also release the corresponding receipt.

Transportation



In order to reach the conference site an efficient Metro is operating in Catania. In the city center you can take the metro in one of these two stations, Giovanni XXIII and Stesicoro. To reach the Conference Venue, you must get out at the metro station Milo, where you will find a shuttle bus connecting with the Department of Physics (Cittadella Universitaria).

Alternatively, the bus line BRT directly connects the city center with the Conference Venue. You can get the BRT in "Piazza Stesicoro" and get out in "via Santa Sofia" (Cittadella Universitaria).

Lecture rooms

Plenary Lectures and the common other events will take place in the main lecture Hall, located in the physics department. The parallel session will

take place in the rooms of the Physics Departments and of the Mathematic Department. The location of the various rooms will be indicated within the buildings.

In the University Campus area are also present two cafeteria, indicated in the above figure.

Plenary sessions

Monday, September 30

12:00 -13:00 **Amos Maritan**
Università di Padova (Italy)
Optimality and Scaling Laws in LivMat

14:00 -15:00 **Ian Robinson**
University College (UK) – Brookhaven Nat. Lab (USA)
Ultrafast Dynamics of Materials studied by Coherent X-ray Diffraction

Tuesday, October 1

09.00 -10:00 **Julia Yeomans**
University of Oxford (UK)
Self-propelled topological defects in active matter

14:00 -15:00 **Christian Schönenberger**
University of Basel (Switzerland)
Engineering van der Waals Heterostructures: the importance of strain and superlattice effects

17.00 -18:00 **Ursula Keller**
ETH Surich (Switzerland)
Attosecond dynamics in solids

Wednesday, October 2

09:00-10:00 **Kai Kaila**
University of Helsinki (Finland)
Ion channels and transporters in neuronal signalling: from basic thermodynamics to brain functions and disorders

14:00 -15:00 **Riccardo Betti**
Rochester University (USA)
Status and prospects for nuclear fusion with lasers

17.00 -18:00 **Stefan Goedeker** University of Basel (Switzerland)

From Levinthal's paradox to the enigma of missing structures: Using Minima Hopping to gain insight into potential energy landscapes

Thursday, October 3

09:00-10:00 **Dirk Van Der Marel** Université de Genève (Switzerland)

The mechanism of superconducting pairing in doped strontium titanate

14:00 -15:00 **Stefan Maier** University of Munich(Germany)

Plasmonic nanoparticles as energy converters for chemical reactions and for the launching of acoustic surface waves

17.00 -18:00 **David Quéré** ESPCI Paris (France)

Friday, October 4

09:00-10:00 **Jukka Pekola** Aalto University (Finland)

Thermodynamics of superconducting quantum circuits

Status and prospects for nuclear fusion with lasers

Riccardo Betti
Laboratory for Laser Energetics, University of Rochester

For decades, scientists have been trying to develop clean and unlimited energy by fusing light nuclei as occurs in the center of the sun. A critical step in the quest for nuclear fusion is the demonstration of thermonuclear ignition of fusion fuel in the laboratory. Giant lasers have been prime candidates to achieve fusion ignition of deuterium-tritium (DT) fuel due to their ability to compress and heat material to pressures of billions of atmospheres and temperatures of millions of degrees. Recent progress in laser fusion has improved the prospects of achieving ignition of millimeter-size capsules with megajoule-class lasers. Laser fusion uses either direct illumination of the capsule (direct-drive) or indirect illumination of the capsule via X-rays produced by laser heating of a metal enclosure called a hohlraum (indirect-drive). Direct-drive is pursued at the OMEGA laser facility of the University of Rochester while indirect-drive is pursued at the National Ignition Facility (NIF) at the Lawrence Livermore National Laboratory. Recent implosion experiments at the NIF have achieved the conditions of pressure and confinement time that are about 70% of the values required for thermonuclear ignition. The improvements came from enhanced control of the hohlraum energetics and use of capsules of more-efficient ablators. When scaled to NIF laser energies, recent direct-drive implosions on OMEGA are expected to produce more than 500 kilojoules of fusion energy. Those implosions have benefited from a significant increase in implosion velocity obtained through larger-diameter targets. A new statistical approach[1] used in designing OMEGA targets has demonstrated a considerable predictive capability, thereby enabling the design of targets with improved performance. A review of the steps leading to this improved performance is presented together with an assessment of future expectations of achieving thermonuclear ignition via laser fusion. This material is based upon work supported by the Department of Energy National Nuclear Security Administration. The support of DOE does not constitute an endorsement by DOE of the views expressed in this article.

[1] V. Gopalaswamy et al.,"Tripled yield in direct-drive laser fusion through statistical modelling", Nature, Vol. 565, p. 581-586 (2019)

From Levinthal's paradox to the enigma of missing structures: Using Minima Hopping to gain insight into potential energy landscapes

Stefan Goedecker
University of Basel (Switzerland)

The number of possible structures of a condensed matter system is growing exponentially with respect the number of atoms in the system. So, for large systems, it is neither in a simulation possible to search over all existing structures to find the geometric ground state structure, nor would it be possible for such a system in nature to find its ground state on any reasonable time scale if it had to visit a large fraction of intermediate structures. This problem has first been noticed in the context of protein folding and is known as the Levinthal paradox. Its solution came also from the protein folding community. The folding of a protein on a short time scale can only be explained if one assumes that the potential energy surface has a funnel like structure that guides the system directly into its ground state without the need to visit a very large number of intermediate structures. The situation is analogous for large molecules, clusters and solids. There is only a realistic chance of finding the ground state structure if the potential energy surface is composed of funnels. Modern structure prediction methods have shed new light on many longstanding structural problems. The structures found by systematic structure prediction simulations for various nano-systems are for instance frequently considerably lower in energy than structures proposed based on chemical/physical intuition. Many systems have a multi-funnel character. In the case of periodic solids, the structures at the bottom of these funnels typically represent different crystalline structures. Even though the number of funnels and therefore the number of possible crystalline structures is typically not huge it turns out that one can find in simulations a considerably larger number of low-energy structures than is known experimentally. I call this fact the enigma of missing structures and I will show what features of the potential energy surface can lead to kinetically inaccessible structures. All the results presented were obtained by a family of methods that are based on the Minima Hopping Method. I will also explain these methods that allow us to find metastable structures, transition states and reaction/transformation pathways on the potential energy surface.

Attosecond dynamics in solids

Ursula Keller

ETH Zurich

In the 1980s, rapid progress in picosecond and femtosecond ultrafast lasers has enabled to start to bridge the gap between electronics and optics with the optical generation of terahertz frequencies for the investigation of ever faster physical processes and device performance. More recently with full electric field control within few-cycle pulses [1] we have continued to fully bridge this gap approaching the petahertz regime. A number of pioneering publications demonstrated that attosecond carrier transport can be resolved with attosecond transient absorption spectroscopy (ATAS) [2-5] and an attosecond interferometry technique at solid surfaces [6,7]. After a general introduction with this plenary talk I will discuss in more details some recent results from our group in diamond [5], GaAs [8,9] and Ti-metal [10]. In addition I will discuss the effective mass approximation in the attosecond regime [11].

[1] H. R. Telle et al., "Carrier-envelope offset phase control: A novel concept for absolute optical frequency measurement and ultrashort pulse generation," Appl. Phys. B 69, 327 (1999)
[2] M. Schultze et al., "Attosecond band-gap dynamics in silicon " Science 346, 1348 (2014)
[3] H. Mashiko, et al., "Petahertz optical drive with wide-bandgap semiconductor," Nature Physics 12, 741 (2016)
[4] M. Schultze et al., "Controlling dielectrics with the electric field of light," Nature 493, 75 (2013)
[5] M. Lucchini et al., "Attosecond dynamical Franz-Keldysh effect in polycrystalline diamond," Science 353, 916 (2016)
[6] R. Locher et al., “Energy-dependent photoemission delays from noble metal surfaces by attosecond interferometry” Optica 2, 405 (2015)
[7] M. Lucchini et al., “Light-matter interaction at surfaces in the spatiotemporal limit of macroscopic models”, Phys. Rev. Lett.115, 137401 (2015
[8] F. Schlaepfer et al., “Attosecond optical-field-enhanced carrier injection into the GaAs conduction band”, Nature Physics14, 560 (2018)
[9] S. A. Sato et al., “Role of intraband transitions in photocarrier generation”, Phys. Rev. B98, 035202 (2018)
[10] M. Volkov, S. A. Sato, F. Schlaepfer,L. Kasmi,N. Hartmann,M. Lucchini, L. Gallmann,A. Rubio,U. Keller, submitted
[11] L. Kasmi et al., “Effective mass effect in attosecond electron transport”, Optica 4, 1492 (2017)

Plasmonic nanoparticles as energy converters for chemical reactions and for the launching of acoustic surface waves

Stefan A Maier

Chair in Hybrid Nanosystems, Nanoinstitute Munich, Faculty of Physics,Ludwig-Maximilians-Universität München, 80539 München, GermanyStefan.Maier@physik.uni-muenchen.de

Abstract - In addition to the well-established electromagnetic hot spots of plasmonic nanostructures, metal nanoparticles can also act as nanoscale energy transformers from electromagnetic into chemical or acoustic energies. Energetic electron/hole pairs formed via plasmon decay enable control over chemical reactions on the nanoscale, and coherent acoustic vibrations of the nanostructures the controlled launching and detection of acoustic surface waves.

We present our recent efforts to unravel both the energetics and the spatial distribution of hot charge carriers generated in metallic nanostructures via the decay of localized surface plasmons. Using a combination of bulk electrochemistry and single-particle spectroscopy, we directly determine the energy of hot holes in Au nanocolloids and their energetic contribution to a polymerization reaction at the nanoparticle's surface [1]. Our results demonstrate that the energy contribution of the "hot" holes is maximized upon excitation at the localized plasmon resonance frequency of the particles.

Such plasmon-enhanced chemistry enables further control over nanoscale self-assembly [2] and also a novel super-resolution imaging scheme of optical absorption [3], based on the controlled cleaving of thiol-bonds via hot electrons excited in top-down fabricated gold nanoantennas. We use this scheme to bridge top-down nanofabrication with bottom-up self-assembly, and further show direct spatial imaging of near-field energy transfer in a Fano cavity.

In addition to hot electron effects, optical excitation of metallic nanoparticles also lead to coherent acoustic vibrations. Using spatially separated source and detector nanoparticles, we demonstrate the launching of acoustic surface waves in the underlying substrate via this scheme (Figure, [4]). This enables nanoscale interrogation of the properties of surface-acoustic waves.

Launching of surface-acoustic waves in the underlying substrate via coherent excitation of phonons in a metallic nanostructure [4].

Pensa et al, Nano Letters 19, 1867 (2019)
Simoncelli et al, ACS Nano 12, 2184 (2018)
Simoncelli et al, Nano Letters 18, 3400 (2018)
Berte et al, Physical Review Letters 121, 253902 (2018)

Amos Maritan

Optimality and Scaling Laws in LivMat

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Via Marzolo 8, 35131 Padova Italy

Living systems are characterized by the recurrent emergence of patterns/regularities independent of their biological/physiological details. In ecological communities species interact forming networks with typical topological structures. Power-law distributions and long-range correlations are pervasive and can be found both at the level of single organisms and at the community level.

The most challenging goal in ecology is to grasp how general trends and behaviors emerge in spite of such complexity.

Forests represent one of the most complex systems with a high degree of structural and functional diversity: in the tropics, there often are hundreds of coexisting plant species with different habitats and thousands of consumers, each of them with interspecific relationships with plant species. This leads to a multitude of interconnected food webs and complex fluxes of matter and energy. We demonstrate an astounding simplicity underlying the apparent bewildering complexity of forests. Our starting point is based on optimization/variational principles and scaling analysis from statistical physics for understanding and making predictions that are in accord with empirical data.

Thermodynamics of superconducting quantum circuits

JukkaPekola

Aalto University (Finland)

I will present our work on thermodynamics of mesoscopic electronic circuits. In the first part of the talk I discuss stochastic thermodynamics in circuits where single electrons can be controlled and detected. This set-up forms a platform for studies of non-equilibrium fluctuation relations, and has allowed us to realize and investigate two types of Maxwell's demons [1-3]. In the second part of the talk I introduce superconducting qubits as a working substance for experiments on quantum heat transport, refrigerators and heat engines [4-6], and I present our efforts towards measuring quantum trajectories by a calorimetric method [7].

[1] Jonne V. Koski, Ville F. Maisi, Jukka P. Pekola, and Dmitri V. Averin, Experimental realization of a Szilard engine with a single electron, PNAS 111, 13786 (2014).

[2] J. V. Koski, A. Kutvonen, I. M. Khaymovich, T. Ala-Nissila, and J. P. Pekola, On-chip Maxwell’s demon as an information-powered refrigerator, Phys. Rev. Lett. 115, 260602 (2015).

[3] J. P. Pekola, Towards quantum thermodynamics in electronic circuits, Nature Physics 11, 118 (2015).

[4] Alberto Ronzani, Bayan Karimi, Jorden Senior, Yu-Cheng Chang, Joonas T. Peltonen, ChiiDong Chen, and Jukka P. Pekola, Tunable photonic heat transport in a quantum heat valve, Nature Physics 14, 991 (2018).

[5] B. Karimi and J. P. Pekola, Otto refrigerator based on a superconducting qubit: classical and quantum performance, Phys. Rev. B 94, 184503 (2016).

[6] Jorden Senior, Azat Gubaydullin, Bayan Karimi, Joonas T. Peltonen, Joachim Ankerhold, and Jukka P. Pekola, Heat rectification via a superconducting artificial atom, arXiv:1908.05574

[7] B. Karimi, F. Brange, P. Samuelsson, and J. P. Pekola, Observing temperature fluctuations of a mesoscopic electron system, arXiv:1904.05041

Ultrafast Dynamics of Materials studied by Coherent X-ray Diffraction

Ian Robinson
London Centre for Nanotechnology, University College, London, UK
Condensed Matter Physics and Materials Science, Brookhaven National Lab

The structure of materials is accessible through X-ray diffraction techniques. In 1936 Lawrence Bragg developed the idea of imaging materials through an X-ray microscope. Today this has become possible with the development of synchrotron radiation sources of X-rays and will move into the ultrafast time domain in the near future with the development of free-electron laser sources.

I will describe my group’s latest Bragg Coherent Diffraction Imaging (BCDI) experiments, which are capable of imaging nanometer-sized crystals in three dimensions [1]. The method is different from many other imaging methods in that it uses data measured around individual Bragg peaks of the crystal studied. For this reason, it is highly sensitive to strain fields present in the crystal under investigation, which are therefore mapped in three dimensions [2]. The latest development is to measure several Bragg peaks from the *same nanocrystal* to reveal multiple components of the displacement field and the resulting strain tensor. The strain induced by ion-beam milling of nanocrystals has been imaged in 3D in this way [3]. I will show recent progress in understanding some of these systems in the first few picoseconds after excitation with a laser [4].

[1] “Three-dimensional Mapping of a Deformation Field inside a Nanocrystal”, Mark A. Pfeifer, Garth J. Williams, Ivan A. Vartanyants, Ross Harder and Ian K. Robinson, Nature 442 63-66 (2006).
[2] "Coherent Diffraction Imaging of Strains on the Nanoscale", Ian Robinson and Ross Harder, Nature Materials 8 291-298 (2009)
[3] “3D lattice distortions and defect structures in ion-implanted nano-crystals”, Felix Hofmann, Edmund Tarleton, Ross Harder, Nicholas Phillips, Pui-Wai Ma, Jesse Clark, Ian Robinson, Brian Abbey, Wenjun Liu, and Christian Beck, Nature Scientific Reports 7 45993 (2017)
[4] Melt-front Dynamics in Polycrystalline Gold Thin Films, Tadesse A. Assefa, Yue Cao, Soham Banerjee, Sungwon Kim, Dongjin Kim, Sunam Kim, Jae Hyuk Lee, Sang-Youn Park, Intae Eom, Jaeku Park, Daewoog Nam, Sangsoo Kim, Sae Hwan Chun, Hyojung Hyun, Kyung Sook Kim, Pavol Juhas, Emil S. Bozin, Ming Lu, Changyong Song, Hyunjung Kim, Simon J. L. Billinge and Ian K. Robinson (2019)

Engineering van der Waals Heterostructures: the importance of strain and superlattice effects

Christian Schönenberger, University of Basel

The active 2D vdW's material, be it graphene (G) or a TMDC, must be encapsulated to achieve stable transport with high mobility. Hence there are at least two interfaces, for example hBN-G and G-hBN in encapsulated graphene, where the relative lattice alignment may play a role. It has been widely observed that the lattice of hBN imprints a potential to graphene, leading to a new bandstructure, the so-called superlattice (SL), where secondary Dirac points (sDP) can emerge. This can strongly effect the electrical properties, such as the electrical resistance and the supercurrent in Josephson junctions made form encapsulated graphene. We have found an excess edge current at gate voltages where van Hove singularities (vHS) appear in the SL bandstructure. We argue that the effective transport time in the bulk increases at the vHSs due to the suppression of the Fermi velocity.

SL effects can be engineered if lattices are intentionally aligned or stacked together with a well-defined rotation angle adjusted to within a fraction of a degree. Until now, only a single SL has been discussed in the literature. However, it is possible that two SLs with two different periods may emerge, since G is in contact with an upper and a lower hBN layer. These new SLs may themselves form a next generation of "2nd order" superlattice (2SL) with an even larger periodicity. We have found evidence for 2SLs in stacks of encapsulated graphene.

Regarding strain, we first show that clean suspended graphene at high tension mechanically resonate with a fundamental mode larger than 1GHz due to the large (uniaxial) tension, corresponding to strain values exceeding 1%. It has been predicted that non-uniform strain can generate a pseudo-magnetic field in graphene which acts on the two different valleys with opposite signs. We strain encapsulated graphene, fabricated on a flexible substrate, by bending the substrate. Compared to suspended graphene, a significant advantage of substrate clamped devices is that the gate capacitance is not affected by bending, which is crucial for high-resolution transport measurements. We have also engineered strain gradients by shaping the graphene stacks in a trapezoid instead a rectangle. First electrical measurements show effects that can be assigned to both a strain-induced scalar and pseudo-magnetic potential.

Acknowledgment: This work has been done by the following list of contributors in alphabetic order: G. Abulizi, A. Baumgartner, M. Calame, A. Eichler, R. Delagrange, J. H. Garcia, D. I. Indolese, M. Jung, M. Kedves, P. Karnatak, A. Kononov, D. Mandrus, M.H. Liu, P. Makk, J. Overbeck, K. Qu, P. Rickhaus, T. Taniguchi, J. Wallbanks, L. Wang, K. Watanabe, J.-Q. Yan, and S. Zihlmann. I am very grateful to them! The work has financially been supported by the Swiss NSF, graphene flagship, H2020-ERC Adv, SNF-QSIT, SNI and further organizations.

Dirk Van der Marel

Université de Genève (Switzerland)

The mechanism of superconducting pairing in doped strontium titanate.

Strontium titanate is a semiconducting material, which can be tuned to become ferro-electric by substituting the heavier 18^O isotope for the natural 16^O isotope. When doped with electrons, the material becomes a good metal with a resistivity that rises with temperature proportional to T^2. The doped material is superconducting at low temperatures, even down to doping levels where the average distance between the conduction electrons is more than 200 Angstrom. This state of affairs has lead to many speculations as to the mechanism that binds the electrons together in Cooper-pairs. Among the many proposals, the interplay between ferro-electricity and superconducting pairing has been particularly prominent in recent years and has lead to the prediction of a very large increase of superconducting Tc with 18^O isotope substitution. We have studied this phenomenon experimentally by preparing these samples, by doping them, and studying their transport and optical properties. I will discuss these experimental data and their theoretical implications for the physics of superconductivity in doped SrTiO3.

Self-propelled topological defects in active matter

Julia Yeomans
University of Oxford (United Kingdom)

Active materials, such as bacteria, molecular motors and self-propelled colloids, are Nature’s engines. They continuously transform chemical energy from their environment to mechanical work. Dense active matter shows mesoscale turbulence, the emergence of chaotic flow structures characterised by high vorticity and self-propelled topological defects.

The chaotic nature of active turbulence means that it is likely to be difficult to harness its energy. Hence it is interesting to consider ways to `tame' active turbulence, channelling the energy input into coherent flows. This can be done by screening hydrodynamics through confinement or friction, and I will describe flow patterns and defect trajectories in active matter in confined geometries.

Moreover the ideas of active matter suggest new ways of interpreting cell motility and cell division. In particular recent results indicate that active topological defects may help to regulate turnover in epithelial cell layers and contribute to controlling the structure of bacterial colonies.

Parallel Sessions

30 Mon

Low-dimensional Materials 1	30 Mon
Materials and devices for renewable energy 1	30 Mon
Active and soft matter and fluids 1	30 Mon
Physics technologies for health	30 Mon
Complex systems, networks and interdisciplinary applications of statistical mechanics	30 Mon

01 Tue

Low-dimensional Materials 2	01 Tue
Materials and devices for renewable energy 2	01 Tue
Active and soft matter and fluids 2	01 Tue
Out of Equilibrium Statistical Physics 1	01 Tue
Cultural Heritage 1	01 Tue
Low-dimensional Materials 3	01 Tue
Materials and devices for renewable energy 3	01 Tue
Active and soft matter and fluids 3	01 Tue
Plasma Physics 1	01 Tue
Advanced computational Methods 1	01 Tue
Biophysics, Biomedicine and modeling 1	01 Tue
Cultural Heritage 2	01 Tue
Materials for environmental applications 1	01 Tue
Nanostructures and Nanotechnologies 1	01 Tue
Novel semiconductors and applications 1	01 Tue

02 Wed

Quantum Information Physics and Technologies 1	02 Wed
Physics meets the brain: biophysical approaches to the neuroscience	02 Wed
Ultrafast phenomena	02 Wed
Plasma Physics 2	02 Wed
Advanced computational Methods 2	02 Wed
Biophysics, Biomedicine and modeling 2	02 Wed
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Materials for environmental applications 2	02 Wed
Nanostructures and Nanotechnologies 2	02 Wed
Novel semiconductors and applications 2	02 Wed

03 Thu

Quantum Information Physics and Technologies 2	03 Thu
Nanostructures and Nanotechnologies 3	03 Thu
Strongly Correlated systems and Spintronics 1	03 Thu
Novel semiconductors and applications 3	03 Thu
Superconductivity 1	03 Thu
Biophysics, Biomedicine and modeling 3	03 Thu
Nanophotonics and plasmonics	03 Thu

04 Fri

Orals

LOW-DIMENSIONAL MATERIALS 1	STEFAN HEUN
MATERIALS AND DEVICES FOR RENEWABLE ENERGY 1	PICCININ/LA MAGNA
ACTIVE AND SOFT MATTER AND FLUIDS 1	JULIA YEOMANS
PHYSICS TECHNOLOGIES FOR HEALTH	PIGNATARO/ARRABITO
COMPLEX SYSTEMS, NETWORKS AND INTERDISCIPLINARY APPLICATIONS OF STATISTICAL MECHANICS	SILVIA SCARPETTA

#001 - POLYMER-PROMOTED GROWTH OF VAN DER WAALS HETEROSTRUCTURES

Filippo Fabbri (I) - NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore,

Research on two-dimensional atomic crystals is intense and is likely to remain one of the leading topics in condensed matter physics and materials science for many years. Looking beyond the study of single material, isolated atomic planes can also be reassembled into designer heterostructures (often referred to as 'van der Waals') made layer by layer in a precisely chosen sequence [1]. In the recent years van der Waals heterostructures were mainly fabricated by stacking single layer materials obtained by means exfoliation process. This method allows to fabricate small area devices, in the order of tens of micron, with a lack of scalability and integration with silicon technology. The direct growth, by means of chemical vapour deposition process, allows to create van der Waals heterostructure by a direct synthesis of the top materials on different 2D platform, overcoming mainly the issue of the scalability. Among the 2D crystals, it is possible to find insulating, as hexagonal boron nitride (h-BN), semiconducting, as the transition metal dichalcogenides (namely MoS_2 and WS_2) and semi-metallic materials, as graphene (Gr), and therefore it is possible to tailor the properties of van der Waals heterostructure by stacking the different 2D-materials.

In this work, we study the direct synthesis of WS_2 monolayer (ML) on different two-dimensional platforms as single crystalline CVD graphene or commercial single layer h-BN. In both cases we find that the polymeric residuals due to the transfer of graphene and/or h-BN promote the synthesis of the WS_2 MLs in terms of size and orientation. However, it is worth noting that the high temperature CVD process (900°C) is detrimental for single-crystal graphene in terms of doping and strain. In the case of commercial h-BN single layer the polymeric residuals protect the h-BN from the expected high temperature degradation [2], by forming an amorphous carbon layer.

Preliminary results of the synthesis of a complex heterostructures composed of WS_2/ Gr /h-BN will be shown.

The WS_2 growth dynamics and the 2D platform stability are studied by means of scanning Raman spectroscopy and secondary electron microscopy.

In conclusion we achieve the polymer promoted direct synthesis of van der Waals heterostructure by chemical vapour deposition by stacking different 2D materials.

[1] A. K. Geim & I.V. Grigorieva Nature **499**, 419-425 (2013)
[2] L.H. Li *et al.*, ACS Nano **8** 21457-1462 (2014)

#002 - MIMIC 1D PROPERTIES ON CONTINUOUS 2D MATERIALS: THE PILOT CASE OF GRAPHENE ON NICX/NI(100)

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Tailoring electronic properties on 2D materials by inducing 1D electronic states via lateral confinement is a well-established research route, with real applications almost exclusively on graphene due to the difficulty of bottom-up synthesis of nanoribbon made of other 2D materials. Here we present a different approach, based on smart choice of the substrate, that allows the creation of 1D stripes embedded on a continuous 2D material, namely graphene grown on Ni(100)[1]. Such stripes are forced to have different electronic properties by the selective formation at the graphene/metal interface of nickel carbide that decouples graphene from the substrate only at selected lanes of 1D moiré. Our results, obtained with combination of microscopy, spectroscopy and diffraction techniques and corroborated by DFT calculations, show that such 1D stripes have electronic

properties that resemble the ones of zig-zag graphene nanoribbons, and that this procedure offers the unprecedented possibility to measure the band structure of 2D materials with 1D states by angle-resolved photoelectron spectroscopy. This approach can in principle be extended to other 2D materials, giving access to characterization of low-dimensional states without passing through bottom-up synthesis of nanoribbons.
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#003 - GRAPHENE MEDIATED GROWTH OF OXIDE-METAL INTERFACES

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Ultrathin oxide films grown on metallic substrates have been intensively investigated in modern surface science [1,2]. A convenient way to tailor the physical and chemical properties of oxide/metal interfaces is the use of a buffer layer, i.e. an ultrathin metallic or oxide film interposed between the substrate and the overlayer. Here, we show that the morphology and electronic properties of oxide films can be tuned by using a buffer layer of graphene stabilized on a Ni(111) surface [3]. By combining X-ray photoemission spectroscopy, low energy electron diffraction and scanning tunneling microscopy/spectroscopy, we compare the structural, chemical and electronic properties of Cr oxide (Cr_xO_y) and Fe oxide (Fe_xO_y) films deposited by means of reactive molecular beam epitaxy on the bare and on the graphene covered Ni(111). Cr_xO_y grows layer-by-layer on the graphene/Ni(111) surface, while Fe_xO_y forms three-dimensional islands. On the other hand, Fe_xO_y develops a smooth morphology on the clean Ni(111) surface, while a rough surface is observed in the case of Cr_xO_y . Atomically resolved images show that the surface of Cr oxide grown on graphene is characterized by a honeycomb structure in which Cr and O atoms are threefold coordinated, with the same lattice parameter of the substrate. On the other hand, the images acquired on the Fe_xO_y surface display a hexagonal lattice with a larger lattice constant, suggesting a weak interaction between the islands and the substrate.
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#004 - DISCLOSING THE PHOTO-INDUCED ELECTRONIC DYNAMICS IN BLACK PHOSPHORUS: A TIME-RESOLVED ARPES STUDY

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Due to unique and promising electronic and optical properties, two-dimensional materials play a crucial role in many technological and engineering applications [1]. Among them, black phosphorus (BP) - the most stable allotrope of the phosphorus family at room temperature and pressure – has shown very singular semiconducting properties such as high hole mobility, tunable band structure and significant sensitivity to external electric field, strain and surface doping [2]. Although the equilibrium properties of BP have been thoroughly investigated in the past, little is known about its response to photo-excitation. We have studied bulk BP by means of femtosecond time- and angle-resolved photoemission spectroscopy (tr-ARPES). Our measurements disclose relevant photo-induced modifications in the electronic properties, affecting both band gap and band structure. The

results will be illustrated in terms of the photo-injected electron-hole pairs and their dynamics. Preliminary comparison with measurements performed on surface-adsorbed samples provide an essential insight on the photo-induced band manipulation, thus offering new prospective for the design of tunable band gap devices.
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#005 - TRANSIENT ELECTRONIC EFFECT IN BLACK PHOSPHORUS AFTER BAND TUNING BY SURFACE DOPING

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Black phosphorus (BP) is a layered semiconductor that is attracting great scientific interest thanks to its high carrier mobility and its anisotropic electronic and optical responses to external stimuli [1]. Its band-gap is extremely sensitive to thickness, pressure and electric field. Besides, it has been recently demonstrated that surface doping by alkali atoms is a powerful mean to fine-tune the band structure of BP, especially in atomically thin samples [2]. In view of this recent finding, understanding transient photo-induced effects in BP is of pivotal importance for practical applications. Here, we investigate bulk BP with time- and angle-resolved photoemission spectroscopy after tuning its band structure by means of alkali atoms surface doping. Photo-excitation triggers carriers dynamics, inducing peculiar band modifications that can counteract the effect of ad-sorption. Our results, combined with the study of photo-induced effects in pristine un-doped samples, provide a previously unexplored opportunity to elucidate the unique aspects of band tuning in a wider class of layered semiconductors.
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#006 - NOVEL SEED-LAYER-FREE ATOMIC LAYER DEPOSITION APPROACHES TO OBTAIN UNIFORM AND ULTRA-THIN AL2O3 LAYERS ONTO GRAPHENE

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The Graphene (Gr) with its peculiar properties, such as atomic thickness, excellent carrier mobility and field-effect tunable ambipolar current transport, is the most studied 2D material for microelectronic applications. Integration of thin layers of high-κ dielectrics on graphene is a key requirement to exploit its potential in electronics. The most promising method to obtain ultrathin and uniform films of high-k, at relatively low deposition temperature, is the Atomic layer deposition (ALD). However, the lack of out-of-plane bonds in the planar sp^2 lattice of Gr is an obstacle to the uniform ALD nucleation and growth [1]. Therefore, pre-functionalization processes and seeding layer depositions on Gr have been reported as method to promote the ALD process. Unfortunately, such approaches involve higher equivalent oxide thickness (EOT) of the high-k and adversely affect the Gr electrical properties [2]. Hence, ALD growth of dielectrics on the Gr surface, without pre-functionalization and seed-layers, is highly desirable.
In this work, we investigated a seed-layer-free ALD deposition of Al_2O_3 on monolayer Gr, as-grown and transferred, on different substrates of interest for electronics. In particular, the nucleation process has been investigated on epitaxial-Gr on SiC and on CVD-Gr on Cu and after compared to nucleation on transferred-Gr. This to clarify the role of the substrate. Nanoscale resolution scanning probe techniques, as AFM and conductive AFM, has been employed to evaluate the nucleation quality and the local electrical properties (leakage current, breakdown field) of Al_2O_3 layer. Raman spectroscopy

analyses allowed to investigate the impact of the ALD deposition on the defectivity and doping of Gr. Finally, top-gated field effect transistors were fabricated on Gr to evaluate the dielectric properties of the Al_2O_3 gate insulator, as well as the transport properties (carrier mobility and doping density) of the Gr channel.
This work has been supported, in part, by the FlagERA project GraNitE.

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#007 - STRUCTURAL AND ELECTRONIC PROPERTIES OF METAL/BLACK PHOSPHORUS NANOHYBRIDS THROUGH STEM/EELS/EDX AT ATOMIC RESOLUTION

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Two-dimensional (2D) nanomaterials have recently attracted tremendous research attention. Their unusual properties, originating from the quantum size effects, have led to many promising applications in nanoelectronics, catalysis and energy storage. Theoretical studies demonstrated that black phosphorus (BP) forms strong bonds with metal adatoms while still preserving its structural integrity, unlike graphene whose atomic lattice is strongly distorted. This unique combination of high reactivity with good structural stability is very promising for potential applications of BP. Structural and spectroscopic study by STEM-EELS have been already reported in literature and unveiled for the first time the atomic structure and electronic properties of pristine BP[1-3], During the present research activity, hybridization of exfoliated black phosphorus with different metals was carried out, either as metal nanoparticles in the case of nickel and palladium or as molecular fragment in the case of rurthenium. Thus, Ni/BP, Pd/BP and Ru/BP have been synthesized and their structural and electronic properties studied by means of Scanning Transmission Electron Microscopy (STEM), Electron Energy Loss Spectroscopy (EELS) and Energy Dispersive X-ray Spectroscopy (EDX) at atomic level. In particular, EELS spectra were numerically simulated by means of Density Functional Theory (DFT) calculations in order to assess the effect of the different metals adatoms on the phosphorene electronic Density of States (DOS), a key parameter to understand the electronic properties of the system.
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#008 - ELECTRON CONFINEMENT EFFECTS IN SILVER FILMS EMBEDDED BETWEEN GRAPHENE AND METALLIC SUBSTRATES

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We have investigated by means of angle-resolved photoemission spectroscopy (ARPES) the electronic structure of Ag multilayers intercalated between graphene (Gr) and Co(0001)[1]. ARPES measurements reveal the formation of Ag *sp*-derived quantum well states, due to finite electron reflectivity across the buried metal/metal interface. This observation provides evidence of flat Ag(111) film growth underneath Gr, in analogy with the layer-by-layer growth of Ag on the corresponding Gr-free surfaces. Band dispersion and spectral properties of the quantum well states reflect primarily the interaction with the supporting substrate, as also proved by similar experiments performed on Ag(111) films intercalated between Gr and Pt(111). Moreover, concerning the electronic structure of Gr, we provide evidence, for the first time by ARPES, of ***n***-doping and band gap opening between π and π^* Dirac cones of Gr on multilayers Ag films. These systems can be considered as prototypes of Gr-protected thin metal films displaying electron confinement effects.

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#009 - GRAPHENE-LIKE SILICENE GROWN ON GRAPHITE SURFACE

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The challenge of designing groundbreaking systems to connect with silicon technology has inspired the study of novel two-dimensional (2D) materials. Experimentally, 2D silicon layers were obtained by depositing Si atoms on metal (M) surfaces [1]. However, due to the strong p-d mixing between Si and M atoms, it is still debated if pure 2D-Si layer has been actually observed [2]. In this study we have used highly oriented pyrolitic graphite (HOPG) as substrate because of its honeycomb structure and chemical inertness. Based on scanning tunneling microscopy (STM), scanning tunneling spectroscopy and Raman spectroscopy, we demonstrate the formation of 2D Si arrangements. In particular, the Raman study shows a new feature located around 542.5 cm^{-1}, never reported so far for sp^3 Si modes, thus suggesting the formation of a genuine sp^2 Si mode assigned to silicene in low buckling configuration [3]. From STM we observed the formation of silicene nanosheets [3,4] and Si three-dimensional clusters on HOPG surface [3,4] and Si 2D sheets intercalated below the outmost carbon atom layer of the HOPG substrate [5]. Theoretical calculations of the structure and energetic viability of silicene nanosheets, of their expected Raman modes, of the strain distribution of the outermost carbon atom layer and of its influence on Raman resonances support the experimental observations.

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#010 - INNOVATIVE TECHNOLOGIES TO REDUCE THE COST OF THE PHOTOVOLTAIC ELECTRICITY OF PV MODULES

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In this paper we report on the efforts for the industrialization of Si heterojunction technology towards volume manufacturing and towards more than 25% efficiency in production, as well as on the activities to overcome the theoretical limits of silicon, aiming at more than 28%, through implementation of tandem cell structures.

#011 - THE MULTILAYER STRUCTURE OF TCO/AG/TCO FOR PV APPLICATIONS: A NEW CONCEPT OF TRANSPARENT ELECTRODES

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Transparent electrodes (TE) are critical materials for many devices in strategic technological areas such as photovoltaics (PV) and flexible electronics. In the case of thin film PV, the thickness of the TE must be reduced with respect to standard bulk solar cells, this being a big issue in terms of electrical properties. In the field of flexible electronics, the robustness and reliability under bending conditions is another hot topic to be considered. The need of simultaneously good electrical, optical and structural properties for TE pushes to study new materials with respect to the standard TCOs (transparent conductive oxides) largely employed today, often containing expensive and toxic elements such as In. Among these new materials, AZO/Ag/AZO multilayer structure (AZO = Al-doped ZnO) has shown very promising capacity of facing all the requirements for being one of the next generation TE. The ultrathin metal layer accounts for a very low electrical resistance (lower than a single TCO layer 10 times thicker) but high optical transmittance in the visible range. A step ahead is a similar multilayer but with a Ag mesh instead of a film, with benefits in terms of optical transparency and mechanical flexibility. To this end, we studied innovative IZO/Ag_mesh/IZO (IZO= In-doped ZnO) structures fabricated via colloidal lithography. Well-defined Ag grids were realized by covering an IZO film with a single layer of polystyrene spheres (1.6 μm and 5 μm in diameter) through the Langmuir-Blodgett process: we fabricated IZO/Ag/IZO multilayers having different Ag grids in terms of thickness and mesh openings. We found excellent electrical properties and a significant enhancement of the infrared transmittance (R_s=16.4 Ω/□ and Transmittance = 66%) with respect to state-of-art transparent electrodes. Furthermore, we have studied the role of interconnected Ag nanoparticles (NP): AZO/Ag NPs/AZO films were grown on glass and plastic (PEN) substrates: TCO were deposited by sputtering technique, while the Ag NP film were obtained by Supersonic Cluster Beam Deposition (SCBD). Here we show that a TCO/Ag Nps/TCO multilayer has superior flexibility, electrical stability and optical transmittance as compared to pure AZO, ITO and TCO/Ag/TCO films. The changes in the electrical resistance after mechanical bending as a function of the radius and number of bendings show a much higher degradation of the electrical properties for all AZO and ITO films with respect to the TCO/Ag Nps/TCO. The ductility of such Ag NPs film, due to its granular nature, is hence increasing the flexibility of the overall structure and the robustness upon bending processes. In summary, we show how very thin TCO/Ag/TCO multilayers, with Ag mesh, or with Ag NP, produces one of the most electrical reliable, structural flexible and optically tunable material to be employed as TE.

#012 - VIABLE STRATEGY TO IMPROVE THE STRUCTURAL STABILITY OF POLYCRYSTALLINE HYBRID PEROVSKITES

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Organic-inorganic hybrid perovskites are nowadays considered as reference materials for optoelectronics and photovoltaics. Their outstanding yields in luminescence, electroluminescence and photoelectric conversions, combined with the easy solution processing, promise large-scale production, wide dissemination and high technological throughput.

However, the well-known structural instability of hybrid perovskites under working conditions limits a real market uptake of all the related technologies. Solutions to guarantee the durability of products are mandatory and can be numerous, if the problem is addressed from different perspectives.

Moreover, the plethora of perovskite materials produced in different laboratories, with preparation procedures changing from lab to lab and from time to time, ask for stabilising treatments that, in a certain extent, reset the starting conditions in a convenient and reproducible manner. This is particularly needed for small grained perovskite layers, on one hand used to implement pinhole-free coverages, but, on the other hand, offering extended lattice discontinuities due to the high surface to volume ratio. In addition to morphology and environment, temperature-related effects are unavoidable during device operation.

In this framework and on the basis of experiment and theory, we draw a general paradigm that reconsiders N_2 not simply being an inert species but rather a small effective healing gas molecule inside a $MAPbI_3$ layer. Nitrogen is soaked into polycrystalline $MAPbI_3$ via a post-deposition mild thermal treatment under slightly overpressure conditions in order to promote its diffusion through the whole layer. We observe a significant reduction of radiative recombination and a concurrent increase of light absorption, with a maximum benefit at 80 °C. Concomitantly, the current of holes locally drawn from the surfaces by a biased a tip with nanometric resolution has increased by a factor 3 under N_2. This was framed by a reduction of the barrier for the carrier extraction. The achieved improvements were linked to a nitrogen-assisted recovery of intrinsic lattice disorder at the grain shells along with a simultaneous stabilization of under-coordinated Pb_{2+}species and MA^+ cations through weak electrostatic interactions. Defect mitigation under N_2 is further supported by the behavior of the absorption coefficient during thermal cycles in comparison to similar data under Argon. We additionally unveil that surface stabilization through N_2 is morphology-independent and can be thus applied after any preparation procedure.Such simple and low-cost strategy could complement other stabilizing solutions when building perovskite solar cells or light-emitting diodes. Just published in Adv. Energy Mater. 2019, 9, 1803450 and NATURE COMMUNICATIONS 2019, 10:2196 |

#013 - SURFACE-PHENOMENA IN HYBRID PEROVSKITES INVESTIGATED BY MOLECULAR DYNAMICS: LIQUID CONTACT ANGLES AND SURFACE EFFECTS ON IONIC POLARIZATION

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Understanding and controlling the properties of surfaces and interfaces of hybrid perovskites (e.g. MAPI) is crucial for the development of a reliable solar cells technology based on hybrid perovskites. The overall properties of perovskites devices require the precise control of the morphology at the nanoscale but this is challenging from an experimental point of view and makes it difficult to correlate structure and properties. Atomistic methods based on molecular dynamics simulations can be useful in this perspective, provided that they are numerically efficient to make affordable the simulations of large models including interfaces. The recently developed Mattoni force-field[1]represents a good compromise between numerical scalability and accuracy and it has been successfully applied to study several large-scale phenomena including molecular disorder[2], defects diffusion, thermal transport and many others[3,4].

Here, we report two recent studies focusing on the surfaces and interfaces of methylammonium lead iodide (MAPI). In the first example[5]we investigate MAPI surfaces and their interaction with different liquids including water. MAPI/liquid interaction depends on the surface quality and the adhesion determines the equilibrium contact angles that can be experimentally measured. We show the possibility to predict the contact angles by directly simulating the dynamics of liquid drops on MAPI. We consider also the case of water discussing the hydrophilic nature of MAPI against the apparent hydrophobic behavior observed in contact angle measurements[6].

A second application of classical molecular dynamics concerns the effect of surfaces and domain boundaries on the dynamics of mobile point-defects and ionic polarization. By simulating the ionic mobility under external bias and modeling the surface-defects interaction we are able to identify close-surface physical mechanisms at the origin of memory effects and current hysteresis, i.e. phenomena of great relevance for hybrid perovskites technological applications[4].

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#014 - RAMAN STUDY OF THE FORMAMIDINIUM LEAD IODIDE PEROVSKITE IN THE FULL FREQUENCY RANGE

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Lead halide perovskites represent the most promising photovoltaic materials for the production of low-cost, high-performance solar cells. In these materials, with general formula ABX_3 (B=Pb, X=Cl, Br, I), an inorganic cage of BX_6 octahedra encloses an organic cation at the A-site (typically methylammonium MA) [1]. Among these substances, the most popular is methylammonium lead iodide ($MAPbI_3$), reaching nearly 20% power conversion efficiency. Most recently, formamidinium (FA) lead iodide ($FAPbI_3$) has attracted significant attention since the large size of the FA molecule gives rise to a symmetric crystal structure and a reduced band-gap value, which allows for a strong near-infrared absorption [2].

Despite many studies on FA-based perovskite structures in thin film solar cells, the intrinsic electrical, optical, and structural properties of $FAPbI_3$ still require further study. At room temperature, $FAPbI_3$ crystallizes as a yellow, non-perovskite d(delta)-phase, which is thermally stable, but is a poor solar absorbent due to a band gap value of ≈2.5 eV. Upon heating up to ≈150 °C, the d-phase undergoes a phase transition to the perovskite black a(alpha)-phase, with electronic properties (in particular band-gap of ≈1.5 eV) favourable for efficient photovoltaic effect [3]. However, the black a-phase is not stable, and tends to transform back to the yellow one in a few minutes [2]. It is thus important to study how the arrangement of the inorganic cage around the FA cation changes after the d=>a structural phase transition.

Since Raman spectroscopy is a powerful tool to detect even subtle changes associated to structural modifications, we performed a detailed Raman study of a $FAPbI_3$ powder sample at ambient conditions in the stable d-phase. After heating the sample, the same measurements were performed in the a-phase. The Horiba-HR micro-spectrometer, employed for the Raman experiments, was equipped with the ultra-low frequency filter, which allows reliable measurements down to 20 cm^{-1}. Measurements in the 800-1700 cm^{-1} spectral range were performed to study how the vibrational spectrum of the FA molecule, well known from the literature [4], is affected by the inorganic cage. Small changes were observed after the d=>a transition. The most interesting results are those obtained in the 20-200 cm^{-1} spectral range (the spectral range below 100 cm^{-1} has never been explored in literature before [2]), where a clear effect of the transition has been observed.

DFT calculations on the aand d-phases allowed us to perform an unambiguous assignment of most phonon modes. Our results might provide novel information on the microscopic mechanism driving the d=>a transition.

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#015 - HYBRID PEROVSKITES FOR PHOTOVOLTAICS: CHALLENGES AND OPPORTUNITIES

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It is undoubted that organic-inorganic hybrid perovskites have been representing a scientific breakthrough in the photovoltaic field since 2009 when they were applied to replace photoactive dyes in hybrid solar cells. Further development has been highly boosted by a large and enthusiastic effort of the worldwide scientific community to improve the response to sun light. The current certified maximum efficiency is 23.7%. The exceptionality of this class of materials resides in their soft nature. The long diffusion lengths of the photo-generated carriers, the wide absorption range, the direct and tunable bandgap are mainstays. It is equally true that the low structural stability of the hybrid perovskites, primary MAPbI$_3$, risks to severely retard their wide-range applications in low cost/high yield devices. A large effort is consequently needed to frame the instability sources and degradation mechanisms in relationship with the operation conditions, including temperature, illumination, humidity, contaminants and boundary materials in the final architecture. One of the most used strategies is this perspective is the changing or mixing different cations, (MA$^+$, FA$^+$ and Cs$^+$) to improve the lattice stability. Although the overall scenario is brighter than years ago, reliable and long-lasting solutions to avoid back-reaction of perovskites to the starting organic and inorganic components and indeed to extend cell durability are under spotlight. For the market uptake, moreover, device architectures, to be produced via simple and sequential steps, being free of contaminants and at low environmental impact, are warmly encouraged to catch the interest of investors. A critical analysis of the available data indicates that degradation under ambient conditions is a defect-generation process that is highly localized on surfaces and interfaces, while it is further enhanced above the tetragonal-cubic transition at ~54 °C. Within this context, we discuss the conservative role of N$_2$ and propose strategies for the emergence of industrially viable hybrid photovoltaics. The paper will thus frame strengths and weaknesses of hybrid perovskites for next-generation photovoltaics in view of their extended use and dissemination in daily life.

#016 - LARGE SURFACE POLARIZATION BUILDUP AND CHARGE DYNAMICS IN LEAD-HALIDE HYBRID PEROVSKITE FILMS UNDER VERY INTENSE OPTICAL IRRADIANCE

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Solution-processed hybrid lead halide perovskites are most highly-performant and cost-effective material systems for advanced thin film solar cells also extremely appealing for high concentrated photovoltaic (HCPV) applications, at extremely high levels of optical irradiance [1,2] and as light emitting devices [3]. In this perspective, the assessment of the impact of intense illumination on the performances and long-term device reliability of hybrid perovskites is still an open research challenge.

We report on the comparative characterization of long-term dynamical evolution of polarization and charge dynamics, photoinduced by intense optical irradiance at 500suns in methylammonium lead iodide ($MAPbI_3$). Polycrystalline $MAPbI_3$ films were deposited by the two step interdiffusion method on charge selective contacts, namely electron-transport-layer (ETL) compact TiO_2 and hole-transport-layer (HTL) PEDOT:PSS, respectively as parts of *standard* and *inverted* solar cells structures.

The analysis was performed in vacuum conditions and in the absence of any electrical bias, by Laser-Assisted Time-Resolved Scanning Electron Microscopy (TR-SEM) technique [3], supported by *in-situ* time-integrated PL measurements.

A large surface positive photovoltage builds up in both systems with a turn-on time of seconds and a much slower decay time of tens of minutes and up to hours. Mixed electron-ionic conduction and defect formation and migration -triggered and driven by strong optical absorption- can be at the origin of the phenomenon. However, the evolution of photoinduced polarization is strongly different in the two cases. Both TR-SEM and PL confirm that the specific nature of the charge selective contact and related interface crucially affect the optoelectronic response of $MAPbI_3$ thin films. Specifically, $MAPbI_3$/PEDOT:PSS films show a *p*-type semiconducting behavior, with reversible photo-excited polarization effects, fast and reversible quenching of PL and some degree of persistent luminescence. $MAPbI_3/TiO_2$ films behave as *n*-type, featuring much slower but non-reversible PL quenching dynamics, no residual luminescence, photo-induced inhomogenous space-charge fields and semi-permanent modifications.

The results of jointly performed TR-SEM and PL characterizations suggest that PEDOT:PSS/$MAPbI_3$ films are more robust in view of high-irradiation applications, while in the case of $TiO_2/MAPbI_3$ films, even in the absence of morphological surface damage, physico-chemical degradation may locally occur in the bulk and at the contact interface, definitely altering the photo-physical response of the material and deserving further investigations.

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#017 - BIMODAL POROSITY AND STABILITY OF A TIO2 GIG-LOX SPONGE INFILTRATED WITH MAPBI3 FOR PEROVSKITE SOLAR CELLS

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We created a blend between a TiO2 sponge with bimodal porosity and a MAPbI3 perovskite. The interpenetration of the two materials is effective thanks to the peculiar sponge structure. During the early stages of the growth of the TiO2 sponge, the formation of 5-10 nm-large TiO2 auto-seeds is observed which set the nano-porosity (<5nm) of the layer, maintained during further growth. In a second stage, the auto-seeds aggregate into hundred-of-nm-large meso-structures by their mutual shadowing the grazing Ti flux for local oxidation. This process generates meso-pores (10-100 nm) treading across the growing layer, as accessed by tomographic Synchrotron Radiation Coherent X-ray Imaging and Environmental Ellipsometric Porosimetry. The distributions of pore size are extracted before (>47%V) and after MAPbI3 loading, and after blend ageing unfolding a starting pore filling above 80% in volume. The degradation of the perovskite in the blend follows a path towards the formation of PbI2 with the concomitant release of volatile species with an activation energy of 0.87eV under humid air. The use of dry nitrogen as environmental condition has a positive impact in increasing this energy by~ 0.1 eV that extends the half-life of the material to 7 months under continuous operation at 60°C.

#018 - LIGHT-MATTER-LIFE INTERACTIONS AT THE MICRON SCALE

Roberto Di Leonardo (I) - Sapienza University of Rome

In 1676, using candle light for illumination and a small glass sphere as the lens, Antonie van Leeuwenhoek revealed to the world the beauty and complexity of a microscopic universe densely populated by living microorganisms. Today, using lasers, spatial light modulators, digital cameras and computers, we investigate the statistical and fluid mechanics of microswimmers in ways that were unimaginable only 50 years ago. With light we can image bacteria as they swim rapidly through 3D environments, apply gentle and controllable force fields or sculpt the 3D structure of their environment. In addition to shaping the physical world outside cells we can also use light to control the internal biological state of microorganisms that are genetically engineered to respond to light signals. I will review our recent work on the interactions between light, matter and bacteria, from the fundamental problems of rectification and non-equilibrium steady states in active matter to the use of genetically modified bacteria as propellers for micro-machines or as a "living" paint that can be controlled by light.

#019 - DYNAMICS AND STATISTICS OF SWIMMERS IN TURBULENCE

Guido Boffetta - University of Torino

I will present recent results on the dynamics and statistics of microscopic active swimmers in turbulent flows. The problem of fluid-mediated collective behavior, spatial segregation and clustering and preferential concentration will be addressed.

#020 - ROTATION AND PROPULSION IN 3D ACTIVE CHIRAL DROPLET

Livio Nicola Carenza - Dipartimento di Fisica, Università degli Studi di Bari - INFN Sezione di Bari

Other Authors: Giuseppe Gonnella (Dipartimento di Fisica, Università degli Studi di Bari and INFN Sezione di Bari), Davide Marenduzzo (SUPA, School of Physics and Astronomy, University of Edinburgh), Giuseppe Negro (Dipartimento di Fisica, Università degli Studi di Bari and INFN Sezione di Bari)

Chirality is an ubiquitous feature of biological matter. Left-right asymmetry may be due to thermodynamic (passive) or non-equilibrium (active) effects. For instance, flagella of some bacteria, acto-myosin filaments as well as microtubule bundles are all examples of intrinsically chiral systems that may eventually apply a non equilibrium active torque on the surrounding fluid environment, thus leading to motility.

Moreover biological fluids are "active" and evolve far from thermodynamic equilibrium, since they are internally driven by continuous injection of energy at the level of the individual constituents. Experiments on concentrated suspensions of bacteria or cytoskeletal extracts have shown that active systems often exhibit orientational order. Indeed they have been successfully modelled by Liquid Crystal (LC) theories, able to reproduce unexpected behaviors arising in active fluids, such as sponteneous flow, active turbulence and superfluidic states [1].

Despite much effort has been taken to understand the hydrodynamics of active nematic/polar fluids in bidimensional environments, much less is known about chiral systems and in general about active matter in three dimensional geometries [2]. In the present study, we consider a system which is inherently chiral and apolar and that can be modelled - in the passive limit - as a Cholesteric Liquid Crystal (CLC). Specifically we examinated the behavior of a 3d CLC droplet with tangential anchoring of the director at its surface.

Previous studies on achiral (nematic) shell showed that activity can only sustain oscillatory motion of topological defects on the surface, while motility of polar droplet is driven by symmetry breaking of its shape [2]. We show here that intrinsically chiral droplets display instead a much richer dynamical behavior. First we find that a force dipole strengthens the equilibrium chiral pattern, enabling a new motility mode, where the rotational motion of surface defects is converted into propulsion. Second, a torque dipole activity sets up a sustained mirror rotation of two pairs of disclination lines exhibiting a "coiling and relaxing" dynamics leading to periodical behavior. Furthermore we explore the effects on the flow and the chiral pattern as the ratio between the radius of the droplet and the cholesteric pitch increases.

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#021 - LAMELLAR ORDERING, DROPLET FORMATION AND PHASE INVERSION IN EXOTIC ACTIVE EMULSIONS

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We study numerically the behaviour of a mixture of a passive isotropic fluid and an active polar gel, in the presence of a surfactant favouring emulsification. Focussing on parameters for which the underlying free energy favours the lamellar phase in the passive limit, we show that the interplay between nonequilibrium and thermodynamic forces creates a range of multifarious exotic emulsions. When the active component is contractile (e.g., an actomyosin solution), moderate activity enhances the efficiency of lamellar ordering, whereas strong activity favours the creation of passive droplets within an active matrix. For extensile activity (occurring, e.g., in microtubule-motor suspensions) we observe an emulsion of spontaneously rotating droplets of different size. By tuning the overall composition, we can create high internal phase emulsions, which undergo sudden phase inversion when activity is switched off. Therefore, we find that activity provides a single control parameter to design composite materials with a strikingly rich range of morphologies. If time permits, the rheological response of an active emulsion under constant shear will be discussed.

#022 - TOPOLOGICAL PROPERTIES OF POLAR ACTIVE POLYMERS

Emanuele Locatelli - University of Vienna

Other Authors: Valentino Bianco (Universidad Complutense, Madrid), Paolo Malgaretti (Max Planck Institute for Intelligent Systems, Stuttgart)

Active systems, due to the local breaking of equilibrium, allow for collective phenomena that their equilibrium counterparts cannot attain. This correspondence between microscopic local equilibrium breaking and the meso/macro-scopic structure formation is a general feature that have been observed in diverse systems including bacteria and synthetic swimmers. A similar behaviour can be observed also in the case of polar active polymers, i.e. polymers made of active monomers whose activity is directed as the local tangent to the polymer backbone. It has been shown that a coil-to-globulelike transition, highlighted by a marked change of the scaling exponent of the gyration radius, takes place for linear active chains. We will show in this contribution that, when the globule-like conformations are dominant, the probability of finding knots increases drastically with respect to the passive case. We will then characterize the knot spectrum for chains of different length and bending rigidity. Further, we investigate the effect of the topology by imposing the chains to be closed, i.e. by investigating unknotted active rings. We show that rings have two different regimes at high enough activity: short rings tend to become "stiffer" and to assume a disk-like conformation, whereas long rings coil up more tightly then linear chains, due to the same kind of instability.

#023 - LIVING POLYMERS GETTING OLDER

Stefano Iubini - University of Padova, Italy

Other Authors: Marco Baiesi (University of Padova & INFN Padova), Enzo Orlandini (University of Padova & INFN Padova)

Surfactants as those in shampoos and lubricants form giant structures of wormlike micellar networks, also known as “living polymers” for their property of constantly rearranging via scission of their arms. Molecular dynamics simulations of coarse-grained models show that in realistic regimes the typical relaxation times related to such rearrangements can become extremely long. As a result, the network exhibits the typical properties of a viscoelastic medium, with aging effects.

#024 - SELF-PROPELLED DIPOLAR NANOCUBES

Martin Kaiser - University of Vienna

Other Authors: Sofia Kantorovich (University of Vienna, University of Ekaterinburg), Yeimy Martinez (University of Cologne) , Annette Schmidt (University of Cologne)

Microscopic active particles, including self-propelled cells, microorganisms and artificial swimming colloids, have gained a lot of attention due to their relevance in such important fields as biology, biomedicine, nanoscience and nanotechnology. The term "active" describes the ability of certain particles or units, to convert energy from their environment into motion, hence, kinetic energy [1]. This highly interesting property can arise from various mechanisms, such as localized concentration gradients, where an asymmetric distribution of reaction products (i.e., chemical fuel) on a coated particle propels the particle by self- diffusiophoresis.

In this study, we use active matter to create a new type of nanomotor, which is oriented by an applied magnetic field and propelled by an active particle. One of those units consists of a dipolar cube that can be directed due to its interaction with a magnetic field, whereas a second non- dipolar active particle with a propulsion force directed into the cubes centre of mass, creates a field controlled swimming unit.

This scenario is investigated using molecular-dynamic simulations, setting the above described unit in an obstacle free environment, while applying a constant magnetic field. By computing the mean-square-displacement, we investigate if the diffusion of the self-propelled motor is enhanced in field direction and look at its dependencies on the unit parameters, which are compared with reported literature [2]. Furthermore, the fine interplay between dipolar and self-propulsion forces is investigated to reveal self-assembly, as well as dynamic properties of clusters containing the active-dipolar cube units.

In collaboration with Dr. Schmidt and Yeimy Martinez from the University of Cologne, those nanomotors are also investigated experimentally. $CoFe2O4$

cubes use an additional platinum cap as a catalyser for the catalytic reaction creating the propulsion force.

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#025 - SENSING AT THE BIOLOGICAL INTERFACE USING NANONEEDLES

Ciro Chiappini (I) - King's College London

Vertical arrays of high aspect ratio nanoastructures are emerging as a minimally invasive approach to investigate and direct intracellular processes. In particular, nanoneedles can rapidly interface with large cell populations *in vitro* and *in vivo* with minimal toxicity, to provide an unprecedented insight into cellular processes. In this talk we will investigate how naoneedles can be engineered to interface with the intracellular milieu of cells, what are the phenotypical effects of the biophysical stimuli that the nanoneedles provide ot the cell membrane, cytoskeleton and nucleus, and how this unique interface can be leveraged to sense biological processes occuring inside living cells in culture or within tissues.

#026 - DISCOVERING UNKNOWN MESSAGES OF CELLS: DEEP LEARNING AND ORGAN-ON-CHIP SYNERGY.

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The synergic integration of microfluidic devices, time-lapse microscopy, and image analysis has attracted attention to the exploitation of the carried information content. Extracted cell motility descriptors may be considered a useful source of information to quantify and to discern relevant biological differences among diverse counterparts of the same scenario. In this talk, the potentialities of data analysis and in particular of the deep learning techniques will be highlighted in different organ-on-chip experimental scenarios where the visualization of reconstituted complex biological processes such as multi-cell type migration and cell-cell interactions are possible.

#027 - LASER SYNTHESIS OF SERS-BASED SENSORS FOR THERAPEUTIC DRUG MONITORING

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Therapeutic Drug Monitoring (TDM) is a clinical practice to assess the drug concentration in a biological fluid, usually blood plasma. TDM is critically important for Narrow Therapeutic Index (NTI) drugs, including Anti-Epileptic Drugs (AEDs), where small differences separate therapeutic from toxic doses. Blood concentration of AEDs is measured with the time consuming and costly Immunoassay tests, or High-Performance Liquid Chromatography+Mass Spectrometry (HPLC-MS). Light scattering with *ad hoc*engineered plasmonic substrates made of noble metal (Au) nanoparticles (NPs) grown by pulsed laser ablation is a fast and comparatively inexpensive TDM approach for AEDs. Ablating in a transparent liquid a colloidal solution of Au NPs is obtained, while in a dense, inert, massive gas (Ar) NPs form in the expanding plasma plume and are deposited on an inert support (100-Si). Ambient gas pressure and laser pulse number in gas-phase synthesis and pulse duration and laser energy density in liquid-phase ablation affect the size, size distribution, shape and optical properties of the NPs and the NP arrays that self-assemble on the support, making possible to adjust the wavelength of the Surface Plasmon Resonance (SPR) peak. Thus, Surface Enhanced Raman Scattering (SERS) on samples of different origin, with various AEDs at concentrations of clinical interest become feasible. Our results on the SERS response of the AEDs Lamotrigine and Perampanel of relevant clinical interest are discussed.

#028 - DISORDERED ARRAY OF AG COATED SILICON NANOWIRES AS EFFICIENT SERS PLATFORM FOR CANCE DNA ANALYSIS AND RECOGNITION

Valentina Mussi - Institute for Microelectronics and Microsystems, National Research Council

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Surface enhanced Raman scattering (SERS) occurring at the surface of rough noble metals is a powerful analytical technique allowing ultrahigh sensitivity and *label-free* recognition of targets with important applications in diverse fields, including medicine, environmental monitoring and trace chemical analysis. Actually, the development of effective SERS materials is the key aspect for the successful transition of the technique to a practical biological and chemical sensing methodology.

Here, we report on highly disordered array of Ag coated silicon nanowires (Ag/SiNWs), combining facile fabrication and full compatibility to the well-established silicon technology, as efficient SERS probe for DNA analysis.

Our data demonstrate not only the ability of the sensing platform to perform simple, rapid and low-cost recognition of different nucleotides, single and double strand molecules for specific Raman database realization, but also the capability to evidence small spectral differences allowing to distinguish cancer DNA molecules with respect to healthy ones coming from the same cell line.

Keywords: Inorganic nanowires, Surface Enhanced Raman Spectroscopy, DNA, cancer cells

#029 - AN IMMOBILIZED ENZYME FOR BIOSENSING OF REACTIVE OXYGEN SPECIES

Stefano Bettati - Department of Medicine and Surgery, University of Parma

Other Authors: Marialaura Marchetti (Biopharmanet-TEC Interdepartmental Center, University of Parma) Luca Ronda (Department of Medicine and Surgery, University of Parma)

Allantoin is produced in humans from the non-enzymatic oxidative degradation of uric acid. The physiological level of allantoin in biological fluids correlates with the presence of reactive oxygen species, making this molecule a suitable candidate marker of acute oxidative stress to be used in biosensing applications. With this purpose, we employed allantoinase, the enzyme responsible for allantoin hydrolization in plants and lower organisms, to setup a fast enzymatic-chemical assay for allantoin quantification. The substrate specificity, catalytic efficiency and stability are pivotal features of allantoinase for its employment as a potential biosensor. We therefore monitored its catalytic parameters and stability after encapsulation in a wet nanoporous silica gel matrix, to investigate biosensor reusability and stability over time. Our results show that, after encapsulation, allantoinase has a catalytic efficiency comparable to that of the free enzyme and the sol-gel entrapped enzyme can be stored for several months retaining more than the 90% of activity. Furthermore, reusability experiments confirmed the suitability of encapsulated allantoinase for the development of durable devices.

#030 - NON-ENZYMATIC ELECTROCHEMICAL GLUCOSE SENSING BY GOLD NANOSTRUCTURES ONTO GRAPHENE PAPER OBTAINED BY LASER DEWETTING

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It is estimated that about 400 million people throughout the world suffer from diabetic pathologies.In this regard, in the insulin-dependent diabetes up to 300 glucose monitoring per month are needed for the patients, making the glucose sensors a highly active area of sensor research both in academic as well as in the biosensor industry.In this work, electrodes for non-enzymatic electrochemical glucose sensing based on gold nanostructures onto graphene paper (GP-AuNPs) have been obtained inducing dewetting, by laser annealing, of 8 nm-thick Au layer deposited by sputtering. Molten-phase dewetting of gold layer, which produces the formation of spherical nanoparticles (AuNPs), was achieved by nanosecond laser annealing using a pulsed (12 ns) Nd: yttrium aluminum garnet YAG laser operating at 532 nm. TheSurface of the electrode presents gold rich regions consisting of graphene nanoplatelets covered by spherical AuNPs. The sizes of AuNPs are in the ranges 10-150 nm. Glucose was detected at a potential of 0.17 V vs SCE, which corresponds to the intense peak of two electrons oxidation. Highest sensitivity of 600 µA mM^{-1} cm^{-2} of glucose detection was obtained. The resulting sensitivity, detection limit and linear range for the glucose detection are very promising since comparable to the actual state of art results for nanostructured gold electrodes which are, however, produced by complex multi-steps processes.

#031 - PCR-FREE MYCOPLASMA AGALACTIAE ELECTROCHEMICAL SENSOR BASED ON AU DECORATED NIO NANOWALLS

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Contagious Agalactia (CA) is an infectious disease of small ruminants endemic in the Mediterranean countries caused by the Mycoplasma agalactiae (Ma). Ma is responsible for a severe reduction and even suppression of the yearly milk production, and occasionally can lead abortion and death of lambs or kids. Due to its morbidity it can rapidly spread in whole flock, causing serious economic losses for farmers. Therefore, a rapid diagnosis of CA is of great importance. Routinary diagnostics is mainly based on isolation of the pathogen in selective media, on serological test and on direct identification of the pathogen DNA using Polymerase Chain Reaction (PCR)-based methods. However, these methods represents a time consuming, costly and elaborated procedures because of the slow Ma growth, the risk of cross-contamination with other species of Mycoplasma, the presence of inhibitors in milk samples which interefere with the reaction, and the low detection limit levels. Recently, PCR-free DNA biosensors have attracted increasing attention due to their rapid, simple and economical testing. In this work we report on a low-cost electrochemical Ma sensor based on Au decorated NiO nanowalls (Au@NiO NWLs) fabricated by Au electroless deposition on NiO nanowalls grown by chemical bath deposition and thermal annealing. This novel nanostructure was characterized by optical microscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD) and electrochemical impedance spectroscopy (EIS). Ma probe ssDNA was successfully immobilized on Au@NiO NWLs surface. Then, the complementary MA ssDNA (0.2-2.5 mM) was detected upon DNA hybridization by monitoring the impedance of Au@NiO NWLs. The reported synthesis method as well as the promising performances of Au@NiO NWLs open the route towards cheap and fast PCR-free detection of Ma.

#032 - BRAIN NETWORK TOPOLOGY MAPS THE DYSFUNCTIONAL SUBSTRATE OF COGNITIVE PROCESSES IN SCHIZOPHRENIA

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Using a novel network analysis of spontaneous low-frequency functional MRI data recorded at rest, we study the functional network that describes the extent of synchronization among different areas of the brain. Comparing forty-four medicated patients and forty healthy subjects, we detected significant differences in the robustness of these functional networks. Such differences resulted in a larger resistance to edge removal (disconnection) in the graph of schizophrenic patients as compared to healthy controls. In this talk we show [1] that the distribution of connectivity strength among brain regions is spatially more homogeneous in schizophrenic patients with respect to healthy ones. As a consequence, the precise hierarchical modularity of healthy brains is crumbled in schizophrenic ones, making possible a peculiar arrangement of region-to-region interaction that, in turns, produces several topologically equivalent backbones of the whole functional brain network. We hypothesize that the manifold nature of the basal scheme of functional organization within the brain, together with its altered hierarchical modularity, contributes to positive symptoms of schizophrenia. Our work also fits the disconnection hypothesis that describes schizophrenia as a brain disorder, characterized by abnormal functional integration among brain regions.

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#033 - CRITICAL DYNAMICS OF ACTIVE AND QUIESCENT STATES IN THE CORTICAL ACTIVITY ACROSS THE SLEEP-WAKE CYCLE: A UNIFYING FRAMEWORK FOR SLEEP REGULATION

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Sleep periods exhibit numerous intermittent transitions among sleep stages and short awakenings, with fluctuations within sleep stages that may trigger micro-states and arousals. Despite the established association between dominant cortical rhythms and emergent sleep stages, the nature and dynamics of sleep-stage and arousals transitions remain poorly understood. Empirical observations of intrinsic fluctuations in rhythmic cortical activity, and the corresponding temporal structure of intermittent transitions in sleep micro-architecture, raise the hypothesis that non-equilibrium critical dynamics may underlie sleep regulation at short time scales, in co-existence with the well-established homeostatic behavior at larger time scales (Scammell et al, Neuron 93: 747-765, 2017). In this talk, I will discuss recent results on the dynamics of dominant cortical rhythms across the sleep-wake cycle that support such hypothesis. I will focus on theta and delta rhythms in rats, which are associated with arousals/wakefulness and sleep, respectively. I will show that intermittent bursts in such rhythms exhibit a complex temporal organization: Theta-burst durations robustly follow a power-law distribution, whereas delta-burst durations follow an exponential-like behavior. Such features are typical of non-equilibrium systems self-tuning at criticality, where the active phase is characterized by bursts/avalanches with power-law distributed sizes and durations, while quiescent periods (inactive phase) are exponentially distributed. By interpreting theta-bursts as active phases and delta-bursts as inactive phases of the cortical activity in the sleep-wake cycle, I will then draw a parallel with other non-equilibrium phenomena, and demonstrate that theta-bursts exhibit a peculiar organization in time described by a single scaling function (Gamma distribution) and closely reminiscent of earthquake dynamics. Overall, such results constitute a fingerprint of critical dynamics underlying the complex temporal structure of intermittent sleep stage transitions at the behavioral level (Lo et al,PNAS,101,2004), and ideally complement previous observations of critical behavior at the neuronal level (we find similar scaling exponent).

#034 - DISSIPATION AND SELECTION IN CHEMICAL REACTION NETWORKS

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Life has originated as a consequence of a selection process taking place in non-equilibrium conditions (e.g. nearby submarine volcanos). In these cases, states which are equally probable at equilibrium can become favourable at stationarity in presence of a symmetry breaking in the rates of some reactions. Here we present a stremlined model for chemical reaction networks in which the particles undergo a diffusion process. It is shown that the selection of states is manifestly driven by the dissipation rate, as previously suggested in literature. States that are able to dissipate at an higher rate become favourable when an external gradient drives the system away from equilibrium. Moreover, localization phenomena in the state space can spontaneously emerge, whose features depend on the whole energy landscape. A microscopic explanation for the thermophoresis is also provided within this framework.

#035 - THE STRUCTURE AND DYNAMICS OF NETWORKS WITH MANY LAYERS

Vito Latora (I) - University of Catania and INFN Catania

Many complex systems are better described in terms of graphs with many-layers. Examples are biological networks whose units can interact through different types of interactions, social systems where the relations/communications among a group of individuals are inherently dynamic and the patterns of connections change over time, or man-made infrastructures consisting of inter-connected networks.

An overview of the novel methods to deal with networks with many-layers, namely multiplex networks, temporal networks and networks of networks will be presented. I will concentrate, in particular, on how to describe mathematically the structure of multiplex networks, and how to model different types of dynamical process occurring over them. I will show cases in which multiplexity gives rise to the emergence of novel behaviors, otherwise unobserved in single-layer networks.

#036 - INFORMATION CAPACITY OF A NETWORK OF SPIKING NEURONS.

Antonio de Candia - Università di Napoli Federico II

We study a model of spiking neurons, with recurrent connections that result from learning a set of spatio-temporal patterns with a spike-timing dependent plasticity rule. We investigate the ability of the network to store and selectively replay multiple patterns of spikes, with a combination of spatial population and phase-of-spike code. Each neuron in a pattern is characterized by a binary variable determining if the neuron is active in the pattern, and a phase-lag variable representing the spike-timing order among the active units. After the learning stage, we study the dynamics of the network induced by a brief cue stimulation, and verify that the network is able to selectively replay the pattern correctly and persistently. We calculate the information capacity of the network, defined as the maximum number of patterns that can be encoded in the network times the number of bits carried by each pattern, normalized by the number of synapses, and find that it reaches a value $\alpha_{max}\approx0.27$, similar to the one of sequence processing neural networks, and almost double of the capacity of the static Hopfield model. We study the dependence of the capacity on the global inhibition, connection strength (or neuron threshold) and fraction of neurons participating to the patterns. The results show that a dual population and temporal coding can be optimal for the capacity of an associative memory.

#037 - EXPLORING GENOME STRUCTURAL REARRANGEMENTS AND HIGHER-ORDER ORGANIZATION WITH POLYMER PHYSICS

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Polymer physics has proven to be a powerful tool to investigate genome architecture in three dimensions and the mechanisms underlying chromatin folding. By combining Polymer Physics and experimental data, it has been shown that it can be used to reconstruct with accuracy the 3D structure of real genomic loci. Here we apply such an approach to explore the rearrangements of the genome spatial organization in different cell types and to give a meaningful structural rationale to the activity changes of the genomic loci during differentiation. Using as a case of study the a- and b-globin and the *HoxD* loci, we discuss the performances of the approach in the description of structural modifications occurring in different cell types. Importantly, the predictive power of our polymer models is tested when extracting higher-order information as multi-way contacts and compared with published independent experimental data produced with recent technologies.

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NOVEL SEMICONDUCTORS AND APPLICATIONS 1	GIANNAZZO/LA MAGNA

#038 - BUILD, BREAK AND ASSEMBLE. GRAPHENE OXIDE AS VERSATILE TOOL TO INVESTIGATE LOW-DIMENSIONAL SYSTEMS ON LARGE-SCALE

Andrea Liscio (I) - Istituto per la microelettronica e microsistemi (CNR-IMM)

The great hype existing around graphene has caused a proliferation of graphene producers, with several hundreds of 'graphenebased' products available on the market [1] with no common agreement on the most important parameters needed to compare different materials. In particular, the lack of a clear metrology and quality control is creating confusion among industrial end users, with many websites and companies selling what should be called graphite powders or thin platelets, rather than graphene. Despite the nomenclature [2] and classification framework [3] that have been proposed for 2D graphene-based materials, a clear agreement on metrology and standards is still missing.We propose operative approaches to face such issues using graphene oxide (GO) as a prototype 2D material to investigate the properties of graphene-based materials at different scales and as well as to produce macroscopic materials with tuned properties.

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#039 - NANOSTRUCTURED FILMS OF GRAPHENE AND TWO-DIMENSIONAL MATERIALS: ELECTRONIC TRANSPORT, NON-LINEAR OPTICS AND THZ PHOTONICS

Felice Torrisi - University of Cambridge

Graphene and related 2D materials (GRMs) hold a great potential for flexible (opto)electronics and photonics for their novel electrical and optical properties. Low temperature production and deposition of nanostructured GRM films from GRM-based solutions is extremely attractive for printed heterostructures in flexible electronics, [1] while the linear dispersion of Dirac electrons and the Pauli blocking in graphene films generates strong optical non-linearity, suitable for ultrafast photonics and optoelectronics. [2] GRM-based inks enable a large range of printed device and integration options, such as digital, lithographic printing and roll-to-roll coating, which are ideal to deposit nanostructured GRM films. Liquid Phase Exfoliation (LPE) of bulk precursor layered materials (such as graphite, MoS_2 crystals, etc.) is a scalable approach ideally suited to produce inks. However, currently LPE has low yield, resulting in a low concentration of dispersed GRMs. I will give a brief overview about the development of high-yield, cost-effective and large-scale production techniques for GRM-based inks,and the portfolio of reproducible deposition processes enabling GRM-based printable and flexible (opto)electronic devices.[3]. Then I will show how careful tuning of the flakes-substrate surface interaction and GRM deposition process enables hybrid heterojunctions from 2D materials, achieving mobility > 100 cm^2 V^{-1} s^{-1}at room temperature.[4] Finally, I will demonstrate how the ultrafast dynamics of graphene is preserved in nanostructured graphene-films [2] and is driven by carrier multiplication and Auger recombination, enabling saturable absorbers operating in near-IR fibre lasers [5] and THz quantum cascade lasers [6].

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#040 - OHMIC CONTACT ENGINEERING IN FEW-LAYER BLACK PHOSPHORUS FIELD EFFECT TRANSISTORS

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Achieving good quality Ohmic contacts to van der Waals materials is a challenge, since at the interface between metal and van der Waals material, different conditions can occur, ranging from the presence of a large energy barrier between the two materials to the metallization of the layered material below the contacts. In black phosphorus (bP), a further challenge is its high reactivity to oxygen and moisture, since the presence of uncontrolled oxidation can substantially change the behavior of the contacts. Here we study three of the most commonly used metals as contacts to bP, Chromium, Titanium, and Nickel, and investigate their influence on contact resistance against the variability between different flakes and different samples. Using the transfer length method, from an analysis of ten different devices, both at room temperature and at low temperature, Ni results to be the best metal for Ohmic contacts to bP, providing the lowest contact resistance and minimum scattering between different devices. Moreover, we investigate the gate dependence of the current-voltage characteristics of these devices. In the accumulation regime, we observe good linearity for all metals investigated.

#041 - ADDRESSING GRAPHENE BASED NANO-ARCHITECTURES FOR SPIN AND PHOTON DETECTION

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There is a general interest in using molecular architectures for downscaling (spin-)electronic devices and here I report on our recent effort along this direction. I shall first present our results in using graphene to realize narrow conducting channels or electrodes to realize three terminal devices with active molecules. In a first case we use perylene as conducting channel showing excellent electrical properties also for devices width as narrow as 100nm [1]. In a second case, we use graphene nanoribbons as photosensitive layer that allow us to realize fully graphene-based photodetectors with high photo-rensponsivity [2, 3]. Electroburning technique then allowed us to further scale dawn the active channel at single molecule scale [4, 5]. We have focused our attention on a prototypical case of TbPc2 magnetic center that was largely used in experiments performed in Grenoble in the last years showing genuine quantum effects. In a first set of experiments we have studied deviations of Landau-Zener effect at crossing of electro-nuclear states that we ascribed to dephasing [6]. Finally I’ll present results of recent experiments in which we study the mechanism spin reversal on a single molecule transistor under application of microwave pulses [7].

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#042 - COLOR SENSITIVE RESPONSE OF GRAPHENE / GRAPHENE QUANTUM DOT PHOTOTRANSISTORS

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Graphene is a promising candidate for the realization of optoelectronic devices, with particular regards for photodetectors. Among the various type of light sensors that have been proposed and reported, the so-called sensitized graphene detectors are gaining increasing interest. This class of devices consists of a graphene layer in the transistor configuration, which is functionalized with light-absorbing materials, such as nanocrystals, nanoparticles and other two-dimensional materials. Following the photon absorption, either electrons or holes are transferred to graphene, while the other type of charge remain trapped into the photo-active center, thus working as an effective additional local electrostatic gate for graphene, where charges are recirculated many times. This mechanism is known as photo-gating effect and it is characterized by high gain (i.e. multiple electrical carriers are detected per incident photon), thus leading to high sensitivity. Previously reported examples of this type of detectors typically have broad absorption spectra, with a threshold depending on the type of the sensitizing element employed, without a specific color (i.e. wavelength) selectivity.

In this work we employ, as the sensitizing material, atomically precise and chemical synthesized graphene quantum dots (GQD), nanoscale fragments of graphene, with non-zero energy gaps due to the quantum confinement effect. Depending on the sizes and structures of the graphene fragments, they absorb and emit light at different wavelengths. By employing GQDs in our photodetectors, we combine high photosensitivity with color selectivity, a feature that could be used in sensing and light processing and harvesting.

We will report the functionalization of cvd-grown graphene with three different type of GQDs, with different chemical structures and optical properties. The photoresponsivity exceeds 10^6 A/W for vanishingly small incident power comparing well with state of the art sensitized graphene photodetectors. More importantly, the photoresponse is determined by the specific absorption spectrum of each GQD, exhibiting the maximal responsivity at the wavelengths corresponding to the absorption maxima. The tunability of the GQD absorption properties make our novel all-carbon photodetectors suitable graphene based light sensors for applications where both low incident power- and color- sensitivity are required.

#043 - MAGNETIC HALLMARKS OF VISCOUS ELECTRON FLOW IN GRAPHENE

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Electrical transport [1-5], thermal transport [6], and scanning gate spectroscopy measurements [7] have been used to identify signatures of

viscous electron flow in graphene, PdCoO2, and GaAs. In this regime of transport, viscosity determines electron whirlpools in the steadystate
current pattern. So far, a direct experimental observation of electron whirlpools and associated backflow is still lacking. We predict
that the profile of the magnetic field generated by hydrodynamic electron flow in confined geometries displays unambiguous features linked
to whirlpools and backflow near current injectors. We also show that the same profiles shed light on the nature of the boundary conditions
describing friction exerted on the electron fluid by the edges of the sample. Our predictions are within reach of vector magnetometry
based on nitrogen-vacancy centers in diamond, a technique that access the details of 2D spatial flow patterns in graphene [8] and combines
the benefits of high spatial resolution, competitive magnetic field resolution, and operability over a wide range of temperatures [9].

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#044 - ELECTRONIC TRANSPORT IN 2D MEMBRANES: REDUCED GRAPHENE OXIDE SINGLE SHEETS VS THIN FILMS.

Alessandro Kovtun - ISOF CNR

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We focus on the study of graphene oxide (GO) and its graphene derivative as a model material system for defining quantitative approaches to describe GBMs, due to its morphology and high-processability. Using strong oxidation procedures in liquid, suspensions of monoatomic layers were prepared in water and shown to be stable over several years.
In general, several detailed studies on the charge transport properties have been performed for single RGO [1-4] sheets, while less work has been devoted to thin films and so a systematic study is still lacking [5-7]. Most studies give an ambiguous interpretation of charge transport phenomena by qualitative plot of resistance vs temperature, while a univocal interpretation of the charge transport phenomenon is still object of debate: Efros-Shklovskii variable-range hopping (ES-VRH) or 2D Mott variable-range hopping (2D-VRH).
We perform a quantitative study of the charge transport properties of such GBMs. The chemical composition [8], film thickness and the lateral size of single layers were monitored quantitatively providing detailed analyses of charge transport properties of RGO thin films. We report a systematic data analysis and modellingof experimental data of the resistance of RGO thin films of different thicknesses. Such films are described as multi-layered networks where hopping events affect the in-plane charge transport whereas out-of-plane transport is quasi-metallic. Based on analysis of the reduced activation energy W(T) [9], we show that the charge transport mechanism strongly depends on hopping events, followingthe same physical model in the whole temperature range, the ES-VRH [10,11].

Moreover, we further correlate the electronic transport mechanisms with the morphology of the RGO film. The probability that charges can circumvent the hopping barriers increases with film thickness, with a corresponding increase in the effective delocalization of the electronic states up to the micron scale [11].

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#045 - LOW TEMPERATURE RESISTIVITY BEHAVIOR IN GRMS FILMS: ROLE OF THE VERTICAL STACKING ORDER

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The unique properties of graphene-related materials (GRMs) have attracted a large interest in the last decade at both the scientific and industrial levels [1]. While the transport of charge carriers has been extensively studied in single flakes or atomically-thin devices [2], less attention has been paid to more structurally complex systems, such as printed films and GRMs-polymer composites, that are the ones usually employed for realistic applications. More specifically, industry-related processes may exploit different film fabrication methods, that in turns may lead to different film structures and hence properties.

The aim of this work is to investigate charge transport in GRMs network films, going towards more complex structures, such as the ones found in realistic devices. In particular, we address here the role of the flakes stacking order along the vertical direction in determining the charge transport properties in films composed by tens, or hundreds, of layers.

We fabricated reduced graphene oxide films with a varying degree of order in the flakes stacking. This has been realized by exploiting different film deposition methods, namely spin-coating, spray-coating and vacuum-assisted filtration. Chemical and morphological properties of the films were characterized by X-ray Photoelectron Spectroscopy (XPS), Atomic Force Microscopy (AFM) and X-ray Diffraction (XRD) analysis.

In order to investigate the different transport mechanisms, we measured the resistivity ρ from room temperature down to 2 K. We also acquired magnetoresistance curves at fixed temperatures.

Exploiting a $\rho(T)$ linearizing approach [3], we self-consistently determine the transport regimes of the samples across the various temperature ranges. We correlate the transport characteristic parameters with the degree of order of our samples and elucidate the role of the flakes vertical stacking, that is of the pi-pi interaction between adjacent layers, in the final transport behavior of the film. Our analysis will help to rationalize the charge transport mechanisms in realistic devices made of GRM multilayers.

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#046 - THEORETICAL MODELING OF FE2O3 ELECTRODES FOR PHOTOCATALYTIC WATER OXIDATION

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Hematite (α-Fe2O3) is a widely investigated photocatalyst material for the oxygen evolution reaction, a key step in photoelectrochemical water splitting. Having a suitable band gap for light absorption, being chemically stable and based on earth abundant elements, hematite is a promising candidate for the fabrication of devices able to split water using sunlight. What limits its performance is the high rate of bulk recombination following the optical excitation, so that few charge carriers are able to reach the surface to perform the redox reactions. In an effort to better understand the light absorption properties of hematite, we perform a theoretical first-principles investigation of its band structure and optical absorption properties [1]. We use state-of-the-art many-body perturbation theory, including the effects of electron–hole interaction by solving the Bethe–Salpeter equation. Using hybrid functional calculations, we then show that holes form small polarons and, depending on the fraction of exact exchange included in the hybrid functional, the site where the holes localize changes from Fe to O [2]. We perform high-level quantum chemistry calculations on small hematite clusters, showing that holes are localized on oxygen atoms, in agreement with recent time-resolved XUV experiments. To model the electrode/electrolyte interface we perform DFT-based molecular dynamics simulation, obtaining a structural model of the electric double layer in the presence of counterions [3]. We extract the capacitance of the double layer, which compares favorably with experimental measurements. Using the variation of the electrostatic potential across the electrode/electrolyte interface we are able to compute the position of the valence and conduction bands of hematite on the electrochemical scale. Finally, using a simplified approach based on adsorption energies of reaction intermediates, we compute the free energy cost of oxidizing water on a hematite surface, identifying the potential-determining step [4].

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#047 - FIRST PRINCIPLE MODELING OF MATERIALS AND INTERFACES FOR SOLAR WATER SPLITTING

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In the context of solar energy exploitation, dye-sensitized solar cells (DSCs) and dye-sensitized photoelectrosynthetic cells (DSPECs) offer the promise of cost effective sunlight conversion and storage, respectively. Dye-functionalization of bot n- and p-type semiconductors (like TiO_2 and NiO, respectively) can be either exploited to build active DS photoelectrodes or tandem DSC and DSPECs devices. Computational modelling has played a prominent role in the development of the DSC technology,whereas the understanding of the interfacial processes in DSPEC is still at its inception, especially for what concerns the electron and hole transfer phenomena, which are central to the efficient device functioning. Here I will discuss the recent advances concerning first principle modelling of materials, interfaces and processes of active photoelectrodes for solar water splitting. Particular emphasis will be put on the characterization of the electronic and structural properties of the complex semiconductor/solvent/dye/interface. We will discuss the main methodological limitations of state-of-the art DFT methodologies in predicting the electronic structure and optical properties of the isolated materials as well as the energy level alignment across the interface and the challenging definition of proper structural models needed to reliably capture the interface complexity.

#048 - AB-INITIO INVESTIGATION OF A NOVEL PHOTOCATHODE: BULK AND SURFACE PROPERTIES OF CUFEO2

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The urgent need to transition from fossil fuels to renewable energy sources is driving several avenues of intense research. Photoelectrochemical (PEC) devices offer the possibility to convert solar radiation into chemical fuels, mimicking the natural process of photosynthesis. Recent experiments have highlighted the delafossite CuFeO2 (CFO) as a promising candidate in the role of the photocathode [1,2], yet in spite of these encouraging results, improvement in the catalytic activity and charge separation is required. Currently, we lack an adequate theoretical characterization to provide insight that can direct further experimental investigations.

In this work, we present the first fully self-consistent Hubbard U investigation of CFO using the linear response approach introduced and refined by Cococcioni, De Gironcoli, Kulic, Scherlis and Marzari [3,4].

The coupling of Density Functional Theory and ab-Initio thermodynamics allows us to characterize the stability of bulk CFO with respect to other iron and copper oxides in the air and in an aqueous environment. On this basis we study the formation energy of native defects of CFO inside its stability region.

The position of the CFO band edges relative to the redox potentials of H2O at the CFO/H2O interface is fundamental for PEC applications. To this end it is necessary to go beyond the bare bulk properties, investigating the energetics of the surfaces and how they interact with water. Given the novelty of the application as a photocathode, little experimental characterization of the surface and interface is available.

Based on our thermodynamic screening we have been able to focus our investigation on two energetically relevant surfaces: a (11-20) cut and a (0001) cut with a complete Fe/O termination. We report on the electronic and geometric properties of these surfaces exposed to the vacuum and H2O.

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#049 - SB2SE3 (100): A STRONGLY ANISOTROPIC SURFACE FOR PHOTOCATALYSIS

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Solar light-driven water oxidation and reduction are achieved, in photoelectrochemical cells (PEC), by utilizing semiconductor materials as photoelectrodes. The realization of low-cost, commercialized PEC is subject to the employment of appropriate inexpensive, easily fabricated and highly stable

semiconductors. Antimony selenide (Sb_2Se_3), a p-type semiconductor belonging to the binary V_2-VI_3 compound family, recently started to be considered a promising photoelectrode. In fact, it combines very convenient properties, such as earth-abundance, low-cost, low-toxicity [i], direct band gap of 1.2 eV and a high optical absorption coefficient [ii] with an excellent resistance to photocorrosion in aqueous environment [iii].
Encouraged by the growing interest in the material and intrigued by the peculiar nature of the cleavage planes, we have studied the structural and electronic properties of freshly cleaved Sb_2Se_3 single crystal surfaces by means of surface science techniques. Indeed, X-ray Photoelectron Diffraction (XPD), Low-Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM) demonstrated that the crystals cleave along (100) planes. This exposes parallel edges of $[Sb_4Se_6]_n$ ribbons along the [010] direction, giving the surface a marked one-dimensional appearance. Angle-resolved Photoelectron Spectroscopy (ARPES) results reflected the strongly anisotropic character of the material, by showing much stronger dispersion along the ribbons than across them.
The obtained results serve as a basis for the investigation of heterostructures and interfaces involving this material, such as those found in PEC, possibly leading to a rational optimization of the device performances.

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#050 - NI-FE ELECTRODES BY IMPREGNATION FOR EFFICIENT OXYGEN EVOLUTION REACTION IN WATER SPLITTING SYSTEMS

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Electrochemical water splitting is considered as a promising approach to acquire clean fuels from renewable energy resources. In this context, one of the major limitations for the realization of a fully integrated solar-to-hydrogen water-splitting system is the difficulty in achieving an efficient anodic oxygen evolution reaction (OER). OER is a demanding step within the water splitting process for its requirement of a high overpotential. Thus to overcome this adverse kinetics, efficient catalyst is required to expedite the process. In this context, we report wet chemically synthesized, low cost, Fe and Fe(OH)X modified Ni foam as OER catalysts. A number of approaches to synthetize the catalysts were attempted. In one of the cases, the prepared catalyst based on Iron hydroxide precipitate shows a promising performance by delivering an overpotential of 270 mV at a current density of 10 mA /cm2 in 1 M KOH solution, an efficient tafel slope of 50 mV/dec and a stable chronopotentiometry with no visible degradation in OER performance. The promising performance of Ni-Fe anode is confirmed also in the overall water splitting phenomenon with inclusion of Pt covered Ni foam cathode. The overall water-splitting reaction requires a potential as low as 1.508 V to afford 10 mA /cm2, suggesting an 81.5% electrical to fuel efficiency. Along with a scanning electron microscopy study to understand the morphological features of the developed catalyst, cross sectional scanning trasmission electron microscopy of Ni-Fe based samples has also been performed to understand the catalysts' chemical composition and microstructure. The main results of this study will be presented and discussed. This work has been performed in the framework of the EU project PECSYS, devoted to the demonstration of large-scale photo-electrochemical systems for solar to hydrogen production.
Keywords: Ni-Fe, oxygen evolution reaction, water splitting

#051 - NI/NI(OH)2 NANOSTRUCTURES AS A SUSTAINABLE AND EFFICIENT CATALYST FOR WATER SPLITTING

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Hydrogen production through solar-assisted water splitting can be a viable solution towards a more environment-friendly energy economy. However, the efficiency of hydrogen production is limited to the high cost of the catalyst and the slow kinetics of the oxygen evolution reaction (OER) in photo-electrochemical cells (PEC). Ni based oxides/hydroxides are known to be one of the most promising Earth-abundant materials for OER [1], for which the activity can be further improved by proper nanostructured modification of the electrode surface.

In this study, we report on a low-cost approach to synthesize Ni/Ni$(OH)_2$ nanostructures acting as efficient catalyst for water splitting. By combining chemical bath deposition and thermal or electrochemical surface oxidation, shape, crystallinity phase and composition of the nanostructures can be varied with the synthesis parameters.

Working electrodes for the OER reaction were fabricated by growing a thin film (0.2 ÷1 µm) of Ni/Ni$(OH)_2$ nanostructures onto Au/ITO substrates. To correlate the electrochemical response with the structural properties of the catalyst, we systematically studied the morphology and chemical arrangement before and after the catalytic reaction through SEM-EDX analysis, while the catalyst loading, its chemical composition and the presence of dopant impurities have been investigated by Rutherford backscattering spectrometry (RBS) and XPS analysis.

The OER catalytic activity was tested in a 3-electrode electrochemical cell under alkaline conditions (1M KOH). Cyclic-Voltammetry (CV), electrochemical impedance spectroscopy (EIS) and chrono-amperometry are performed to kinetically measure the OER catalytic activity. We observed a significant difference in the OER catalytic activity by changing shape and morphology of the Ni based nanostructures, with a marked increase in OER activity when a Ni/Ni(OH)2 core/shell nanostructure is employed

Our findings confirm how the facile synthesis of Ni/Ni$(OH)_2$ nanostructures can be used as a viable method to produce a low-cost platform catalyst for efficient OER.

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#052 - SMART CATALYST DEPOSITION BY 3D PRINTING FOR LOW TEMPERATURE FUEL CELLS

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Polymer Electrolyte Membrane Fuel Cells (PEMFC) are arguably the most robust and integrated into various industry sectors among fuel cells, as they operate at low temperature and exhibit short start-up time. Currently, PEMFC manufacturing is transitioning from low-volume to mass production. However, the major hindrance against their massive use consists of high materials costs, low power density and relatively short lifetime. Notably, the need for employing platinum as a catalyst promotes exploring more convenient and effective manufacturing routes. The present work focuses on applying a microextrusion-based 3D printing system to deposit catalyst layers onto the Membrane-Electrode Assembly (MEA). A commercial 3D printer was modified to support the MEA substrate; furthermore, a peristaltic pump was inserted to supply the microextrusion printhead with the catalyst-endowed ink, finally released by a syringe.

The main objectives of this work were to provide optimized compositions of catalyst inks suitable for MEA preparation and to assess the effectiveness of the microextrusion-based 3D printing technique in yielding homogeneous coatings.The ink was a mixture of distilled water, ethanol and graphite. Granulometric and rheometric analyses were carried out to characterize inks in a quest for low viscosity and short drying time. Repeatability of released flow rate and ink homogeneity onto the GDL target surface were also evaluated by statistical analysis. The final assessment of the coated substrates was performed by measuring the characteristic polarization curve. The results suggest that microextrusion-based 3D printing can be considered as a promising technology for fuel-cell manufacturing.

Key words: PEMFC, micro-extrusion, 3D printing, MEA, catalyst inks

#053 - ANIONIC POLYSULFONE BASED MEMBRANES FOR AMFC

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Alkaline membrane fuel cells (AMFCs) can be considered a valid alternative to overcome polymer electrolyte fuel cells (PEFCs) limitations such as a difficult oxygen reduction reaction (ORR), higher fuel cross-over, high CO poisoning and use of precious metal catalysts. In this context, the development of anion exchange membrane (AEM) with good hydroxyl conductivity and polymer stability, is a key factor for (AMFC) applications. Polysulfone-based AEMs have been widely studied due to their good solubility in aprotic polar solvents, high thermostability, high chemical and mechanical resistance, and easy film preparation.

In this work, a series of quaternary ammonium-functionalized polysulfones were successfully synthesized by chloromethylation two-step method. Different functionalization degrees from 60 to 150% of original chloromethylated polysulfone connecting triethylamine and trimethylamine were investigated,in order to point out the optimal functionalization degree for greater efficiency in fuel cell. ^{1}H-NMR spectroscopy confirmed that ammonium-polysulfones were successfully synthesized to the desired degree of functionalization. Using a doctor-blade casting method anionic membranes were prepared starting from each obtained polymer with a good homogeneity of thickness. The resulting membranes were chemical-physical and electrochemical characterized to evaluate the key parameters such as ion exchange capacity, water retention and anion conductivity as a function of the functionalization degree and the used quaternary agents.

#054 - ELASTIC COLLOIDAL MODELS: A NEW LOOK AT THE STRUCTURE AND DYNAMICS OF SOFT COLLOIDS

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Thanks to the advances in the chemical synthesis it is now possible to design colloidal particles with an internal polymeric architecture that deform,
interpenetrate and shrink in response to external stimuli such as temperature or pH changes. These “soft colloids” are exploited not only for technological applications but also to unravel fundamental problems in soft matter physics such as the glass and jamming transitions.

In this context, numerical simulations represent a powerful tool for understanding the microscopic mechanisms at the basis of several experimental observations. Despite their potentialities, theoretical and numerical predictions are based on simple models which do not account for the internal degrees of freedom of the single particle; colloidal models are usually designed as penetrable particles that can overlap to a given extent but cannot shrink or deform as real particles do, making the concept of softness different in experiments and simulations. During the talk I will show the potential of a new class of models of soft particles that can deform and shrink and thus posses a new phenomenology with respect to standard soft matter models.

With one particular type of these models, i.e. the elastic polymer rings (EPR)[1], it has been recently shown that some interesting phenomena observed experimentally can be also reproduced numerically. For instance, the model provides a microscopic explanation of the faster than exponential relaxation observed in gel networks, and establishes a connection between softness and dynamics at high concentrations. Such work has paved the way for a new class of soft particles that truly possesses elastic properties as in real soft colloids, being able to deform and deswell. While in the EPR model elasticity is provided complementing polymer rings with an internal repulsive field placed at their center of mass, the new generation of numerical models of soft colloids rely on a
Hamiltonian in which elasticity is described by the Mooney-Rivlin hyperelastic model[2]. In this way the bulk and shear moduli are explicit parameters of the Hamiltonian and they can be modified to obtain particles with tunable softness and macroscopic properties.

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#055 - DNA WITHOUT DNA: WATSON-CRICK SELECTIVITY CONTROLS THE SELF-ASSEMBLY OF MONONUCLEOTIDES

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The transfer and memory of genetic information relies on Watson-Crick selective base pairing of DNA and RNA chains, universally considered a defining characteristic of these polymers. We found that the self-assembly of mononucleotides triphosphates (NTP) into columnar chromonic liquid crystal (LC) phases retains the same selectivity: among all solutions of adenosine, cytosine, guanine and thymine NTPs and their mixtures, liquid crystal ordering is found only in the A-T and C-G combinations. X-ray diffraction demonstrates that these phases are formed by columnar stacks of paired bases, a geometry that closely resembles the famed double helical structure. In stoichiometrically unbalanced mixtures, the system phase separates, expelling unpaired bases from the LC matrix, thus providing a molecular selection mechanics [1].

In parallel, we have found that LC ordering of DNA and RNA oligomers has a significant effect on the chemical binding of their terminals: the ligation rates are boosted, and the resulting elongated chains are linear, while the formation of circular chains is dominant in isotropic media [2,3].

The combination of these results suggests that NTP could spontaneously polymerize when prompted by their LC ordering. If this were true, DNA and RNA would emerge as a bona fide “self-synthesizing material”, i.e. a system that catalyzes the formation of molecules that stabilize their own structure [4].

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#056 - INTERACTIONS BETWEEN NANOPARTICLES IN A POLYMER MELT: EFFECTS OF CHAIN POLYDISPERSITY AND MULTIBODY TERMS

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Polymeric materials containing nanosized particles are experiencing an intensive investigation, mainly due to their improved physical properties [1] which allow for many industrial applications [2]. These materials are typically formed by filling a polymer matrix with inorganic particles whose typical dimensions are of the order of a few nanometers. In this context, a well defined control of the underlying interactions in nanocomposites is crucial in order to investigate the stability of the nanocomposite and its resulting chemical-physical properties. By applying a computer-simulation-based approach, the main obstacle to overcome concerns the long times usually required to get a proper relaxation of the system.

Here we present a hybrid particle-field molecular dynamic approach [3], well suited for guarantee an efficient relaxation of polymeric material with even high molecular weight [4]. Such an approach is applied to silica-polystyrene nanocomposites, which show a large variety of intriguing and non conventional behaviors [5], in particular when nanoparticles (NPs) are grafted with polystyrene chains. By calculating the two-body potential of mean force (PMF) between ungrafted NPs, we show that a bidisperse distribution of polymer chains increases the strength of attraction, in comparison with a unimodal distribution. If the NPs are grafted, the effective interaction crucially depends on bidispersity and grafting density. Moreover, we estimate the three-particle contribution to the total PMF and its role in regulating the phase separation on the nanometer scale. In particular, the multi-particle contribution to the PMF is able to give an explanation of the complex experimental morphologies observed at low grafting densities. More in general, we propose this approach and the models utilized here for a molecular understanding of specific systems and the impact of the chemical nature of the systems on the composite final properties.

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#057 - MOSAICS OF PATCHY RHOMBI: FROM CLOSE-PACKED ARRANGEMENTS TO OPEN LATTICES

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In the realm of functional materials, the production of two-dimensional structures with tunable porosity is of paramount relevance for many practical applications: surfaces with regular arrays of pores can be used for selective adsorption or immobilization of guest units that are complementary in shape and/or size to the pores, thus achieving, for instance, selective filtering or well-defined responses to external stimuli.

This simple principle is valid at both the molecular and the colloidal length scale.

Here we provide simple design directions to combine the anisotropic shape of the building units -- either molecules or colloids -- and selective directional bonding [1]. Our model - hard rhombi with localized interactions sites - has been proven to mimic the steric and attractive interactions of tetracarboxylic acids, small rigid organic molecules with functional carboxylic groups [2,3].

We show that regular rhombic platelets decorated with attractive and repulsive interaction sites target specific tilings, going smoothly from close-packed arrangements to open lattices. The rationale behind the rich tiling scenario observed can be described in terms of steric incompatibilities, unsatisfied bonding geometries and interplays between local and long-range order.

We are confident that the design principles we found through exploring various tuning parameters will guide the way to building new interesting materials. In particular, the ability to fine tune the lattice porosity leads us to speculate about lattices that can dynamically and reversibly switch between close-packed and open structures. The colloidal junctions [4] might prove to be the experimental realization of these dynamically switchable tilings.

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#058 - SELF-ASSEMBLY OF HOLLOW COLLOIDAL SILICA CUBES

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Among the multitude of recently synthesized non-spherical colloids, hollow silica cubes distinguish themselves by their charged surface and the strong influence of van der Waals forces on their behavior. While their self-assembly has been observed in experiment, its origins have not yet been fully understood. Gaining control of the underlying self-assembly mechanisms of charged cubes is the basis for designing new soft materials with desired rheological and optical properties.

Using MD simulations that take the superball model of cubes, developed in [1] for the study of hematite cubes [2], and expand it to consider the electrostatic aspects of the system, we investigate the electric double layer surrounding the cubes. The anisometric cubical shape of the colloids leads to an overall anisometry of the counterion distribution near the surface, studied on the level of a single cube. Based on the acquired knowledge, we are able to compute the interaction potential of two weakly charged cubes as a function of their mutual orientation, allowing for the effects of Van der Waals forces[3]. Doing so, we also investigate the influence of the intercube distance and their mutual orientation on the distribution of counterions. Obtained quantities show the preference of two cubes to approach each-other corner to corner, slide along the edges and only then assume a final face to face configuration.

In combination with experimental observations and calculated trajectories, we then examine the microstructures formed by small clusters of cubes, which differ significantly from those exhibited by comparable spheres. These investigations give us a multifaceted understanding of the behavior observed in these systems and pave the way for future applications.

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#059 - CHARACTERISATION OF THE MAGNETO-MECHANICAL RESPONSE OF NANOSCOPIC MAGNETIC FILAMENTS IN APPLIED FIELDS.

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Construction of materials with sophisticated magnetic response by incorporating magnetic nanoparticles within permanently cross-linked structures, opens up the possibility for synthesis of more complex, highly magneto-responsive systems.[1] Nanoscopic magnetic filaments (nMF's) are magnetic, nano-sized colloids, crosslinked into polymer-like linear chains, and are a promising platform for engineering new magnetically controlled filtering and flow control elements in micro-fluidic devices. Recent advances, advocating an assembly mechanism where the structure building instructions are embedded into nanoparticles via DNA origami frames, finally opened the door towards synthesis of nMF's with desirable mechanical properties. It has been shown that a pre-defined set of different DNA-framed nanoparticles, along with DNA polyhedral frames, enable designing diverse planar constructs, 1D, 2D and 3D frameworks, which allow for significant flexibility while maintaining structural integrity [2,3]. Notably, particle size can, among other factors, significantly alter the self-assembly within such a manufacturing process. We suggest using magnetic DNA-framed nanoparticles for constructing similar superstructures.

In this contribution, we show that structural inhomogeneities together with inter-particle Van der Waals forces can significantly alter the equilibrium properties and the magnetic response of nMF's. We compare the mechanical and magnetic response of filaments, to static and rotating magnetic fields, for ferromagnetic and super-paramagnetic colloids within different crosslinking scenarios. Firstly, without central attraction, we show that filaments consisting of super-paramagnetic colloids loose little in terms of overall filament magnetisation, while having a more predictable magnetic response, regardless of crosslinking approach. Overall, filament properties turn out to be most sensitive to the crosslinking scenario and conformation length, when Van der Walls attractions are screened. For plain crosslinking, where colloid rotation is decoupled form the filament backbone, persistence length doesn't exceed three nanoparticles, even under strong applied magnetic fields. For constrained crosslinking however, it can reach eight particles. Persistence length reflects the magnetic susceptibility of filaments, which we discuss in detail. Non-screened central attractions mostly affect filaments consisting of super-paramagnetic colloids, even for constrained crosslinking of colloids. This makes the interplay between central attraction and anisotropic magnetic dipolar interaction a key control parameter for tuning macroscopic response of nMF's.

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#060 - HYDROGEN DYNAMICS IN LIQUID MIXTURES WITH NEON: AN INELASTIC NEUTRON SCATTERING STUDY

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We have measured the dynamic structure factor of liquid neon-hydrogen mixtures (T=30.1 K) at two different H_2 concentration levels (namely, 3.4% and 10%) making use of inelastic neutron scattering. This system has been selected since the presence of heavy Ne atoms strongly influences the dynamics of the H_2 centers of mass via the formation of short-lived cages, which act both on the vibrational and the diffusive parts of the single-particle motion. Experimental neutron spectra were analyzed through a generalization of the Young and Koppel model, and the H_2 center-of-mass dynamic structure factor was finally extracted for the two liquid samples. Important physical quantities (namely, single-particle mean kinetic energy and self-diffusion coefficient) were estimated from the experimental data and then compared with quantum dynamical calculations, which also provided simulations of the velocity auto-correlation functions for Ne atoms and H_2 centers of mass. The latter estimates, in the framework of the well-known Gaussian approximation, were used to simulate the H_2 center-of-mass self dynamic structure factor in the same kinematic range and thermodynamic conditions of the neutron scattering one. The comparison between measured and calculated spectra turned out to be qualitatively good, but some discrepancies, especially in the low-frequency part, seem to reinforce the idea of the existence of relevant non-Gaussian effects as in the case of pure hydrogen and H_2-D_2 mixtures.

#061 - ANOMALOUS DYNAMICAL SCALING AND TRANSPORT IN OSCILLATOR LATTICES

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Understanding non-equilibrium properties of classical and quantum many-particle systems is one of the goals of contemporary statistical mechanics. Besides its own interest for the theoretical foundations of irreversible thermodynamics (e.g. of the Fourier's law of heat conduction), this topic is also relevant to develop innovative ideas for nanoscale thermal management with possible future applications to nanotechnologies and effective energetic resources [1]. We review anomalous transport and scaling in classical anharmonic chain and the connection with Kardar-Parisi-Zhang physics. Some recent results on the effect of almost-integrability [2] and long-ranged interactions [3] will be also presented.

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#062 - ONSAGER RECIPROCAL RELATIONS WITH BROKEN TIME-REVERSAL SYMMETRY

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Onsager reciprocal relations are a cornerstone in nonequilibrium statistical physics. Due to their fundamental relevance, such relations have been called the fourth law of thermodynamics. As the other principles of thermodynamics, they introduce fundamental constraints on heat to work conversion. Violation of Onsager relations, as expected when time-reversal symmetry is broken, would allow, in principle, to have finite power at Carnot efficiency. Indeed, in such situation, the second law of thermodynamics is consistent with the possibility to have non-dissipative currents, generated by thermodynamic forces. Here we show instead that the Onsager reciprocal relations remain valid even in presence of a generic magnetic field breaking the time-reversal symmetry. Our results show that the Onsager reciprocal relations are much more general than previously assumed. Correspondingly, breaking the time-reversal symmetry does not remove the thermodynamic constraints imposed by the Onsager relations.

#063 - ACTIVE INTERFACES: A UNIVERSAL APPROACH

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Other Authors: Martin R. Evans, Davide Marenduzzo (University of Edinburgh)

The essential features of many interfaces driven out of equilibrium are described by the same equation---the Kardar-Parisi-Zhang (KPZ) equation. How do living interfaces, such as the cell membrane, fit into this picture?
In an endeavour to answer such a question, we proposed in [F. Cagnetta, M. R. Evans, D. Marenduzzo, PRL 120, 258001 (2018)] an idealised model for the membrane of a moving cell.

Specifically, we identified the key ingredient for the physics of the system in the mechano-chemical coupling between the membrane and associated proteins.
Then, guided by the principle of universality, we wrote the simplest interaction compatible with a membrane whose motion is orchestrated by a collection of protein.
The result is an active twist on both the KPZ equation and the problem of the dynamycs of tracers embedded into a fluctuating medium.

In fact, the effects of activity are dramatic. The membrane, for instance, develops an oscillatory dynamics on top of the scale-invariant roughening typical of fluctuating interfaces. The particles, instead, rather than follow chaotically the medium fluctuations, self-organise into clusters that "surf" the membrane ripples.
In the talk I will discuss the principles that led us to the model, and review its most intriguing implications for both membrane-protein system
and the more general problem of motion in fluctuating media.

#064 - NOISE-DRIVEN DYNAMICS IN METASTABLE AND MULTISTABLE FAR-FROM-EQUILIBRIUM SYSTEMS

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The noise-driven dynamics and the nonlinear relaxation of three far-from-equilibrium systems are investigated. In particular we analyze: (i) the Josephson junction as a threshold detector for Lévy noise; and the residence time problem of a particle subject to a non-Gaussian noise source in arbitrary potential profile; (ii) the escape from a quantum dissipative metastable state in the presence of an external driving; and (iii) the growing dynamics of conductive filaments in memristors.
(i) We propose a threshold detector for Lévy-distributed fluctuations based on a Josephson junction. We discuss a theoretical model, which allows characteristic features of the Lévy fluctuations to be extracted from a measured distribution of switching currents. Moreover, we obtain exact analytical results for the statistical characteristics of the residence time for anomalous diffusion in the form of Lévy flights in a fully unstable potential profile. The noise enhanced stability phenomenon is observed in the system investigated.
(ii) We show here that dissipation can enhance the stability of a quantum metastable system strongly interacting with a thermal bath. We find that the escape time from the metastable region, with an unstable initial condition, has a nonmonotonic behavior versus the system-bath coupling and the temperature, producing a stabilizing effect. Moreover, the combined effects of strong Ohmic dissipation and monochromatic driving affect the stability of a quantum system with a metastable state. The escape time from the metastable state has a nonmonotonic behavior as a function of the thermal-bath coupling, the temperature and the frequency of the driving. The quantum noise enhanced stability phenomenon is observed in the system investigated. These results shed new light on the role of the environmental fluctuations in stabilizing quantum metastable systems, to control the escape dynamics to engineer dissipative environments, and exploit dissipation induced steady states for quantum computation.
(iii) We propose a model for the growing of conductive filament in memristors based on an overdamped Brownian diffusion motion in a tilted potential profile. Preliminary results, based on the related Fokker-Planck equation, on the stationary probability distribution and relaxation times of defects are presented.

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#065 - EFFECTIVE METAL-INSULATOR NONEQUILIBRIUM QUANTUM PHASE TRANSITION IN THE SU-SCHRIEFFER-HEEGER MODEL

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The steady-state behavior of observables in the Su-Schrieffer-Heeger (SSH) and in the one-dimensional transverse field quantum Ising models, after a sudden quantum quench of the parameter controlling the gap, is studied. In the thermodynamic limit, and for long times, nonanalyticities are found even in simple local observables as a function of the quench parameter. This behaviour signals a nonequilibrium quantum phase transition. The occurrence of this nonequilibrium quantum phase transition is attributed to an effective metal-insulator transition occuring at the level of the generalized Gibbs ensemble which describes the steady state of the equilibrated system. Studying the robustness of such transitions, in the paradigmatic case of the SSH model they are found to persist both for quantum quench protocols of finite duration in time as well as for thermal initial states. The presence of fermion-fermion interactions and finite-size effects on the other hand tend to wash out the transition.

#066 - DYNAMICAL TRANSITIONS IN A DRIVEN DIFFUSIVE MODEL WITH INTERACTIONS

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Driven diffusive models are an active research topic in nonequilibrium statistical physics and are inspired by biological and vehicular traffic processes. A basic instance is the Totally Asymmetric Simple Exclusion Process (TASEP): the steady state of this model with open boundary conditions was solved exactly, moreover a dynamical transition, which corresponds to a singularity in the relaxation rate of the system, was discovered and exactly located in the phase diagram. This transition does not coincide with any change in the steady state properties, it separates a slow phase, in which the relaxation rate depends on a control parameter, from a fast phase, in which the relaxation rate reaches a maximum and becomes constant.

Cluster mean-field like approximations reproduce many exact steady state properties of the TASEP and give a dynamical transition line which is close to the exact one. In this work we apply such approximations to investigate the dynamical transition in a driven diffusive model with local interactions [1], supporting the results with Monte Carlo simulations, numerical evidences and a modified Domain Wall Theory (mDWT). This phenomenon occurs in this model as well and exhibits new features when the interactions are strongly ntakattractive.

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#067 - COEXISTING PHASES WITH DIFFERENT EFFECTIVE TEMPERATURES IN SYSTEMS OF ACTIVE BROWNIAN PARTICLES

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Active matter usually reaches a stationary state but the steady state distribution is different from the Boltzmann one and can not be, in general, described by a single temperature. To define an effective temperature in a system of self propelled particles, we consider the parameter that replaces the bath temperature in the fluctuation-dissipation relations between the time-delayed correlations and linear responses of the same observables. It can be shown that there exists an effective temperature taking the same constant value for all observables that evolve in the same time scale and that this quantity plays the same role as the equilibrium thermodynamic temperature (for example it controls heat flows). We focus on its dependence on the global density and on the activity in a system of spherical active Brownian particles. To measure the linear response we exploit recently developed methods that do not imply the application of a perturbation of vanishing strength. Firstly, with the help of molecular dynamics simulations, we study the behavior of the effective temperature in homogeneous systems and we found that the effective temperature decreases monotonously with increasing density. Secondly, we investigate the temperature behavior when the system undergoes motility induced phase separation and we found that the two phases coexist with different effective temperatures.

#068 - MULTISTABILITY IN NONLINEAR SYSTEMS WITH COLORED NOISE AND APPLICABILITY OF UCNA

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We investigate analytically and numerically probability characteristics of nonlinear dynamical system perturbed by colored Gaussian noise in the form of Ornstein-Uhlenbeck random process. Based on the result given by Unified Colored Noise Approximation (UCNA) and numerical simulation of Langevin equation, a possibility of bimodality in the steady-state probability density function (PDF) even in a monostable potential is shown. This bistability can be also observed in a non-stationary state. We explore the mechanism responsible for emergence of bimodal stationary states in general static single-well potentials. The boundary between unimodal and bimodal regimes is found for a quartic potential. The new procedure to construct the stationary PDF in the form of an expansion in small correlation time of colored noise is proposed for an arbitrary smooth potentials and the first three approximations are found analytically. Comparing our results with UCNA, we demonstrate that UCNA gives the correct result only in the first order in small parameter (correlation time), but coincides with the exact solution in the case of a linear system.

#069 - RAMAN ANALYSIS OF GEMS AND GEMSTONES: COMPARISON BETWEEN MOBILE AND FIXED INSTRUMENTATIONS.

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Raman spectroscopy has proven to be a very efficient tool in the analysis of gems being a fast and non-invasive technique. Important characteristics for the applications in the gemological field are the capability to discriminate between similar materials and the possibility to analyze many materials, crystalline and amorphous, organic and inorganic. This allows to identify simulants and treatments and to have information on the chemical composition and sometimes on the origin of the gems.

In recent years, the commercial availability of many kinds of mobile Raman spectrometers made possible the in situ analysis of gems. Thanks to the novel instrumentation, it is possible to measure priceless gems directly in the collections or museums, to study gems mounted on archaeological objects, etc. Even the analysis of gemstones directly on the outcrops is now possible.

In this work, we compare the different information obtainable with the different instrumentations. The possibility offered from the high space and spectral resolutions of fixed micro-Raman apparatus (as the analysis of fissures and inclusions) are compared with the results obtainable on small portable Raman systems. The performances in gem analysis of different classes of mobile Raman spectrometers, with different laser excitations, are also evaluated

#070 - TIME THROUGH COLORS: A KINETIC MODEL OF RED VERMILION DARKENING FROM RAMAN SPECTRA

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Darkening of Red Vermilion (cinnabar) is a well-known phenomenon which needs, at the moment, a full comprehension of its nature. Some paintings reveal a disfiguring process of blackening degradation of Red Vermilion, albeit other relics preserve the original color during the time. The presence of Cl- ions, in addition to the light exposition, represents the most consolidated cause for explaining the phase transition from alpha-cinnabar (red) to beta-cinnabar (black). However, the real effect of chlorine impurities is still not completely understood. In this study we propose a kinetic model of mutual composition of alpha/beta cinnabar as a function of ageing time by analyzing the Raman spectra of ancient cinnabar pigments. This model has been validated with the experimental darkening of pure alpha cinnabar doped with Cl- ions and treated under UV light.

#071 - TOWARDS MODELLING THE DEGRADATION OF COLOURED PIGMENTS

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Several of the historical coloured pigments belonging to the paintings of the late 1800 and early 1900, are undergoing an irreversible degradation process, causes of which are still unclear. In the specific case of the brilliant yellow pigment that takes its colouration from cadmium sulfide (CdS), a II-VI wide-gap semiconducting compound, the role of structural defects and impurities (Zn, Se, and Cl) is the subject of a still on-going research that aims to link the history of the material to the reactivity of the pigment surface.

The key idea is based on the fact that *different* types of defects in the surface of the pigment – whose concentration depend on the history of the pigment itself - influence the surface reactivity in *different* ways, facilitating the formation of *different* secondary compounds experimentally observed. This fact might be considered as a precursor of the photo-oxidation reactions invoked by experimental results.

The aforementioned study is carried out by means of a fully theoretical approach based on the density functional theory. We demonstrate how vacancies and impurities have a dramatic effect on the absorption spectra of CdS, and give rise to the color changes often seen in masterpieces from that era.

As opposite to novel materials, in the field of Cultural Heritage where pigments already possess their long history, a theoretical method becomes secondary to the experimental analysis but still it represents a very good complementary tool extremely useful in the interpretation of complex mechanisms not easily accessible by experiments.

#072 - THE USE OF ELECTRONIC SPECKLE PATTERN INTERFEROMETRY AS NDE TOOL ON ARTWORKS

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In this contribution we have shown the use Electronic Speckle Pattern Interferometry as non-destructive tool for cultural heritage artifacts diagnostics. The technique is non-invasive, contactless, at full field and can be applied on almost any type of archaeological finds, providing relevant information about their state of conservation and even helping to evaluate a restoration process [1]. The applications include the whole structure analysis, as well as the detection of detachments, micro-cracks, hidden damages and inclusions through the analysis of the correlation fringes showing the deformations of the object, due to a perturbation, with micrometric sensitivity [2]. The diagnostic investigation can be carried out before, during and after a restoration. It is also possible the real time monitoring of the behavior of the object according to the environment thermo-hygrometric changes. Examples of analysis on different artworks are illustrated but the main attention has been focused on painting on canvas that are most difficult items to be analyzed cause to their sensibility to the vibrations.

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#073 - LOW-ENERGY ION BEAM ANALYSIS APPLIED TO CULTURAL HERITAGE

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When a solid is bombarded with energetic primary particles such as photons, neutrals, ions or electrons, “secondary” particles are emitted from the surface of the solid. Most of these species emitted are neutral and leaves the surface together with electrons, atoms, and molecules. However, a small fraction of secondary ions is generated during the bombardment and can be detected using a mass spectrometer. This technique is called secondary ion mass spectrometry (SIMS). In SIMS experiments, single ions or cluster of ions are accelerated (typically between 20 and 60 keV) and focused on the solid surface. The energy of the accelerated particles is transferred to the atoms of the solid by a collision process. A collision cascade occurs and some of these collisions come back to the surface generating the emission of atoms and molecules.

Unfortunately, this kind of investigation approach cannot be used in the cultural heritage field because of its destructive nature. However, using a very low primary particle flux density (10^{12}ions/ cm^2) it is possible to statistically guarantee that no point on the surface will be impacted more than once by a primary ion during an analysis session. This is called staticSIMS.

Static SIMS is one of the most powerful surface investigation techniques that provides elemental and molecular information of the outermost atomic layers (1-2 nm) of the sample under analysis. Its use in archeology and cultural heritage is quite recent and mainly focused on the study of organic compounds. It can be considered with XPS as the principal surface analysis technique. In particular, the continual development of new liquid ion source, delivering cluster projectiles, permits to characterize surface and in-depth compositions of molecular species with minimal damage, excellent spatial (<60 nm) and depth resolution (1 nm) and increased sensitivities for imaging applications. In the last decade, static SIMS has been successfully applied for the chemical characterization of different artworks ranging from paintings, metal artifacts to archeological objects.

#074 - ANALYSIS OF EARLY BRONZE AGE POTTERY FROM THE SITE OF VALCORRENTE - SICILY (ITALY)

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Ceramic, thanks to its resistance to ageing and to its copious production in almost any historic period, is one of the most important sources of information about the prehistoric sites. In addition to the study of typology and style of artifact it is fundamental to obtain data from archaeometric study, concerning clay and finite product compositions, inclusions and trace elements, providing indication on the origin, the realization techniques and their evolution with time.

Valcorrente is situated on a low hill on the south-western slopes of the volcano Etna, on the outskirts of the plain of Catania, less than 20 km from the sea. It was fortuity identified in 2005 during some agricultural works, and was systematically excavated from 2012 to 2015 by the University of Catania and the Local Archaeological service with three large trenches: two located in proximity to a rescue excavation conducted in 2005, and another one 80 m to the east, so as to ascertain the overall extension of the site. This issue was also tackled through an extensive survey that was carried out in 2013 and led to a hypothesis that during the EBA an area of about two hectares had been frequented [1-3].

The excavations revealed three main periods of occupation/frequentation, which date respectively to the end of the Neolithic period, to the end of the Chalcolithic period, and to the Early Bronze Age, dated with C14 and TL methods between the end of fifth mill. BC and the half of the second mill. BC. The different pottery fabrics recognized, belonging to different periods, seem to be mostly locally produced, although it is likely that different technological choices are related to the function of the different classes of materials.

Analysis has been focused on different ceramic class and utilization type, with shards coming from different stratigraphic units, in order to perform diachronic and synchronic comparison.

The chemical composition of pottery shards has been be analyzed with the non-invasive IBA techniques PIXE and PIGE, in order to obtain the major and minor components, from Na to heavier elements. These techniques have been extensively used for the study of ancient pottery thanks to their capability of giving a multi elemental analysis with very low detection limits and small uncertainties.

Chemical investigations on Valcorrente pottery complex will provide many indications about the ceramic production technology in that area and its evolution in different periods. Further information to confirm and complement the results will also be available in a multi-technique approach, by coupling other measurements to be done in the next future

#075 - MULTIDISCIPLINARY ARCHAEOMETRIC INVESTIGATION OF DECORATED POTTERY FRAGMENTS (XIX CENTURY A. D.) FROM AGSU SITE (AZERBAIJAN)

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The present work is aimed at the non-destructive or micro-destructive investigation, at different spatial scales from elemental to microscopic domain by combining optical microscopy (OM), scanning electron microscopy – energy dispersive spectroscopy (SEM-EDS), X-ray diffraction (XRD), prompt gamma activation analysis (PGAA) and synchrotron radiation (SR) based Fourier transform infrared (FTIR) spectroscopy, of the ceramic bulk and pigmented glazed surfaces of ancient ceramics dated back XIX century A. D. and coming from the charming archeological site located in the Medieval Agsu town (Azerbaijan) [1]. This geographic area is of special interest due to the ancient commercial routes between China, Asia Minor and Europe. The acquired information reveals useful for the identification of the provenance, the reconstruction of the firing technology, and, finally, the identification of the pigments used for decoration.

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#076 - EXCITONIC INSULATOR IN LONG-RANGE INTERACTING SYSTEMS

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Fifty years ago a few outstanding physicists, including Leonid Keldysh and Walter Kohn, put forward a heretic paradigm of a strongly correlated insulator: If a narrow-gap semiconductor (or a semimetal with slightly overlapping conduction and valence bands) failed to fully screen its intrinsic charge carriers, then excitons---electron-hole pairs bound together by Coulomb attraction---would spontaneously form. This would destabilize the ground state, leading to a reconstructed 'excitonic insulator' that would exhibit a distinctive broken symmetry, inherited by the exciton character, as well as peculiar collective modes of purely electronic origin. Intriguingly, the excitonic insulator, which shares similarities with the Bardeen-Cooper-Schrieffer superconducting ground state, could display unusual macroscopic quantum coherence effects. So far, the observation of this phase has been elusive. The crux of the matter is the trade-off between competing effects in the semiconductor: as the size of the energy gap decreases, favouring spontaneous exciton generation, the screening of the electron-hole interaction increases, suppressing the exciton binding energy.

Very recently, novel low-dimensional systems seem to renew the promise of the excitonic insulator, as they combine optimal band structures, poor screening, truly long-ranged interactions, and giant excitonic effects. In this talk I will discuss our theoretical predictions [1-3], based on the combination of first-principles and model approaches, concerning: (1) armchair carbon nanotubes (2) MoS_2 at high pressure (3) monolayer MoS_2 in the *T'* phase, a 2d topological insulator.

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#077 - LOCAL AND MACROSCOPIC ELECTROMAGNETIC FIELDS IN BILAYER CRYSTALS

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Optical contrast experiments [1] can distinguish in between the number of constituent planes of a 2D crystal, but a proper theoretical analysis of the optical response of a 2D material is missing already for the bilayer case [2]. In this presentation, I will illustrate a complete theory for the optical response of a bilayer material [3]. Focus will be on the bilayer hexagonal Boron Nitride (hBN). In the viewpoint of optics, being an insulating dielectric, this is the simplest example of a bilayer crystal.

The theory shows that, if the distance ***d*** between the two planes far exceeds the lattice constant ***a***, the two atomic planes can be macroscopically treated as two separated monolayers. In this case, for both layers, the local field is connected to the macroscopic field via an expression identical to the one for the monolayer. On the other hand, for shorter distances, although it is still possible to define a surface polarization and hence a surface current for each single plane, the local fields are coupled to the macroscopic fields in both layers. Because of this, it is meaningful to provide a volume susceptibility s rather than a surface susceptibility s_s(for this last quantity I would obtain different results for the two planes). It is possible to compare the surface susceptibility for the monolayer with the susceptibility for the bilayer, I obtain $s_s > s \times d$ where the equality holds only when $d >> a$.

The comparison of this theory with the optical contrast measurements confirms that the interaction in between the two atomic planes alters the optical response of the bilayer crystal.

This approach can be extended to study multilayer structures, up to a thickness where the bulk susceptibility is found. There still are open questions to address. All the fields considered in this presentation travel in the vacuum, so one may wonder how a polarization wave that propagates with the speed of light divided by *n* emerges (*n* being the refractive index), and how many layers do we need in order to have a layer independent refractive index.

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#078 - INTERACTING TOPOLOGICAL EDGE CHANNELS

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Electrical currents in a quantum spin Hall insulator are confined to the boundary of the system. The charge carriers can be described as massless relativistic particles, whose spin and momentum are coupled to each other. While the helical character of those states is by now well established experimentally, it is a fundamental open question how those edge states interact with each other when brought in spatial proximity. We employ a topological quantum point contact to guide edge channels from opposite sides into a quasi-one-dimensional constriction, based on inverted HgTe quantum wells. Apart from the expected quantization in integer steps of 2e2/h, we find a surprising additional plateau at e2/h. We explain our observation by combining band structure calculations and repulsive electron-electron interaction effects captured within the Tomonaga-Luttinger liquid model. The present results may have direct implications for the study of one-dimensional helical electron quantum optics, Majorana- and potentially para-fermions.

#079 - LEVITONS IN INTERACTING HELICAL EDGE STATES OF TWO-DIMENSIONAL TOPOLOGICAL INSULATORS

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One-dimensional edge states are one of the building blocks of the so-called electron quantum optics. It is a fast developing field aiming at performing quantum optics experiments using single-electron excitations in solid state devices instead of photons on optical tables [1]. In this respect, a prominent role is played by a peculiar kind of one-dimensional excitation which features one electron above the Fermi sea accompanied by *no* disturbance below it [2]. These remarkable excitations are known as levitons [2]. They have been experimentally detected in non-interacting systems [3] and they have been predicted to survive also in (strongly interacting) single edge states in the fractional quantum Hall regime [4].

Here we demonstrate the existence of levitons in yet another system: the interacting helical edge states of two-dimensional topological insulators (2DTI), which represent an ideal playground for further and exciting developments of electron quantum optics [5]. We carefully study the spectral properties of levitons (accessible via spectroscopic measurements) and highlight the novelties associated with the presence of two counter-propagating and interacting channels. We also discuss a scheme which allows to detect one of the most striking signatures of levitons, *i.e.* the vanishing excess noise associated with their tunneling across a quantum point contact (QPC). Our results are timely in view of the very recent experimental breakthrough in building QPC in 2DTI [6], which paved the way for a concrete development of electron quantum optics with topological insulators.

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#080 - ELECTRONIC AND STRUCTURAL PROPERTIES OF FEW LAYERS CRI3

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The recent reports of ferromagnetic order in two dimensional crystals sign the beginning of a new chapter in the field of 2D materials. Bulk CrI_3 is a layered van der Waals ferromagnet and, in its monolayer form, a 2D ferromagnet. In contrast, few-layers CrI_3 present an AFM interlayer coupling. In this study, we address the interplay between stacking and interlayer exchange coupling for CrI_3 2D crystals using first-principles calculations and an effective interlayer coupling model. We also explore the possibility of using 2D ferromagnets in a new type of spin valve, in which a 2D nonmagnetic conductor is intercalated between two ferromagnetic insulating layers. In this setup, the relative orientation of the magnetizations of the insulating layers can have a strong impact on the in-plane conductivity of the 2D conductor. We first show this for a graphene bilayer, described with a tight-binding model, placed between two ferromagnetic insulators. In the antiparallel configuration, a band gap opens at the Dirac point, whereas in the parallel configuration, the graphene bilayer remains conducting. We then compute the electronic structure of graphene bilayer placed between two monolayers of the ferromagnetic insulator CrI_3, using density functional theory. Consistent with the model, we find that a gap opens at the Dirac point only in the antiparallel configuration.

#081 - HIGHLY-ORDERED SINGLE-LAYER MOS2 ON THE ANISOTROPIC AG(110)

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Transition-metal dichalcogenide (TMDC) single layers, such as $MoS_2$and WS_2on Au(111), could be grown by physical vapor deposition with a single-orientation and high-quality making them suitable for their exploitation in applications in valleytronics devices. In that case, the templating effect and the crystalline symmetry of the *fcc* substrate have been accounted for the high-quality and single-orientation of the TMDC single layer. Herein, we show that it is possible to grow highly-ordered single-layers of MoS_2on the anisotropic Ag(110) surface. The growth is achieved in two steps, with an initial formation of MoS_2 nanoclusters that act as seeds for the growth of the complete layer. By means of core-level and valence band photoemission spectroscopy, we investigate the electronic structure of the interface, revealing a metallicity of the single-layer MoS_2induced by the Ag substrate. X-ray photoelectron diffraction (XPD) reveals the coexistence of an equal amount of mirror-oriented MoS_2crystalline domains on the surface. Low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) measurements show the formation of a complex superstructure, accounting for additional moiré-induced electron diffraction spots and striped patterns in the STM topography images. Based on the analysis of these results, we identify a structural atomic model for the MoS_2/Ag(110) interface, with the formation a moiré superstructure and a strain of the MoS_2lattice of about 3% along the [1-10] direction of the substrate.

#082 - VERTICAL WS2/MOS2 VAN DER WAALS HETEROSTRUCTURES BY ONE-STEP LIQUID-PRECURSOR CVD GROWTH

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In recent years, transition metal dichalcogenides (TMDs) have attracted large attention as promising semiconducting materials for next generation optoelectronic devices. This class of semiconductors, in fact, shows a unique relation between the number of atomic layers and the nature of band gap: MoS_2, for instance has an indirect band gap at 1.3 eV when grown as bulk material, but also shows a direct band gap at 1.9 eV in the in the monolayer limit [1]. Because of the direct band gap, together with long exciton life and coherence times, monolayer TMDs usually show large light-matter interaction and remarkably intense photoluminescence (PL) [2]. Such that, TMDs appear to be the ideal building blocks for future high-performance, ultra-small, flexible optoelectronic devices.

In addition, since the atomic layers of these materials are held together by weak van der Waals (vdW) interactions, many layers of different TMD materials can be easily stacked together without any lattice constrains [3]. Van der Waals vertical heterostructures are usually obtained by either sequentially growing different TMDs in 2 steps or more [4], or by deterministically transferring them one on the top of each other [5]. Furthermore, the properties of the final device can be manipulated by engineering the vdW gap and the lattice strain in the heterostructure by carefully choosing the TMD building block and their reciprocal orientation [6].

In this work, we will present vertical WS_2/MoS_2 heterostructures obtained by one-step liquid-precursor chemical vapour deposition (LPCVD). The water solution based precursors lead to the growth of single-crystal flakes of vertical WS_2/MoS_2 with lateral size of tens of microns. Microscopic and spectroscopic characterizations reveal that the flakes are monolayer oriented with a 0° angle. In comparison with the sequential assembling of these structures previously reported, this method gives the advantage of systematically obtaining vertical heterostructures that show clean interfaces and are aligned at the atomic level. The structural and optical properties of this vdW heterostack as well as its applicative potential will be thoroughly discussed and presented. From these preliminary results, LPCVD appears to be a very promising technique for the one-step growth of high-quality atomically-aligned TMD heterostructures for future optoelectronic devices.

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#083 - UNCOVERING THE ROLE OF CONTACTS RESISTANCE AND GRAIN BOUNDARIES IN THE ELECTRICAL PROPERTIES OF CVD MOS2 TRANSISTORS BY CONDUCTIVE ATOMIC FORCE MICROSCOPY

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Transition metal dichalcogenides, such as MoS_2, have recently gathered a lot of interest as promising candidates for post-Si CMOS devices [1] and novel heterostructure transistors [2]. Despite many progresses in the chemical vapour deposition (CVD) of MoS_2, uniformity on large area still needs to be improved. Furthermore, the impact on the electrical properties of extended defects, e.g. grain boundaries, in CVD polycrystalline MoS_2 have to be further elucidated [3]. In addition, several processes (contacts, dielectrics, mobility engineering) need to be improved to achieve optimal MoS_2 transistors performances [4,5]. In particular, current injection mechanisms from metals to MoS_2 are still object of intense debate, due to their implications in the final device performances.

In this work, ultrathin MoS_2 films consisting of single and bilayer triangular domains separated by grain boundaries were obtained by optimized CVD onto a SiO_2/Si substrate [6]. After preliminary inspection by optical microscopy, Raman, photoluminescence, and atomic force microscopy, back-gated MoS_2 field effect transistors (FETs) were fabricated to get information on the key electrical properties (on-resistance, carrier mobility) [7]. Characterization of these FETs showed non-linear current onset in the output characteristics at low drain bias and a field effect mobility of approx. 0.1 cm^2/Vs. Nanoscale current mapping and local I-V measurements by CAFM [8] were employed to uncover the mechanisms limiting electronic transport in these devices. First, the distribution of the local metal/MoS_2 Schottky barrier heights within individual domains was evaluated, showing an average value of approx. 0.3 eV, consistent with the nonlinear current onset observed in the FETs characteristics . Furthermore, a large conductance drop associated to grain boundaries between neighboring MoS_2 domains was directly imaged for the first time. This can be responsible, in part, of the low mobility values in CVD MoS_2. The demonstrated nanoscale characterization approach will be an essential tool to evaluate further improvements in CVD MoS_2 material and devices.

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#084 - 2D-MATERIALS: NEW PLATFORM FOR NEXT-GENERATION ENERGY DEVICES

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Two-dimensional (2D) materials are entering several application areas,[1-5] improving the performance of existing devices or enable new ones.[1-5] A key requirement for the implementation of 2D materials in the energy field is the development of industrial-scale, reliable, inexpensive production processes,[2] while providing a balance between ease of fabrication and final product quality.

In this context, the production of 2D materials by solution processing[2,6] represents a simple and cost-effective pathway towards the development of 2D materials-based energy devices, presenting huge integration flexibility compared to other production methods. Here, I will first present our strategy to produce 2D materials on large scale by wet-jet milling[7] of their bulk counterpart and then an overview of their applications for energy devices.[3,8,9,10,11,12,13,14]

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#085 - SOLAR SELECTIVE COATING FOR HIGH VACUUM FLAT SOLAR THERMAL PANELS

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The Selective Solar Absorber (SSA) is a key component of solar thermal panels. SSA should absorb the solar radiation and it should not emit the thermal radiation. Due to the Wien's law, the optimal transition wavelength from high absorbance to high reflectance depends on the absorber working temperature [1].

The new developed high vacuum flat solar thermal panel [2] has moved the operating temperature of flat panel from about 80°C up to 200°C. Under high vacuum at such temperature the main heat loss is due to absorber emitted radiation and the absorber radiative properties have to be optimized for the new working temperature.

Intrinsic selective materials are not satisfactory for solar thermal application and optical absorbing coatings on a conductive substrate are required to obtain the desired performances. The optimum optical package is obtained using multi-layered structures consisting of different materials. The complete package has to be transparent in the infrared region, so that the spectral averaged emissivity is dominated by the low emissivity substrate. An antireflective (AR) coating is used to reduce the optical losses due to refractive index mismatch between the absorbing coating and the vacuum. We present the simulation and experimental results obtained using Cr2O3, Ti and Cr as absorbing layers on aluminium film substrate. The presence of a Silicon oxide as AR coating was also simulated. The thin films were deposited by electron beam evaporation without breaking the vacuum. Structural, optical and infrared characterizations of the single layer and of the multilayer structures will be presented. New proper optimized structures reduce absorber emissivity improving the panel thermal efficiency.

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#086 - FREE-STANDING AND HIGHLY CONDUCTIVE PEDOT:PSS

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A low cost and fast method to obtain a free-standing, flexible, thick and conductive polymer foil from a mouldable paste is presented. The procedure is based on the phase separation of PEDOT from PSS, induced by acidification of the solution until its complete saturation and is as easy as writing with an ink-pen. The samples obtained have been electrically characterized and have shown a sheet resistance ranging between 0.90 and 0.30 Ohm/sq, depending on the processing used to produce them. These values correspond to conductivities within 370 and 1000 S/cm. The samples are easily detachable from the substrate and then can be handled as free-standing foils. A qualitative mechanical analysis of the free-standing specimens have shown that they are flexible and can be repeatedly bent without exhibiting damage. The morphological and chemical characterization has been carried out by Scanning Electron Microscopy and Raman analysis, and have shown that the material is constituted of nm-size grains where both PEDOT and PSS species are present. The results have been explained in terms of a new material structure arrangement made of PEDOT and PSS agglomerates in which a core made of PEDOT and PSS is surrounded by a PEDOT-based shell. The charge transport then goes through the conducting PEDOT-enriched shells functioning as percolation channels. The material can be prepared through industrial techniques such as screen printing, doctor blade, inkjet printing and roll-to-roll, i.e. it is scalable. Therefore, in future perspectives, the synthesized material can be considered as a good alternative to other organic conductive materials and to the common and more expensive metallic contacts.

#087 - HYDROGEN STORAGE IN FULLERENES

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A new class of hydrogen storage materials has taken hold in the last years: the so-called alkali-cluster intercalated fullerides (A_xC_{60}, $x \geq 6$) in which the *fcc* structure of C_{60} is intercalated by partially ionized alkali metal clusters. These materials are able to uptake high amounts of hydrogen via a reversible chemisorption mechanism at modest temperatures and dehydrogenation enthalpies.

The hydrogen sorption mechanism was investigated by: 1-“in situ” neutron diffraction by following the evolution of the structure on increasing the temperature under hydrogen pressure and 2- muon spin rotation spectroscopy thanks to the capability of this technique to follow the muonium reactions (a muon-electron bound state similar to an hydrogen atom).

The evolution of the structure under hydrogen pressure on increasing temperature shows that in the case of x=6, the hydrogenation of C_{60} is the first process to occur eventually associated with a *fcc* to *bcc* structural phase transition. At moderate degree of C_{60} hydrogenation, a segregation of LiH is observed which progressively reduces the nuclearity of the intercalated clusters.

During desorption, both processes (hydride formation and fullerene hydrogenation) reverse and the original material is fully restored.

On the other side, implanted muons can also probe the chemisorption process through the formation of muonium, which is an isotope of hydrogen. The observed formation of a muon adduct radical confirms that C_{60} hydrogenation is the first process to occur, but its efficiency, related to the amplitude of the radical signal, increases on lowering the temperature down to 5K. This indicates that the cluster mediated hydrogen dissociation is the process requiring the relatively high temperatures needed for the storage process.

In conclusion, the combination of in-situ neutron diffraction and muon spectroscopy allowed to disclose the hydrogenation mechanism of these new type of hydrogen storing materials. The results obtained give suggestions on how to further improve the (already satisfying) performances of these systems.

#088 - DIRECT GROWTH OF ZIF8 FILMS ON CU FOILS FROM SOLUTION FOR LITHIUM ION BATTERY

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Metal Organic Frameworks (MOFs) are hybrid porous complexes in which periodic arrangements of metal clusters are connected by organic ligands. They represent promising materials for a wide range of applications, like gas and energy storage, chemical sensing and nanodevices. MOFs are characterized by a high specific surface area, low density, tunable pore size and good thermal stability. In addition, thanks to the possibility to achieve surface functionality and modulate pore size they result versatile and suitable materials for host-guest chemistry. Among all possible MOFs topologies, ZIF8 that consists of $Zn(MeIm)_2$ (HMeIm: 2-methylimidazolate), presents a crystal bcc structure featuring large openings of 11.6 Å accessible through six-membered ring apertures of 3.4 Å. There are several examples of ZIF8 films obtained mainly by synthetic methods based on layer-by-layer deposition (LBL), solvothermal, microwave and electrochemical protocols. However, to guarantee the covalently anchoring of ZIF8 onto the surface, different substrates have been functionalized with OH or NH_2-terminated Self assembled monolayers (SAMs). Here, through direct growth from methanol solution ZIF8 thick films were grown on copper foils. The high surface basicity has allowed to accelerate the homogenous and heterogeneous nucleation compared to other surfaces leading to amorphous thicker films. Samples were characterized by XRD, SEM and FTIR spectroscopy. In addition, post-synthetic treatments based on doping with lithium acetate were carried out to obtain Li-doped ZIF8 films, whose behavior during the charge/discharge profile of lithium ion cell has been investigated. Indeed, Li-doped ZIF8 and ZIF8/Cu have been assembled in lithium ion cells and characterized by voltammetry cyclic and galvanostatic measurements.

#089 - SYNTHESIS OF METAL NANOPARTICLES/GRAPHENE HYBRID COMPOSITES AND EXPERIMENTAL STUDY OF THE CHARGE TRANSFER EFFECTS

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Hybrid composites, fabricated by the synergistic combination of graphene and metal nanoparticles (NPs), are considered promising candidates for the design and production of innovative and functional sensing, energy production/storage, electronics, catalytic devices [1,2]. The physico-chemical response of such devices is dictated by the properties arising from the combination of the properties of both components. In particular, noble metals nanoparticles (Au, Pt and Pd NPs) have received great attention by scientific community due to the huge surface-volume ratio compared to the correspondent bulk materials and their optical, electrical and magnetic properties, which make them useful for many applications in catalysis, hydrogen storage, direct alcohol fuel cell and reduction of environmental pollutants. Furthermore, graphene is the favorite substrate to load NPs due to its good electrical conductivity, high surface area and mechanical strength. So, loading metal NPs on graphene can leads to nanocomposites with larger active surface areas and improved electron transport for enhancing catalytic reactions, electronic and optics devices, sensors and fuel cells, due to charge transfer effects between graphene and NPs. This effect can be investigated through the value shift of the 2D peak of the graphene's Raman spectrum [2-4]. Here we present an approach to fabricate graphene-metal NPs hybrid composites and we provide some experimental results related to the metal/graphene charge transfer effects.

In particular, we present a laser-assisted synthesis method for the production and processing of mono- and bi-metallic Pt, Pd, Au, PtPd and AuPd NPs. It is based on the nanosecond-pulsed laser ablation, in liquid environment. Also, the NPs have been used to decorate graphene substrates to fabricate hybrid nanocomposites and these nanocomposites were characterized by Raman spectroscopy and by Conductive Atomic Force Microscopy (C-AFM) in order to analyze the NPs-graphene interaction. The amount of the Raman 2D signal shift and some current-voltage curves obtained by C-AFM demonstrate that the chemical composition of the metal nanoparticles drives the charge transfer phenomena. A combined analysis of these results allow us to draw a general framework for the interpretation of charge transfer mechanisms in graphene-NPs hybrids.

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#090 - SUPER-ACTIVATED BIOCHAR FROM POULTRY LITTER FOR ELECTRODES IN SYMMETRIC SUPERCAPACITORS

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Supercapacitors (SCs) are rather promising devices for energy conversion and storage, capable to bridge the gap between conventional capacitors and rechargeable batteries. Electrical double-layer capacitors (EDLCs) exploit the very large specific surface area (SSA) of polarizable porous carbon electrodes (typically 1000-2000 m^2/g) and the very short distance between charges at the electrode/electrolyte interface (few nanometers) to bring the resulting capacitance to values of the order or 100 F/g, hence much higher than flat plate capacitors. Moreover, with respect to secondary batteries, SCs show much longer cycle life (> 100000 cycles) and higher power densities (> 1 kW/kg), although energy density values are still lower (of the order of few Wh/kg) [1].
Recently, highly porous activated carbons obtained from biochar, namely the carbon side-product in the pyrolysis/gasification of residual waste biomasses, started to receive a widespread attention in the field of the electrical energy storage, thanks to its hierarchical porous structure inherited from biomass precursors, its excellent chemical and electrochemical stability, high conductivity, high surface area and inexpensiveness [2].
In this study, we report for the first time the production of a novel hierarchically porous super-activated carbon with SSA exceeding 3000 m^2/g starting from the biochar generated by the pyrolysis of poultry litter. This waste material is the solid waste resulting from chicken rearing, which nowadays, due to the fast growing of the poultry industry, is posing important disposal and pollution problems [3]. The chemical activation, performed with KOH and subsequent HCl washing, proved to be efficient to remove all impurities other than carbon present in the raw material and to enhance the fraction of sp^2 carbon, which locally organizes to form few layered graphene-like nanosheets structures. The very large SSA, together with the optimal hierarchical mesoporous and microporous structure of this material, allowed to reach remarkable performances in SCs operating either with KOH, or with Na_2SO_4 environmental friendly electrolyte, which delivered specific capacitances of up to 229(13) F/g [4]. These findings suggest possible large-scale applications for such devices, for example in the field of transportation or in renewable energy-grids, but also in the field of bio-medicine.

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#091 - PREDICTIVE MODEL OF BIFACIAL PV SYSTEMS PERFORMANCE

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Recently, a relevant development of bifacial PV devices has occurred and for the next years a remarkable market share growth is foreseen [1]. But for such devices two relevant questions exist:

the lack of a standard method for their electrical characterization and their performance optimization. Some studies have recently deal with such questions, by proposing different models [2-4].

In this work, a novel analytical model to forecast the electrical performance of bifacial PV devices is presented and the main validation results are shown and discussed. By comparing the model forecasts to relevant experimental cases on a bifacial module, we observe very low deviations (order of 1%). Finally, the model proposed is used to predict the electricity generation of a bifacial PV system at different latitudes.

Our model is suitable for any geographical location. It considers the beam, diffuse and reflected components of the solar radiation to estimate the global irradiance on the PV module inclined surface and on the ground. To evaluate the ground albedo, the normal incidence reflectivity was measured in the 300-1100 nm wavelength range, for the materials over which the solar devices were located. For each PV cell, we evaluate the short circuit currents of its front and back sides, by considering the EQE spectra measured for the front and back cell sides, the incident solar spectrum on a bifacial module front surface and on the ground, and the ground albedo. The cell overall photocurrent is determined by adding such currents. The cell electrical characteristics are calculated according to the PV cell classic single-diode model. Then, the bifacial module I-V characteristics are determined by the characteristics of the cells in series making up it. The module temperature is evaluated via the NOCT equation, as a function of the ambient temperature [5] and then compared to experimental data. Our model allows to foresee the electrical performance of a PV system made up by several modules too.

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#092 - MESOSCALE DYNAMICS AND PLASTICITY OF SOFT-GLASSY MATERIALS

Mauro Sbragaglia (I) - University of Rome "Tor Vergata"

Soft-glassy materials (SGM) are key for many industrial and technological applications. These materials usually consist of a disordered collection of soft elementary constituents (e.g. droplets, bubbles, etc) jammed together in a packed configuration. Such systems are elastic and typically out of equilibrium and their fluidization takes place via a succession of elastic loadings followed by plastic rearrangements. In this lecture I will address the mesoscale dynamics of such plastic rearrangements in two relevant situations.

In the first part of the lecture I will concentrate on the dynamics of coarsening, i.e. the process that drives the system towards equilibrium in absence of any external load. The coarsening dynamics causes the soft constituents to change in size and eventually rearrange abruptly. The effect of rearrangements is propagated throughout the system via the intrinsic elastic interactions and may cause rearrangements elsewhere, resulting in intermittent bursts of activity and “avalanche” behaviour. Here we aim at quantitatively characterizing the corresponding avalanche statistics (i.e. size, duration, and inter-avalanche time).

In the second part of the lecture I will focus on situations where SGM are driven with external loadings. The importance of rearrangements on the flow properties is particularly prominent in the flow of SGM in microchannels, where bulk rearrangements are coupled with boundary rearrangemens, triggered by the boundary roughness. I will present a comprehensive study of SGM flowing in microfluidic channels, one wall of which is patterned with micron-size equally spaced grooves oriented perpendicularly to the flow direction. We find a scaling law describing the roughness-induced fluidization as a function of the density of the grooves, thus fluidization can be predicted and quantitatively regulated. Numerical simulations confirm these views and provide a direct link between fluidization and the spatial distribution of plastic rearrangements.

#093 - DROPLET MICROFLUIDICS FOR BIOLOGICAL APPLICATIONS

Davide Ferraro (I) - University of Padova, Italy - Institut Curie, France

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Microfluidics is defined as the science and technology of systems that manipulate small amounts of fluids (pL and nL ranges), using channels having dimensions between tens to hundreds microns [1]. Nowadays, these systems are currently undergoing an exponential development and are starting to take a major place in the new generation of biological and medical analysis instruments. In fact, the typical sample volume can be reduced down to one million-fold as compared with conventional approaches, and a high level of spatiotemporal control is possible, facilitating highly parallelized assays with drastically increased throughput and reduced cost.

For biological applications, the compartmentalization of assays is one key element to obtain independent and large data sets. In daily life biological laboratory, this is achieved by distributing different solutions in independent wells of a microtiter plate, an operation that nowadays is performed manually or by pipetting robots. An improvement of this compartmentalization can be easily achieved through a branch of microfluidics risen in the past two decades: droplet microfluidics [2]. Here, two (or more) immiscible fluids are put into contact by specific geometrical channel networks (like flow-focusing, T-junction, etc.), to produce a controlled emulsion of droplets of one phase dispersed in the other. For biological applications, the emulsions are typically composed by aqueous-phase droplets dispersed in oil mixed with specific surfactants. In this way, each droplet can be considered a single small reactor, which guarantees stable separation of chemicals, bio-molecules and even cells, as well as tiny liquid volumes of the dispersed phase and much reduced contamination risks with the surroundings environment. Nowadays, several operations can be achieved with droplets, including high-throughput generation (up to kHz), merging, splitting, incubation, sorting and solid particles manipulation.

During this talk, the main features of droplet microfluidics will be highlighted, with particular attention to the capability of manipulating solid-phase particles, such as magnetic beads [3,4], hydrogel [5] and nanoparticles [6]. As a matter of fact, this specific skill is paving new research directions in several biological applications, leading to strong improvements in the limit of detection of low abundance molecules and introducing new way of barcoding.

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#094 - UNIDIRECTED MOTION AND NEGATIVE VISCOSITY IN MICROPHASE SEPARATION WITH AN ACTIVE POLAR COMPONENT

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Active fluids are systems where active components present in the fluid (microtubules with molecular motors such as kinesin or actomyosin bundles) display interesting collective ordering properties. Active fluids also exhibit peculiar rheological properties. Depending on the characteristic of the active stress, activity is capable to heighten viscosity, enough to develop shear-thickening properties in contractile systems (e.g. an actomyosin solution) or induce, in extensile suspensions (e.g. materials based on bacterial suspensions), a ”superfluid” regime under suitable conditions.

We present results of Lattice Boltzmann simulations of an emulsion made of an active polar component and an isotropic passive fluid. Different flow regimes are found by varying the values of shear rate and extensile activity. By increasing activity, a transition first occurs from linear flow regime to spontaneous persistent unidirectional macro-scale flow, followed by another transition to (low shear) intermittent flow regime with coexistence of states with positive, negative, and vanishing apparent viscosity, or to (high shear) symmetric shear thinning regime. The different behaviors can be explained in terms of the dynamics of the polarization field close to the walls. In addition a maximum entropy production principle selects the most likely states in the intermittent regime. For contractile activity shear thickening behavior is observed.

#095 - OPTO-MICROFLUIDIC PLATFORM IN LINBO3 FOR SENSING SYSTEMS

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In the last 50 years microfluidic has received great attention from the scientific community due to its wide range of applicability, from chemical to biological analysis and sensing. Although nowadays many efficient and compact microfluidics devices are available, in most of the cases they still require external coupled systems to provide for optical investigation of fluids and dispersed phases within present, often needing for long post processing analysis which make unfeasible real-time sensing. For this reason, a lot of attempts have been made to combine on the same substrate different stages, both optical and fluidic, to overcome this lack of integration and make more feasible the use of optofluidic chips for sensing applications. To this aim, a good candidate is surely Lithium Niobate ($LiNbO_3$), which is a well-known material in photonics, thanks to its excellent properties, such as large piezoelectric and non-linear coefficients and significant photovoltaic and electro-optic response. As a matter of fact, lithium niobate has been recently demonstrated to be a promising material also for fluidic applications, thus paving the way for a full integration of its optical potentialities with the tools typical of microfluidics. Different techniques, such as Laser Ablation, Focused Ion Beam and optically-grade dicing, have been successfully implemented for creating microfluidic circuits on pure $LiNbO_3$ substrates with both T-shaped and cross-junction geometries, by testing their performance as droplet-generators. Moreover, this material has been proved also as viable substrate for actuating on droplets, particles dissolved in liquids and liquid crystals, by means of the strong photovoltaic electric fields and charge accumulations induced at its surface via proper light illumination. These results represented the first step toward the combination of both fluidic and optical stages on $LiNbO_3$, but a full integration has been achieved only in the last year. In this work we present the first fully-integrated opto-fluidic platform realized in $LiNbO_3$ for droplet and liquid crystals actuation and monitoring. On a commercial $LiNbO_3$crystal the microfluidic circuit has been realized by optically-grade dicing the surface and it was coupled with an array of optical waveguides previously realized in the same substrate by means of titanium local doping. In this way, a self-aligned optofluidic platform has been realized on lithium niobate, able to detect and characterize objects and droplets flowing inside the fluidic channels. Finally, the chip was sealed with a Fe-doped $LiNbO_3$ sample, which is capable of actuating on liquid crystals and monitoring their reorientation induced by light-controlled photovoltaic fields, thus creating a optofluidic optical switcher and polarizer.

#096 - OPTOFLUIDIC PLATFORM USING LIQUID CRYSTALS IN LITHIUM NIOBATE MICROCHANNEL

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We demonstrate the all optical control of the molecular orientation of nematic liquid crystals confined in microfluidic channels engraved in lithium niobate. Microchannels are obtained by a novel approach based on femtosecond pulse laser micromachining carried on in controlled atmosphere. The combined effect of photovoltaic and pyroelectric fields generated by light in lithium niobate crystals on the liquid crystal orientation, is reported for the first time. The total space charge field and its dependence on the incident light intensity can be controlled by changing the direction of pump light propagation through the microfluidic chip. The results reported in this manuscript demonstrate that liquid crystals and lithium niobate can efficiently be combined in microfluidic configuration, in order to push forward a novel class of optofluidic devices.

#097 - MULTI-SCALE RELAXATION IN AGING GELS: FROM LOCALIZED PLASTIC EVENTS TO SYSTEM-SPANNING 'QUAKES'

Stefano Buzzaccaro - Politecnico di Milano

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Relaxation of internal stresses through a cascade of microscopic restructuring events is the hallmark of many materials [1,2], ranging from amorphous solids like glasses and gels to geological structures subjected to a persistent external load. By means of Photon Correlation Imaging, a recently developed technique blending the powers of scattering and imaging, we provide a spatially and temporally resolved survey of the restructuring and aging processes that spontaneously occur in physical gels originating from arrested phase separation. We show that the temporal dynamics is characterized by an intermittent sequence of spatially--localized `micro-quakes' that eventually lead to global rearrangements occurring at a rate that scales with the gel age. Notably, these dramatic upheavals of the gel structure are heralded by a progressive acceleration of the microscopic gel dynamics that originates from recognizable active spots and then spread at a large but finite speed through the gel. Within the `slack' phase between two of these `macro--quakes', the fluctuations of the degree of temporal correlation obey a non-Gaussian statistics described by a generalized logistic distribution, while the distribution of the strongest micro--quakes within is in full agreement with the predictions of an Extreme Value Analysis. The evidence we obtained suggests a strong connection both with the stress relaxation processes taking place in earthquake sequences [3] and with recently proposed self-organized oscillator mechanisms of crystal plasticity [4]. Exploiting these analogies, we find that a simple model based on assuming the occurrence of a slow viscoelastic relaxation, added to a standard elasto--plastic description, may help to rationalize our findings.

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#098 - TUNING DROP MOTION AND SHAPE BY MEANS OF VERTICAL OSCILLATIONS

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The manipulation of small (micro-/nano-liter scale) discrete amount of liquid is a subject of great interest for applications in many fields, from chemical synthesis to biological analysis. We can distinguish mainly two branches of Microfluidics dealing with the actuation of droplets: two-phase flows in closed micro-channels and sessile drops motion on open surfaces. Focusing on the latter, it is possible to control the motion and the shape of sessile droplets by means of vibrations of the substrate.

Wehave studied the one-dimensional motion of few microliters drops of liquids with different viscosities and surface tensions on inclined plate subject to vertical sinusoidal oscillation with frequency ranging from tens up to hundreds of Hz. We have taken into account both surfaces with finite contact angle hysteresis and Lubricate-Infused Surfaces (LIS), characterized by low hysteresis ($< 5°$). Properly tuning oscillation amplitude and frequency the drop can be displaced along the incline both downhill, at low amplitude, and, surprisingly, uphill against gravity, above certain amplitude. The main difference between the two substrates is the presence of drop pinning in the case of finite hysteresis for low amplitudes and for amplitudes corresponding to the switch between sliding down and climbing up. These dynamics is due to the asymmetric variations of the front and rear contact angles of the drop producing a net displacement in the oscillation period. In particular, the climbing drop experiences a much bigger variation in its profile during an oscillating period.

We have also studied the interfacial morphologies of water confined to the hydrophilic top face of rectangular posts subjected to vertical vibrations. In response to mechanical driving, an initially flat liquid channel is collected into a liquid bulge that forms in the center of the rectangular post if the acceleration exceeds a certain threshold. The bulge morphology persists after the driving is switched off, in agreement with the morphological bistability of static interfacial shapes on posts with large length-to-width ratios. To explain the dynamic bulging of the liquid interface, we propose an effective lifting force pulling on the drop’s slowly moving center of mass in the presence of fast oscillation modes.

#099 - TANAKA-LIKE TRANSITIONS IN MAGNETIC GRANULAR SYSTEMS

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We investigate the phase separation of a shaken mixture of glass and magnetised steel spheres after a sudden quench of the shaker amplitude. In experiment we focus on quasi 2D system, whereas in molecular dynamics computer simulations also 3D systems are accessible. We observe transient networks of steel spheres emerging in the experiment, as well as in simulations. Analyzing the network evolution by network specific parameters like the mean number of neighbours or network efficiency we have uncovered three regimes (Kögel et al. Soft Matter **14** 2018), previously established by H. Tanaka (2000) for the viscoelastic phase separation of dynamically asymmetric mixtures.

Here we present new results for the network evolution particluraly focusing on the influence of system dimensionality. It turns out that in 3D the dynamics is significantly faster and the observation of all three regimes becomes much more sensitive to the system parameters.

#100 - RESEARCH ACTIVITIES ON PLASMA PROPULSION FOR SPACE APPLICATIONS

Tommaso Andreussi (I) - SITAEL S.p.A.

Since the beginning of the twentieth century, when the concept of Electric Propulsion (EP) was first proposed, the idea to use an electric power source to accelerate a propellant brought about the development of several technological concepts. In particular, plasma-based EP technologies proved capable of significant performance improvements over traditional chemical systems and, consequently, made great technological and commercial progress over the past decades [1]. The development of plasma-based EP technologies relies on the study of basic, low temperature plasma (LTP) dynamics. Understanding the physics behind the operation of these devices can help improving their performance to make them even a more promising choice for a wide variety of space missions. However, despite several experimental, theoretical and numerical investigations, several questions directly related to the plasma state still remain unanswered [2].

In this talk, I will present some of the most active research areas on EP, focusing in particular on the development and testing challenges, as well as on plasma diagnostics, plasma-material interactions, modelling and simulations.

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#101 - TOWARDS APPLICATIONS OF LASER-PLASMA LIGHT ION ACCELERATION AT THE INTENSE LASER IRRADIATION LABORATORY

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Recently, ion acceleration based on ultra-intense lasers has been advancing rapidly due to the dramatic progress of laser technology capable of delivering higher power laser pulses. Research and development in the firle dof laser-driven acceleration is shifting from pure scientific exploration to practical applications. In this scenario, the accelerating process known as Target Normal Sheath Acceleration (TNSA) represents a robust mechanism to accelerate light ions from laser interaction with thin foil targets [1].

An overview is given about the ion acceleration activities ongoing at the Intense Laser Irradiation Laboratory within the TNSA regime [2].

The activity with the 200 TW laser bean line aims at establishing a beam-line of > 10 MeV protons to be coupled with a beam transport line that will provide an advanced test facility for the development and exploitation of laser-driven ion sources [3].

The 10 TW laser beam-line is designed to serve as an R&D platform for the assessment and development of a compact few MeV proton beam-line for proton irradiation in *ambient air,* e.g., to perform Particle Induces X-ray Emission (PIXE) and to produce single-dose specific amounts of

radioactive isotopes for biomedical imaging within suitably devised integrated high-yield microfluidic-based setups.
The description of the main components of the system is given, including the laser source, the beam transport line, the interaction chambers, and the diagnostics. The main results obtained so far are reported, including details of the laser-plasma interaction and ion beam characterization.

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#102 - LASER INDUCED BREAKDOWN SPECTROSCOPY AS A TOOL FOR IN-SITU CULTURAL HERITAGE APPLICATIONS: FROM PORTABLE TO HANDHELD INSTRUMENTATIONS

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Other Authors: Giorgio S. Senesi (CNR Istituto per la Scienza e Tecnologia dei Plasmi)

Over the last years mobile Laser Induced Breakdown Spectroscopy (LIBS) instrumentations have been developed and improved for *in-situ* cultural heritage investigations. LIBS offers many competitive features for the analysis of cultural heritage objects such as simultaneous multi-element analysis under atmospheric conditions in a very short time, micro-invasiveness, simplicity of instrumentation, almost no sample preparation, and no restriction of sample shape and size. Most artifacts are unique and precious, thus non-invasive techniques are required for analytical purposes. Further, some of them cannot be transferred to the analytical laboratory. This implies the need to dispose of mobile instruments for *in-situ* analysis.
As already well known, LIBS is a plasma-based atomic emission spectroscopy technique that permits rapid qualitative and quantitative multi-elemental analysis. It relies on ablating and evaporating a material by focusing the radiation from a pulsed laser onto the surface of the target so forming a hot plasma in which atoms and ions are excited and emit characteristic lines that can be analyzed spectroscopically. Thus, elemental information can be obtained via specific atomic or ionic transitions and associated emanating photons[1]. LIBS spectra can provide quantitative information on the element concentration in the sample also, if a predictive model, i.e. a calibration curve, is constructed by plotting the peak intensities versus the known concentrations of standard materials.
A conventional LIBS equipment consists of a laser, a spectrometer, a number of lenses and optical fibers, a data acquisition system, and a control and synchronization system between the laser and the spectrometer.
Mobile LIBS instruments have shown a promising performance in micro-destructive, *in-situ*, multilayer diagnostic analysis and in-depth elemental profiling of encrustations and impurities even for highly inhomogeneous layered crusts prior to conservation treatments. Repetitive laser shots at the same spot can ablate a thin weathered (~100 mm thick) layer of the material so recording changes in composition as the underlying bulk material is approached. Handheld LIBS instrumentations recently introduced in the cultural heritage field[2] appear to be very promising for *in-situ* measurements on outdoor monuments, because of their capabilities (spectral ranges from ultraviolet to near-infrared, argon purging, rastering and portability) that rival traditional bench-top instruments.

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#103 - SOLAR PLASMA PHYSICS

Francesca Zuccarello (I) - University of Catania

The Sun, our closest star, can be considered a huge laboratory in which we can study a plasma characterized by temperatures in the range 10^3 – 10^7 K, as well as phenomena of interaction of the plasma with localized magnetic fields. This wide range of temperatures and the presence of magnetic fields, gives rise to a number of processes and phenomena that are currently studied by means of new generation telescopes (both ground-based and onboard of satellites), 3D magnetohydrodynamic simulations and models. The state-of-the-art of our knowledge of these processes and how this knowledge might be improved in the next decades will be described.

#104 - PROTON-PROTON COLLISIONS IN TURBULENT WEAKLY-COLLISIONAL PLASMAS: HYBRID BOLTZMANN-MAXWELL SIMULATIONS

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The mechanism of heating for hot, dilute and turbulent plasmas represents a long-standing problem in space physics, whose implications concern both near-Earth environments and astrophysical systems. The energy injected at large scales as gradients is transferred to increasingly larger wave-vectors, producing smaller scale fluctuations - as in typical turbulence processes. Plasma vortices and magnetic coherent structures are routinely recovered in space and astrophysical plasma measurements and observations support the standard picture of intermittent, inhomogeneous features of the turbulent cascade. When the turbulent cascade reaches these small spatial and temporal scales, the energy associated with fields fluctuations can be transferred to the particle velocity distribution function, where it is eventually dissipated. Significant efforts have been devoted to understand plasma dynamics at such scales and different dissipation mechanisms have been invoked. Several of the proposed heating mechanisms explicitly neglect the role of inter-particle collisions. Despite collisions are usually ruled out from the description of these systems, it has been recently shown that plasma collisionality may be locally enhanced by the presence of fine structures in velocity space.

Here, in order to explore the possible role of inter-particle collisions, collisional and collisionless simulations of plasma turbulence have been compared using Eulerian Hybrid Boltzmann-Maxwell simulations, that explicitly model the proton-proton collisions through the nonlinear Dougherty operator. Although collisions do not significantly influence the statistical characteristics of the turbulence, they strongly suppress the production of non-thermal features in the proton distribution function. The latter consists in a suppression of the enstrophy/entropy cascade in the velocity space, damping the spectral transfer towards large Hermite modes. Moreover, we observe that dissipation is located within regions of strong current activity, confirming that the heating process in turbulent plasmas is spatially inhomogeneous.

#105 - VALIDATION OF RADIATION-HYDRODYNAMIC CODE DUED USING HIGH-PRECISION OMEGA AND NIF EXPERIMENTS ON EXPLODING PUSHER IMPLOSIONS

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Exploding pusher targets, i.e. gas-filled, large aspect-ratio shells, driven by a strong laser-generated shock, are widely used as pulsed sources of neutrons and fast charged particles. Due to small convergence ratio, exploding pushers are little affected by fluid instabilities and are weakly sensitive to irradiation nonuniformities. Development of high space- and time-resolution neutron and X-ray diagnostics allows for detailed comparison of experimental data with simulations, and for validation of simulation models. In particular, we refer to simulations with the DUED code of a series of direct-drive experiments performed at the OMEGA laser (reported in Refs [1, 2], and others currently being analyzed) and two indirect-drive NIF shots [3]. Comparisons provided evidence for the transition from a nearly fluid behaviour to a kinetic one, as the implosion Knudsen number Kn (ratio of ion mean-free path to compressed gas radius) becomes comparable or larger than one [1]. Agreement between predicted and measured observables worsens as Kn grows. Ion separation effects occur also for Kn < 1, i.e. in a quasi-hydrodynamic regime [2]. Here we show that in the quasi-hydrodynamic limit simula- tions reproduce DD and DT reaction yields, bang times, burn-widths, burn radii, compressed fuel radius, reaction-averaged ion temperatures. (For gas fills also containing 3He, the delay between D-3He bang time, instead, is not predicted.) Instrumental to the achievement of such an agreement was the introduction of ion viscosity, of a smooth transition between ion viscosity and artificial viscosity, of an appropriate limiter for momentum flux, of bulk fluid motion in the Monte Carlo neutron synthetic diagnostics.

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#106 - AB INITIO PLASMONICS OF EXTERNALLY DOPED SILICON NANOCRYSTALS

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Heavily doped semiconductor nanocrystals (NCs) represent a novel class of plasmonic materials with different applications in nanoscience and nanotechnology [1]. In particular, their localized surface plasmon resonance (LSPR) can be tuned, by static or dynamical doping [2], in the near-infrared region (NIR). The plasmonic properties of doped semiconductor NCs have been mainly modeled using (semi)classical theoretical approaches [1,3,4], in contrast to conventional metallic NCs for which ab initio plasmonics based on Time-Dependent Density Functional Theory (TD-DFT) calculations have now become the standard reference. In this work, we report atomistic first-principles TD-DFT calculations of the externally doped silicon semiconductor NCs [5]. Silicon has been chosen as a model semiconductor and due to recent investigations in which silicon has been proposed for plasmonics [6]. We have considered spherical NCs of different sizes (up to a diameter of 2.4 nm) embedded into an external polarizable medium. Results show the presence of a plasmon peak in the NIR with an intensity increasing with the number of excess electrons. We use the recently proposed Generalized Plasmonicity Index [7], with a novel implementation and interpretation in terms of transition densities [5], to verify the plasmonic properties of this peak. Our analysis demonstrates that the peak in the NIR is a plasmon resonance, but it is strongly screened by the valence electrons. A detailed comparison between TD-DFT and classical results shows that the latter can be safely applied only for NCs with a diameter larger than 2 nm. The present TD-DFT results can also be used as a reference for other theoretical approaches that aim at modeling quantum effects beyond the classical regime in non-conventional plasmonic materials.

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#107 - REACHING CHEMICAL ACCURACY WITH A JASTROW SINGLE PFAFFIAN WAVE FUNCTION

Claudio Genovese - SISSA

Other Authors: Tomonori Shirakawa (SISSA), Sandro Sorella (SISSA)

Quantum Monte Carlo (QMC) indicates a family of simulation techniques that proved to be very effective for the study of the electronic correlation and that in the years have been successfully applied to electronic structure calculations.

Among these methods the Variational Monte Carlo (VMC) allows the sampling of a given wave function (WF) and the optimization of the total energy with respect to its variational parameters, yielding the best solution for the Schrödinger equation in the given ansatz. Moreover, the WF calculated in this way can also be used to perform the so called Diffusion Monte Carlo (DMC). This method provides a much more accurate solution of the Schrödinger equation, depending only on the quality of the WF nodes obtained with the VMC.

Unfortunately, until now, it has been very difficult to improve the WF and the corresponding nodes without increasing enormously the computational cost needed to sample and optimize the WF. For instance, the use of a linear combination of Slater determinant WFs (FCAS) can improve the quality of the solution, but the number of determinants that have to be taken into account scales exponentially with the size of the system.

The ideal goal is to find a WF ansatz that can describe accurately the exact solution maintaining a reasonable computational cost. I will show that the use of a generalized pairing function, known as Pfaffian, with a Jastrow factor allows us to reach an accuracy comparable to the multi determinant WFs with a computational cost similar to a QMC calculation of a single determinant.

#108 - STRUCTURE PREDICTIONS IN WET ENVIRONMENTS FOR ETHANOL AND WATER ADSORPTION ON ANATASE TIO2 (101) SURFACES

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Titanium dioxide exhibits superior photocatalytic properties, mainly occurring in liquid environments through molecular adsorptions and dissociations at the solid/liquid interface. The presence of these wet environments is often neglected when performing ab initio calculations for the interaction between the adsorbed molecules and the TiO2 surface. In this study we consider two solvents, i.e. water and ethanol, and show that the proper inclusion of the wet environment in the methodological scheme is fundamental for obtaining reliable results. Our calculations are based on structure predictions at a density functional theory level for molecules interacting with the anatase (101) surface under both vacuum and wet conditions. A soft-sphere implicit solvation model is used to describe the polar character of the two solvents. As a result, we find that surface oxygen vacancies become energetically favorable with respect to subsurface vacancies at the solid/liquid interface. Ethanol molecules are able to strongly passivate these vacancies, whereas water molecules only weakly interact with the (101) surface, allowing the coexistence of surface vacancy defects and adsorbed species. Infrared and photoluminescence spectra of anatase nanoparticles exposing predominantly (101) surfaces dispersed in water and ethanol support the predicted molecular-surface interactions, validating the whole computational paradigm. The combined analysis allows for a better interpretation of TiO2 processes in wet environments based on improved computational models with implicit solvation features.

#109 - DENSITY FUNCTIONAL PERTURBATION THEORY FOR LATTICE DYNAMICS WITH FULLY RELATIVISTIC ULTRASOFT PSEUDOPOTENTIALS: THE MAGNETIC CASE

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We extend density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials [1] to magnetic materials.

We avoid the computation of the response at **-q** by using explicitly the time-reversal operator and applying it to the Sternheimer linear system and to its self-consistent solutions.

Moreover, we discuss how to symmetrize the density and magnetization responses and the dynamical matrix including the symmetry operations of the magnetic point group which require the time-reversal operator. We validate our implementation by

comparison with the frozen phonon method in fcc Ni and in a monatomic ferromagnetic
Pt wire, and present an application to MnBi.

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#110 - MULTISCALE MODELING FOR MATERIALS SCIENCE APPLICATIONS

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Multiscale modeling is nowadays a general trend in computational physics and industrial mathematics, as it allows the numerical simulation of complex processes and phenomena that would be otherwise impossible to study solely by means of first principles methods. The basic idea is to approach a simplified problem through accurate calculations, extracting appropriate parameters that can be successively used to calibrate theoretical models that are computationally less demanding. Often, the atomistic mechanisms and related parameters are investigated and calculated accurately in the quantum framework of the Density Functional Theory (DFT) and/or within DFT-based Molecular Dynamics (MD). Such ab initio approaches theoretically evaluate the atomic properties of materials specifying their constituents (atoms and electrons), without any relevant approximation. The basis of the predictability potential for the simplified models derives from the proper matching of the DFT/MD calculated “information” (e.g. material parameters, atomic configuration, migration/diffusion paths, energetics, electronic structure, etc.) to simplified simulation schemes. The calibrated approaches can then efficiently simulate large systems for long times, i.e. at the scales of interest for experiments. Here we will discuss examples from our studies for such coupled numerical techniques considering the case of low-dimensional materials and hybrid perovskites.

#111 - VAN DER WAALS INTERACTIONS IN DFT USING WANNIER FUNCTIONS WITHOUT EMPIRICAL PARAMETERS

Pier Luigi Silvestrelli - Universitá di Padova

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A new implementation is proposed for including van der Waals (vdW) interactions
in Density Functional Theory (DFT) using the Maximally-Localized Wannier
functions (MLWFs), which is free from empirical parameters.
With respect to the previous DFT/vdW-WF2 method, in the
present DFT/vdW-WF2-x approach, the empirical, short-range, damping
function is replaced by an estimate of the Pauli exchange repulsion,
also obtained by the MLWFs properties.
Applications to systems contained in
the popular S22 molecular database and to the case of an Ar atom interacting
with graphite, and comparison with reference data,
indicate that the new method, besides being more physically founded,
also leads to a systematic improvement in the description
of vdW-bonded systems.

#112 - AB INITIO MODELING OF TRANSITION METAL COMPOUNDS USING THE EXTENDED DFT+U+V WITH SELF-CONSISTENT HUBBARD PARAMETERS

Matteo Cococcioni - University of Pavia

Transition-metal compounds are central in many applications of unquestionable technological relevance as, for example, catalysis and photo-catalysis, rechargeable batteries, photovoltaics, advanced electronics, spintronics, superconductivity.

For the first-principles modeling of these materials to be quantitatively predictive the localization of valence electrons on atomic-like states (e.g., of d or f shells) must be captured under various conditions. While most approximate exchange-correlation (xc) functionals used in actual implementations of density-functional theory are unreliable for the modeling of these materials because of the over-delocalization of valence states, several corrective schemes have been developed to improve the description of localized and possibly correlated electrons.

In this talk I will show how a simple additive correction of approximate xc functionals, based on the extended Hubbard model with on-site (U) and inter-site (V) interactions (named DFT+U+V), offers the necessary flexibility to capture electronic localization in a broad variety of different systems, most notably those characterized by significant hybridization. As an example of application I will discuss materials for cathodes of Li-ion batteries and I will show how this approach stabilizes mixed-valence ground states during the charge and discharge transients of the devices (i.e. at intermediate Li concentrations). In particular, I will show that it predicts a digital variation of the oxidation state of transition-metal ions that proves crucial to reliably evaluate the energetic balance of the process (in particular, the average voltage) for a broad range of various systems. Highlighting the importance of computing the effective interactions (U and V) self-consistently for quantitative predictions on several properties, I will also present a new linear-response approach to calculate their value that, based on density-functional perturbation theory with monochromatic (wave-length-specific) perturbations, allows for a significant reduction of computational costs and for a notable improvement of the level of automation.

#113 - MULTIPLE PATHWAYS AND MORPHOLOGIES IN PROTEIN SELF-ASSEMBLY

Vito Fodera' (I) - University of Copenhagen

Deposits of protein aggregates, often appearing as fibrils, are associated with the onset of pathologies such as Alzheimer´s and Parkinson´s diseases. Equally important is the impact that protein aggregates may have on the quality of a protein drug product. Finally yet importantly, protein aggregates have unique structural, physico-chemical and mechanical properties, making them appealing bio-inspired materials for applications. Either one looks at protein aggregation in the context of diseases, drug development or biomaterials, understanding how protein-protein (PPIs) and protein-solvent interactions (PSIs) determine self-assembly kinetics and morphology of the aggregates is a *conditio sine qua non* to unravel the mechanisms ruling the self-assembly reaction.

In our group, we have reported the possibility for a large number of proteins to form a variety of protein aggregates, not limited to amyloid fibrils [1]. I will present our approach based on advanced fluorescence microscopy, small angle X-ray scattering and spectroscopy and aimed at identifying the key interactions responsible for such variability in structures and morphologies [2-6]. We use surfactants, salts, alcohols in bulk and microfluidic setups to finely tune the interactions between proteins and, consequently, control the self-assembly process. Our results show that subtle changes in the PPIs and PSIs do not only affect the kinetics, but they may also have a dramatic effect on the 3D arrangement, microscopic structures, mechanical properties and stability of the final species. Our findings provide a scenario in which a pool of heterogeneous structures can be generated as a result of interconnected aggregation pathways, being this aspect of key relevance for a deeper understanding of the generalized protein energy landscape as well as for the design of protein tailored materials.

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#114 - BIOPHYSICAL EXPERIMENTAL TOOLS FOR THE STRUCTURAL CHARACTERISATION OF EXTRACELLULAR VESICLES (EVS)

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Extracellular vesicles (EVs) are nanometer-sized particles secreted from different cell types and operating as potent signal transducers and cell-cell communicators. Also, their bioavailability and stability, along with their mild toxicity and immunogenicity, make them exploitable as nano-delivery systems with targeted cellular uptake.

Within the VES4US project (funded by the Horizon 2020-Future and Emerging Technology Open programme, under grant agreement No 801338) we aim to develop an innovative platform for the efficient production of extracellular vesicles (EVs) from a natural renewable biosource, and then use them as safe and efficient tailor-made nano-materials (https://ves4us.eu). We identified a natural

source to constitute a cost-effective and sustainable source of EVs and then we are optimising the experimental activities for harvesting, manipulating, storing, characterizing and treating EVs.
Here, we focus on the first basic step of our novel bioprocessing approach, that is an extensive characterisation of their structural properties. Specifically, combined experiments of Atomic Force Microscopy (AFM), Dynamic Light Scattering (DLS) and Nanoparticle Tracking Analysis (NTA), along with a dedicated analysis, are used to cope with the heterogeneity of such complex systems. Our effort is dedicated to the development of Standard Operating Procedures which may guide the characterisation of size distributions in EV sample and meet the minimal requirements for studies of EVs (MISEV).
Also, we show how the structural organization of the lipid bilayer of the nano-sized extracellular vesicle membrane may be determined by Small-Angle X-ray Scattering (SAXS) and Small-Angle Neutron Scattering (SANS). The combination of SAXS and SANS measurements on the same sample becomes crucial to clearly identify the structural features of the lipid belayer in such a complex and heterogeneous system.
Our study provides the means for a comprehensive structural characterization of EVs, which is expected to be crucial in the design of engineered vesicles to be employed in different field, such as nanomedicine, nutraceutics and cosmetics.

#115 - EXPLORING THE PH SENSITIVITY OF POLY(ALLYLAMINE) PHOSPHATE SUPRAMOLECULAR NANOCARRIERS FOR INTRACELLULAR SIRNA DELIVERY

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Silencing RNA (siRNA) technologies emerge as a promising therapeutic tool for the treatment of multiple diseases. An ideal nanocarrier (NC) for siRNAs should be stable at physiological pH and release siRNAs in acidic endosomal pH, fulfilling siRNA delivery only inside cells. Here, we show a novel application of polyamine phosphate NCs (PANs) based on their capacity to load negatively charged nucleic acids and their pH stability. PANs are fabricated by complexation of phosphate anions from phosphate buffer solution (PB) with the amine groups of poly(allylamine) hydrochloride, as carriers for siRNAs. Their assembly is driven by electrostatic and hydrogen bonding interactions between the positively charged amine groups of the polyamines and the negatively charged phosphate ions. From Transmission Electron Microscopy (TEM) and Dynamic Light Scattering (DLS) the critical PB concentration for PANs formation was determined. Below this critical point, Small Angle X-ray Scattering (SAXS) studies revealed that small PAH-phosphate aggregates coexist with not complexed or weakly complexed polymer chains in solution and that the presence of the phosphate ions increases the Kuhn length of the polymer chains until that only spherical aggregates are present in solution. PANs are stable in a narrow pH interval from 7 to 9, and that they disassembly at pHs higher than 9 and lower than 6. We show that the formation of complexes is particularly suitable for encapsulating and delivering siRNAs. NCs with encapsulated siRNAs are stable in cell media without disassembling. Once internalized in cells, following endocytic pathways, the NCs will not be any longer stable and disassembly at the low endosomal pH releasing the siRNA into the cytosol. The efficacy of this approach is shown for the silencing of the Green Fluorescence Protein (GFP) protein in the GFP-A549 cell line. Confocal Laser Scanning Microscopy (CLSM) experiments using Green rhodamine labelled PANs (GR-PANs) and Cy3-labelled siRNA show from co-localization experiments that siRNAs are released from the PANs. Co-localization experiments with labelled endosomes and either labelled PANs or siRNAs prove the translocation of PANs and siRNAs into the cytosol. As a proof of concept, it is shown that PANs with encapsulated green fluorescence protein (GFP) siRNAs are able to silence GFP in A549 cells expressing this protein. Silencing efficacy was evaluated by flow cytometry, CLSM and western blot assay. These results open the way for the use of poly(allylamine) phosphate nanocarriers for the intracellular delivery of genetic materials.

#116 - HIGHLY TUNABLE PROTEIN MICROSPHERES FOR DRUG DELIVERY

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It is well-known that protein amyloid aggregation has profound implications in several neurodegenerative diseases. In contrast, a natural role for amyloid structures as protection, adhesion and storage materials in living system is also reported, promoting protein aggregates as an interesting platform for the design of multifunctional biomaterials. Among the broad range of different amyloid structures protein particulates deserve special attention; they are spherical protein aggregates with radius ranging from hundreds of nm to few um which are readily formed in solution at pHs values near the isoelectric point of the protein they are made of. Interestingly, particulate appears to be a generic aggregation state for globular proteins and they are not related to any disease. Moreover, they can be produced from easily available and low-cost proteins. All this makes these microspheres a good candidate for different applications as biomaterials.

Here we present an experimental study in which particulates are formed from alpha-lactalbumin, a well-known model protein from bovine milk. Microparticles with modified ability of uptaking small molecules or with modified surface layers can be created allowing material functionalization without using complex chemical procedures. Using a combination of bulk spectroscopies and quantitative fluorescence microscopy methods, we highlighted particulates features both at the level of the structure and size as well as their stability and capability to load molecules. These features can be tuned by modifying solution conditions. Our results show how general laws regulating protein macromolecular assembly can be exploited to create a platform for the development of a new generation of biocompatible materials for drug delivery.

#117 - POLYVINYLPYRROLIDONE/HYALURONIC ACID-BASED BILAYER CONSTRUCT: A MULTIFUNCTIONAL WOUND DRESSING

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Wound healing is a complex succession of biological events divided into 4 phases: hemostasis (0 h after the injury), inflammation (1-3 days), proliferation (4-21 days), and remodeling (21 days – 1 year). Sometimes this process can be interrupted due to bacterial infections or particular physiological states such as diabetes, leading to a chronic and non-healing condition. The management of wound repairing is considered an immense social and financial burden for society and affects the quality of life of over 20 million people worldwide. Therefore, the development of new, inexpensive and intelligent wound dressings that can ensure effective protection and elimination of bacterial colonization of the wound, and at the same time the tissue regeneration is still an imminent needed and a great challenge.

Here, we present the fabrication of a transparent multifunctional bilayer construct for the sequential release of a cutaneous antiseptic and a widely used antibiotic, with anti-inflammatory and regenerative properties potentially suitable for wound healing applications. The polyvinylpyrrolidone/hyaluronic acid-based material was fabricated using a scalable waterborne and eco-friendly solution casting process. The obtained construct showed satisfactory self-adhering strength to human skin and a sustained release of the antibiotic over a period of 5 days. The bilayer resulted in being biocompatible, hemocompatible, and active against *Staphylococcus aureus*, *Escherichia coli,* and *Pseudomonas aeruginosa*. *In vivo* tests demonstrated its capacity to be completely resorbed by the wound, reduce the levels of inflammatory mediators such as TNF-α, IL-6, and IL-1β and accelerate the healing process.

#118 - HIGH-DENSITY ZNO NANOWIRES FOR CELLULAR BIOINTERFACES: A NEW ROLE AS MYOGENIC DIFFERENTIATION SWITCH

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The design of artificial platforms for expanding undifferentiated stem cells is of tremendous importance for regenerative medicine [1]. We have recently demonstrated that a ZnO nanowires (NWs) decorated glass support permits to obtain a differentiation switch during proliferation for mesoangioblasts (MABs)– i.e. multipotent progenitor cells which are remarkable candidates for the therapy of muscle diseases [2]. We have optimized the ZnO NWs synthesis on glass surfaces by numerical simulations and experimental systematic investigations, considering zinc speciation and supersaturation [3]. In particular, we demonstrated by numerical simulations that the ligand ethylenediamine, at the isoelectric point of the ZnO NWs tips, can effectively control – at 1:1 stoichiometric ratio with zinc – both speciation and supersaturation of zinc in the nutrient solution. In this regard, we employed ethanolamine (a safer precursor) for ***in-situ*** producing ethylenediamine by means of a zinc-catalysed amination reaction of ethanolamine by ammonia. The obtained high-quality ZnONWs-cells biointerface allows cells to maintain viability and a spherical viable undifferentiated state during the 8 days observation time. Simulations of the interface by theoretical models [4] and our experimental investigations by SEM and confocal microscopy demonstrate that NWs do not induce any damage on the cellular membrane, whilst blocking their differentiation. More specifically, the myosin heavy chain, typically expressed in differentiated myogenic progenitors, is completely absent. Interestingly, the differentiation capabilities are completely restored upon cell removal from the NW-functionalized substrate and regrowing onto a standard culture glass dish. These results open the way towards unprecedented applications of ZnO NWs for cell-based therapy and tissue engineering [5].

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#119 - COMPETITION AND COOPERATIVITY IN THE SIMULTANEOUS BINDING OF DRUGS AND FATTY ACIDS TO ALBUMIN

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Human serum albumin binds a wide variety of drugs with different structure and affinity and accommodates them into two main binding sites, drug site I (DS1) and drug site II (DS2), which partially or totally overlap with fatty acid (FA) sites. Although multiple binding sites are available for endogenous compounds, fatty acids are the primary physiological ligands of albumin and their competition in the occupancy of sites DS1 and DS2 affects the binding of exogenous molecules, with a possible impact on drug delivery.

In this work we have investigated the consequences on the dynamics and thermal stability of albumin due to the simultaneous binding of ibuprofen, warfarin and palmitic acid, under both physiological and denaturing conditions, by using a combination of experimental and computational methods. The two drugs are widely used for their anti-inflammatory (ibuprofen) and anticoagulant (warfarin) effects, and can be also considered as model compounds to probe site DS2 and DS1, respectively. Palmitic acid is the most important fatty acid from a physiological point of view, and also the one with the highest binding affinity.

The results show that both drugs induce a higher thermal stability of albumin, with a domain-specific effect on the protein lobe where each corresponding binding site is located. Such local stabilization extends on the global protein dynamics, and may have a dominant enthalpic or entropic character depending on specific features of the drug. In the presence of palmitic acid, the calorimetric profile of albumin shows a biphasic trend with a lineshape depending on ligand concentration. Palmitic acid increases the binding capacity of both drugs, indicating a synergic cooperative influence due to allosteric effects. The overall results provide insights on the dynamics of the albumin/ligands complex, and on the effects of the presence of fatty acids on the drug binding capacity of the protein, which in turn has important pharmacokinetic and pharmacodynamic implications.

#120 - NEW DEVELOPMENTS IN ACCELERATOR BASED ANALYTICAL TECHNIQUES AT CEDAD

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Accelerator based analytical techniques have shown nowadays their potential in cultural heritage diagnostics, in particular AMS (accelerator Mass Spectrometry) radiocarbon dating and IBA (Ion Beam Analysis) methods. We review in this paper recent instrumental developments and case studies at CEDAD (Centre for Applied Physics, Dating and Diagnostics) at the University of Salento. In particular we underline the potential of the combined use of AMS and IBA methods for the study of the same archaeological context or even object. Different case studies are reported spanning from the analysis of ancient bronze statues, the study of prehistoric contexts and the use of ^{14}C for dating non-standard sample material such as lead carbonate. The enormous potential resulting in cultural heritage studies from the use of the recently installed combined IRMS-AMS set-up is also presented. The performances of the system are reviewed showing how, in a single measurement run, carbon and nitrogen stable isotopic ratios and radiocarbon concentrations can be measured on the same sample with masses in the microgram range. We show the potential of this approach in the field of cultural heritage where the reduction of a factor 100 in the required mass is surely an enormous advantage in the analysis, for instance, of organic residues on ancient pottery, the analysis of precious objects and poorly preserved bones.

#121 - MACHINA THE PROJECT FOR A MOVABLE ACCELERATOR FOR CULTURAL HERITAGE IN-SITU NON-DESTRUCTIVE ANALYSIS

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We are facing a continuously increasing interest for of low-cost, compact, small footprint and possibly transportable systems able to produce MeV ion beams. This is a feature of great interest in many fields, such as for example material science, environmental studies and cultural heritage. For this last field, ***in-situ*** compositional analyses are of great interest, due to the large number of artworks that cannot be moved (owing to, for example, their weight, dimensions, value). Unfortunately, at present, Ion Beam Analysis (IBA) techniques, which can provide an insight into the structure of artworks, impossible to obtain with other techniques, are possible only in laboratory, as no transportable accelerator has been developed yet.

To overcome this limitation, the European Organization for Nuclear Research (CERN) and the Italian National Institute for Nuclear Physics (INFN) have jointly started the MACHINA project, dedicated to the development of a transportable accelerator system. The pillars of such a project are the competencies:

- developed at INFN-Labec, for external beam IBA studies in C.H. field,
- at CERN, concerning beam dynamics for a high frequency radiofrequency quadrupole cavity (HF-RFQ)
- both at CERN and at INFN-Labec, in the development, use and application of particle accelerators.

In this presentation, the current status of the MACHINA project after about one and half year from its beginning will be presented, together with the activity forecasted for the next months.

#122 - STATISTICAL APPROACH FOR ED DETERMINATION IN HISTORICAL MORTARS DATING

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The possibility of using mortars to evaluate the chronology of a historical building has been studied over the years and to date important results have been achieved in luminescence dating field. However, the study on the evaluation of the bleaching degree during mortar laying, which may affect the accuracy of the equivalent dose calculation, is still open. In this work, four mortars (IM1, IM6, IM7, IM9) were sampled from already dated “Terme dell’Indirizzo”, the best preserved thermal baths in the Roman Empire located in the historic center of the Catania (Italy). Bleaching degree was studied for quartz fractions of two different size extracted and measured in small aliquot through Optically Stimulated Luminescence (OSL). Equivalent Dose (ED) measurements on small aliquots of two different quartz fraction, inclusion (90 μm<Ø<150 μm) and coarse grain (180 μm<Ø<212 μm) quartz, were performed by optically stimulated luminescence and single aliquot regeneration procedure. In order to choose the more suitable age model to be used, the bleaching degree was studied through a deep statistical approach using ED frequency distribution, Q-Q plot and Shapiro-Wilk normality test. The results show that ED from coarse grain could be statistically associated to normal distribution and then Central Age Model (CAM) can be used for Archaelogical dose calculation; the quartz inclusion data not follow a normal distribution, and then Minimum Age Model (MAM) can be used. Archaelogical dose results obtained in two different cases were in good agreement with each other.

#123 - CLIMATE AND CULTURAL HERITAGE: THE CASE STUDY OF REAL SITO OF CARDITELLO

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In the last years monitoring campaigns, performed to understand the environmental pressure on an important archaeological site became always more important in order to assess the effects of atmospheric pollution and changes in the climate of the structure (outdoor site) and to evaluate the conditions of conservation and fruition of the artworks indoor rooms).

In the present paper, a case study has been realized at the monumental complex of the Real site of Carditello, which realization of started in 1787, when Ferdinando IV di Borbone entrusted the construction to Francesco Collecini (1724-1804), a pupil and collaborator of Luigi Vanvitelli.

In detail, the following parameters have been measured : i) Temperature, Humidity, NO2, SO2, Brightness (indoor room); ii) Temperature, Humidity, NO2, SO2, O3, PM, Rainfall, Anemometry, Visible and Ultraviolet Radiation (outdoor).

At the same time, non-invasive and non-destructive investigations were carried out to: (i) identify constituent, restoration and/or degradation materials belonging to the wall paintings on the main floor; (ii) assess their conservation state under the current environmental conditions detected during the monitoring phase.

The results obtained from the environmental monitoring campaign provide parameters values within the regulatory thresholds, even if the area in which the historical site is located has undergone significant anthropic impacts over time .

The in-situ investigations (IR thermography, infrared reflectography, UV fluorescence, X-ray fluorescence) have been aimed to identify the pigments, the execution technique and to evaluate previous degradations or alteration persistent causes. Chemical markers allowed to date in an indirectly way the restoration works carried out during the nineteenth and twentieth centuries as a result of damage suffered during insurrections and war events. The imaging techniques have localized the retouching or remake and detachments areas on the analyzed painted surfaces, providing a useful support for future consolidation operations. All information are reported in a web platformand has been acquired by the guides who, during the visits, illustrate to visitors the scientific results to confirm the historical retrace of the wall paintings.

The research were carried out in the context of the project "Innovative methods and technologies for the conservation, valorisation and use of cultural heritage: environmental and archaeological analyses", within the CULTURA CREA program (MIBACT), which goal is to implement innovative services for the knowledge, conservation and enhancement of cultural heritage, through environmental and archaeometric analyses.

#124 - “GREEN” SENSING ELEMENT BASED ON BACTERIAL CELLULOSE

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Green sensors and transducers represent an emerging research area that regards the development of devices based on new materials and innovative technologies. The main aim is obtaining systems having the prerogatives of being: eco-friendly, bio-compatible [1,2], recyclable, environmentally safe, and biodegradable. In this context, recently, we started investigating the possibility of Bacterial Cellulose (BC) as a suitable compound for realizing green sensors [3,4]. BC is a substitute of plant-derived cellulose and it presents the advantage to be much more eco-friendly and green, in particular, during the realization and the purification process, as respect the classical cellulose. In literature, manuscripts are available demonstrating the properties of mechano-electric transduction of this family of compounds, however the field of sensor based on BC is somehow new and few papers started to appear in the scientific community [5]. In particular, BC with Ionic Liquids (ILs) and polymeric electrodes has been investigated to realize mass and deformation sensors [3,4].

In order to study the sensing properties of the composite, the following setup has been used: a shaker, to mechanically excite the cantilever-structure, a signal generator to drive the shaker, an oscilloscope, for data acquiring and two laser sensors, used to measure the displacement of the sensor at the tip and at the anchor. For the validation of the sensing principle, several different mechanical excitations have been applied and various analyses have been pursued. In particular the output FFT of the sensor for several applied sinusoidal waveforms has been investigated and it shows the resonant frequency of the BC beam and, in accordance with the theory [4], the spike decreases in frequency when the device is driven by frequencies different as respect its mechanical resonant frequency. The analysis in terms of step response shows that in correspondence of a tip displacement of about 1.5 cm, an output voltage of about 2 mV has been obtained. The work is in progress for an exhaustive characterization of BC-based transducer, its features and novel applications and measurement systems also in the field of cultural heritage.

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#125 - SUPERHYDROPHOBIC TIO2-FLUORINATED POLYSILOXANE NANOCOMPOSITES WITH PHOTOCATALYTIC CLEANING ACTIVITY FOR CULTURAL HERITAGE APPLICATIONS

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Superhydrophobic surfaces with a water contact angle (CA) greater than 140° attracted tremendous attention for researchers because of its great importance in fundamental research, as well as its potential in cultural heritage applications as consolidants and/or protective materials [1]. Herein, we report a simple method for fabricating fluorinated polysiloxane/metal oxide nanocomposite coatings. In particular, the copolymer matrix was realized from hydride terminated polysiloxane with silane coupling agent 1H,1H,2H,2H-perfluorooctyltriethoxysilane via dehydrocoupling and hydrosilylation reactions, followed by mixing with TiO_2 nanoparticles and coating formation [2], [3]. Their structure was exhaustively characterized by FTIR, NMR, XPS, AFM and contact angle measurements. The results show that 0.5% loading of TiO_2 led to the formation of superhydrophobic surfaces with a contact angle increasing up to 140° from 110° for undoped systems. In addition, the photocatalytic activity of the coated surfaces was investigated by observing the degradation of the methylene blue dye (MB). The results showed that fluorinated nanocomposite films loaded with TiO_2 nanoparticles exhibit high photodegradation activity when irradiated by UV light. In particular, a 5 fold increase of the photocatalytic efficiency in the degradation of MB was observed when 35 % of TiO_2 was loaded to fluorinated polysiloxanes. By employing doped TiO_2 the photocatalytic process can be activated by visible light, thus offering an effective strategy for self-cleaning consolidant and protective smart nanocomposites. We are actually employing these materials for cultural heritage applications, especially by natural lapideous systems. The project AGM4CuHe (ARS01_00697, PON R&I 2014-2020) is acknowledged for funding.

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#126 - PRELIMINARY ASSESSMENT OF THE USE OF A GREEN NANOMATERIAL FOR POLYCHROME PAINTINGS CONSERVATION

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In last years, interest is growing in the production and use of new materials in cultural heritage conservation. Many products with different characteristics were developed for removing dust films from the surfaces of paintings and for providing effective cleaning tools. The material must be easily controllable by reducing the solvent permeation into underlying paint layers and not dangerous for human health and the environment. This contribution is related to a research activity aimed to assess new nanomaterials alternative to traditional restoration treatment towards artefact, operators and environment.In this occasion, we present a preliminary study regarding the application on easel paintings of a material constituted by nano-titaniato test its self-cleaning performances. The nanostructured material was obtained by Pulsed Laser Ablation in Liquids (PLAL) that represents a versatile, economical and “green” methodology that avoids the use of chemical reagents and reaction products, solving the problem of purification of nanomaterials. The prepared nanostructured coating is water-based and the dispersed titania particles have dimensions of about 40 nm. In order to test this coating, painting substrates are prepared in laboratory using the most used historical vehicles and pigments according to old recipes. The pigments selected for the study are documented in the historical fonts and in restoration manuals. The paints were prepared mixing the pigments with wet medium with a fixed ratio. The binary mixtures were mixed with egg tempera, siccative oil and casein. After brushing application on samples of the TiO_2 based nanomaterial, the hydrophobic/hydrophilic features were assessed through contact angle measurements and water absorption tests carried out on uncoated and coated samples. Then, SEM on stratigraphic sections and spectrophotometric analyses were carried out in order to highlight the penetration depth of treatments, the interaction between products and substrates and to identify the chemical-physical and chromatic modifications induced by coating application. For evaluating the efficiency in terms of cleaning performance of the TiO_2 based nanomaterial, the samples are dusted and they are subjected to UV irradiation cycles at different times in cabinet light. The cleaning efficiency is evaluated by spectrophotometric analysis with attention to the colorimetric coordinates and optical modification occurring before and after the cleaning procedure.

#127 - NANOMATERIALS AND POLYMERIC NANOCOMPOSITES FOR WATER PURIFICATION APPLICATIONS

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In the last decades the development of efficient and ecologically-friendly methods to remove contaminants from water has become of fundamental importance, since pollution is increasing drastically. Recent advances in nanotechnology suggest that many of the issues involving water quality could be resolved using nanoparticles, nanofiltration or other products resulting from the development of nanotechnology. Among the different nanomaterials, carbon nanostructures and metal oxides nanostructures provide an interesting example of materials suitable for water remediation processes.Several papers in the literature show the use of TiO_2 powder, carbon nanomaterials or a combination of both, dispersed directly in the solution that is going to be treated. After the photocatalytic process, the photocatalysts have to be removed from water by means of processes not always easy and fast to be carried out, and, furthermore, they cannot be easily used again. A possible solution to get rid of this problem is to incorporate the photocatalytic nanoparticles in polymeric membranes, that can be removed from water, regenerated and used again several times. In this presentation an overview of nanomaterials useful for water pollutants removal (i.e. organic contaminants, bacteria) will be given, with particular attention to graphene oxide, reduced graphene oxide, titanium dioxide and bismuth oxide. The preparation and characterization of nanocomposites based on the incorporation of nanomaterials into suitable sulfonated polymers will be discussed. Finally, the adsorption ability and the photocatalytic and antibacterial properties of nanomaterials and nanocomposites will be described and compared, highlighting pros and cons for each kind of material.

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#128 - ALL-POLYMER PLANAR PHOTONIC CRYSTALS AS AN INNOVATIVE TOOL FOR THE ANALYSIS OF AIR

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Polymer distributed Bragg reflectors (DBRs) are gaining attention thanks to mass fabrication technologies, lightweight, and flexibility unconceivable with other photonic structures.[1]They are indeed increasingly studied for lasing,[2]fluorescence enhancement,[3-5]and optical switching.[6,7]Moreover, their easy assimilation with packaging fabrication technologies[8]makes them interesting integrated transductors for barrier polymers employed in smart packaging and in the encapsulation of moisture-sensitive devices.

We demonstrates that, in polymer DBR structures, the intercalation of molecular pollutants occurs with characteristic kinetics ruled by the chemico-physical interaction between polymer and analytes.[9-11] Then, the kinetics of the DBR optical response allows to discriminate the pollutant and their environmental concentration without using any chemical target. Moreover, it also permits to assess ***in-situ*** the analyte diffusion parameters within the polymers. Such effects consents to esteem diffusivity and allows simple colorimetric selective label-free transductors of a variety of pollutants.

Because of the available DBR mass-scale fabrications and integration with packaging,[12] we believe that this method will be industrially relevant both for environmental monitoring and for the ***in-situ*** assessment of diffusive process of degradation by-products, humidity or even oxygen in smart packaging for foods and optoelectronic devices.

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#129 - MOLECULAR IMPRINTING OF TIO2 PHOTOCATALYSTS FOR THE SELECTIVE DEGRADATION OF PESTICIDES FROM WATER

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The selective oxidation of high-toxic pollutants is a challenging issue in TiO_2-based photocatalysis. Indeed, water effluents usually contain low concentrations of dangerous compounds (as pesticides), together with high concentrations of less-toxic substances which are preferentially degraded with conventional photocatalysis. In this work we report a fascinating approach, based on the combination of the molecular imprinting process, used to obtain the selectivity towards a specific pesticide, with the photocatalytic process, used to degrade that specific compound. The TiO_2 photocatalysts were imprinted without using any organic or inorganic matrix, thus avoiding a multistep procedure and easing the materials synthesis. The chemical-physical properties of the TiO_2 photocatalysts were assessed by various characterization techniques (SEM, XRD, FTIR, N_2 adsorption-desorption measurements), while the photo-activity was evaluated both under UV than solar irradiation. Moreover, the non-toxicity of the investigated materials has been demonstrated through biological tests. The remarkable increase of the photocatalytic activity of the imprinted samples with the corresponding pesticides-targets compared to bare TiO_2 highlighted the synergism between the molecular imprinting and the photocatalysis process. The good performance of the molecularly imprinted TiO_2 materials allows to consider this strategy an efficient method to obtain a selective photocatalytic process.

#130 - SOLVENT EFFECT ON LASER TREATED TIO2 NANOPARTICLES FOR ENHANCED PHOTOCATALYTIC ACTIVITY

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In the recent years, the laser irradiation process has shown to be a simple, efficient, low cost and ecofriendly method for semiconductors engineering. Varying the laser irradiation process parameters is possible to specifically change the dimension, morphology, crystalline phase and chemical structure of semiconductors as titanium dioxide (TiO_2). In the last years, photocatalysis with TiO_2 was applied successfully to several processes, including hydrogen production via water splitting and decomposition of organic pollutants in water. The efficiency of these processes depends on the morphology and the chemical, electronic and crystalline structure of titania. Many investigations have demonstrated that Ti^{3+}-containing (blue) TiO_2nanoparticles, possessing oxygen vacancies, exhibit significant photocatalytic activity in the visible and UV regions. Solvents, used for dispersion of nanoparticles, can be chemi- or physi-sorbed on these defects affecting the resulting reactivity of Titania. In this work, the interaction of dispersing medium (water or ethanol) with Titania nanoparticles surfaces was experimentally investigated by IR and photoluminescence spectroscopy and theoretically studied by structural simulations at Density Functional Theory level. Starting from these observations, titania colloids in water or ethanol were subjected to a laser irradiation process by using nanosecond pulsed laser beams and the obtained chemical and structural modifications of colloids were correlated with experimental parameters (laser wavelength and fluence, irradiation time, dispersing medium, initial titania crystalline phase). During the laser irradiation, different modifications on the morphology, chemical, electronic and crystalline structure of titania colloids were induced by melting and solidification processes resulting in the formation of blue, sub-micrometer spherical titania particles. The morphology of the produced samples were investigated by electron microscopies; the chemical, crystalline and electronic structure of modified samples were analyzed by IR, microRamanand photoluminescence spectroscopy, respectively. Moreover, the effects of laser induced modifications on the photocatalytic activity of Titania colloids were measured by the amount of hydrogen produced by photocatalytic water splitting for laser modified Titania samples with respect to untreated samples.This enhancement was correlated to the laser irradiation process parameters. The as-developed strategy may open up a new avenue for designing and functionalizing semiconductors in order to enhance visible light absorption, to get band gap narrowing, and improve photocatalytic activity.

#131 - SELECTIVE PHOTODEGRADATION OF PARACETAMOL BY MOLECULARLY IMPRINTED ZNO NANONUTS

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One of the main limits of the traditional photocatalysts is the lack of selectivity. Indeed, when a photocatalyst is used to treat wastewater, the organic pollutants at high concentration are efficiently degraded, while pollutants at low concentration (often the most toxic ones) are removed with less efficiency. Therefore, nowadays photocatalysis-based technologies are striving to find a methodology able to selectively degrade specific contaminants. As valid solution, we propose here molecularly imprinted ZnO, through the chemical method of the co-precipitation. ZnO has been imprinted with one of the most diffused analgesic-antipyretic drugs: acetaminophen (commonly called “paracetamol”), today considered a dangerous emergent pollutant. The molecularly imprinted nanonuts have been deeply characterized and the interaction between ZnO and paracetamol has been elucidated. The photodegradation of paracetamol in aqueous solution has been demonstrated under UV light irradiation. The selectivity of the photodegradation process has been investigated thanks to the comparison with the degradation of methyl orange and phenol, other two common water pollutants.Imprinted ZnO nanonuts have shown a great affinity and selectivity for the paracetamol, being able to degrade all the paracetamol present in the solution in only three hours. The results demonstrate as the imprinting methodologies can be successfully applied to obtain highly selective photocatalytic material.

#132 - MECHANICAL COMPACTION OF MOF POWDERS: DEFINITION OF A FULLY PRESERVING TABLETING METHOD FOR CU-BTC.

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Metal–organic frameworks (MOFs) are a new class of microporous hybrid materials, characterized by high crystallinity, very high surface area and large pore volume [1]. Because of the huge number of possible combinations of metal clusters with organic linkers composing the frameworks, tens of thousands of different MOFs have been already successfully synthetized and then it is possible to find a large variety of physicochemical properties, resulting in a wide range of interesting potential applications [1]. In the last years MOFs are finally getting closer to being used in commercial applications. In fact, in 2016, the first commercial application of a MOF technology was announced [2]. However, the full accomplishment of this fundamental objective requires a tableting method of MOF powders, aimed to maximize their packing density, mechanical strength, stability in reactive environments and many other properties. In this context, a key role is played by Cu-BTC, as it is one of the most promising and studied MOF, also because of its commercial availability in powder form. Unfortunately, any previous attempt to compact powder of such MOF has failed, as the collapse of a large fraction of the pristine crystalline structure has been observed [3]. Here we prove that, contrary to all of those previous reports, tableting of Cu-BTC powders without any damage of the lattice is possible and easy to get if a new protocol is followed [4]. For the first time, this kind of investigation has been performed by taking advantage of the strong potentialities of the Electron Paramagnetic Resonance (EPR) spectroscopy [4]. Thanks to this approach, we were able to explore in details all the smallest changes induced in the paramagnetic paddle-wheel units by the application of a variable mechanical pressure on the material. Our study has also permitted us to unveil that water molecules adsorbed by the powdered sample before tableting is the main source of structural instability of Cu-BTC during compaction, and finally to establish a proper compaction protocol [4]. Our conclusions are also fully supported by the results obtained by Powder X-Ray Diffraction, water sorption isotherms, Thermogravimetric Analysis, Fourier-Transform Infrared Spectroscopy, and surface area estimation with the Brunauer–Emmett–Teller method: all the data proved that the tablet of Cu-BTC obtained by our protocol actually preserves the crystal structure and porosity of the pristine powders[4]. A morphological characterization has also been conducted using a combination of optical and Atomic Force Microscopies.

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#133 - TOWARDS ELECTRIC CONTROL OF MAGNETISM: MAGNETOELECTRIC COUPLING IN NANOSTRUCTURED MATERIALS

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In recent years, the possibility of controlling the magnetization of a thin film with an electric field has driven a tremendous research effort.[1] Unfortunately, the materials that display a natural magnetoelectric coupling, known as multiferroics, are scarce in nature and generally display weak ferromagnetic response.[2] The absence of multiferroics with the desired properties has pushed towards the investigation of heterostructures in which two components with different ferroic orders are coupled through an interface to obtain enhanced performances.[3] The most typical example of this process is represented by ferromagnetic films deposited onto ferroelectric substrates. Three main mechanisms are reported in literature as responsible of the interfacial magnetoelectric coupling: charge accumulation or depletion at the interface, strain-mediated effects and ion migration. In this contest, we will present studies in which the strain mediated effect give rise to magnetic transitions [3,4] and to huge change in the observed anisotropy [5]. For this reason, the strain mediated mechanism is nowadays regarded as the solution for new electronics with low power consumption. However, beside the well know and understood effect of the change of the lattice parameter we discover a new mechanism that influence the magnetic response of the ferromagnetic film in hybrid heterostructures: morphoelectric effect. This effect which was never reported until now and origins in the change of the ferroelectric substrates morphology as a function of the applied bias and this in turn affects the magnetic response of the ferromagnetic overlayer [6]. This observation paves the way to design new possible magnetoelectric devices with new functionalities.

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#134 - RASHBA SPIN-ORBIT COUPLING IN HOMOGENEOUS AND HETEROSTUCRURED NANOWIRES

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We use $\boldsymbol{k \cdot p}$ theory to estimate the Rashba spin-orbit coupling (SOC) in homogeneous and inhomoegeneous III-V semiconductor nanowires, and specifically investigate the gate control of SOC ensuing from symmetry and electron density modulation. This is a crucial aspect to engineer hybrid nano-devices supporting zero-mode Majorana states. Both low (linear SOC) and high (non-linear SOC) carrier density regimes are investigate. We show that in core-(multi-)shell nanowires specific interface-induced symmetry breaking results in stronger SOC with respect to homogeneous structures. We analyze recent experiments in light of our calculations and we expose wavefunction engineering strategies to enhance and control SOC [Appl. Phys. Lett. 114, 073102 (2019)].

#135 - ELECTROBURNED GRAPHENE AS ELECTRODE FOR ELECTRONIC AND OPTO-ELECTRONIC DEVICES

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In the last years, a wide variety of electronic and opto-electronic applications have been developed from molecular and organic materials and 2d-heterostructures. In this context, the integration of such materials in electrical circuits is still challenging, mainly due to small size and high contact resistance between those materials and the metals commonly used as electrodes.

In this framework, we present the implementation of graphene electrodes[1], obtained via the electroburning technique[2], in the realization of a novel concept of electronics and opto-electronic devices. With respect to traditional metal contacts, the use of graphene offers the advantages of low-dimensionality and affinity with other carbon-based structures.

Here we demonstrate a novel concept of device, where chemically-synthesized Graphene Nanoribbons (GNRs) are employed as the active channel and graphene as the electrodes[3]. GNRs are one-dimensional stripes of graphene, where quantum confinement can open a direct bandgap, the gap is greatly influenced by the lateral size of the ribbon. Via chemically precise synthesis it is possible grow GNRs of different with and structure, so with different electrical proprieties[4][5].

Firstly, we employed a continuous GNR layer as the device channel and graphene electrodes with gap sizes of few hundreds of nanometers, obtained by electron beam lithography. We demonstrate field-effect transistor devices with on/off current ratio as high as 10^4. These devices are particularly appealing for opto-electronic applications and light sensors, as we report photoresponsivity as high as 6 x 10^5 A/W in the visible-UV range orders of magnitude higher than pristine graphene[6].

Finally, we fabricate graphene electrodes separated by a gap of 10-50 nm, suitable to contact individual or few GNRs. We report a systematic study using GNR with different morphologies, corresponding to different electrical properties. We show that the electrical behavior of the devices is in qualitative agreement with the expected band-gap as calculated by theory[7].

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#136 - SYNTHESIS OF N-DOPED GRAPHENE FOAM BY CHEMICAL VAPOR DEPOSITION

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C-based materials cover a central role in the field of modern nanoelectronics, sensing and energy. In particular, graphene seems to be one of the most promising materials thanks to its many fascinating properties, such as giant electron mobility, extremely high thermal conductivity and extraordinary elasticity and stiffness.

Recently, a great attention has been focused to three dimensional (3D) graphene structures. Indeed, these 3D structures provide graphene-based materials with very high specific surface areas (~850m^2/g), strong mechanical strengths and fast mass and electron transport kinetics. All these properties make them interesting for applications in many fields where the available surface area plays a central role. In this contest, a proper doping of the surface can be challenging. Indeed, introducing dopants like nitrogen canbe used to induce a charge polarization in the carbon lattice, modifying its electronic properties and surface wettability, or to create anchoring sites for chemical reactions often used in organic chemistry to functionalized surfaces, enabling specific reactions and catalysis processes.

In this work we investigated the realization of 3D N-doped graphene foams by chemical vapor deposition on Ni foams used as templates. We used CH_4 and H_2 as gaseous precursors and NH_3 as N-doping source. The growth kinetics and mechanism was investigated as a function of the growth parameters, like growth temperature, gas fluxes and cooling rates, focusing the attention on the various steps of the CVD graphene growth process on Ni. The obtained samples were deeply investigated by scanning electron microscopy, X-ray photoelectron spectroscopy and Raman spectroscopy. The mechanism by which the nitrogen precursor decomposes in N atoms which rearrange into the carbon network is finally described.

This work represents an important result in the field of emerging heteroatom-doped graphene materials for new future fascinating applications in energy, photocatalysis or sensing.

*Keywords:*graphene, foam, nitrogen, doping, chemical vapor deposition

#137 - MICROWAVE ASSISTED TUNNELING IN HARD-WALL INAS/INP NANOWIRE QUANTUM DOTS

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Charge transport in Quantum Dots (QDs) depends on the tunneling process that, in turns, is related to the electron wavefunctions and ultimately to the shape and size of the QD. Tightly confined QDs defined in heterostructured InAs/InP nanowires[1] exhibit different tunneling regimes associated to the population of charge state with different axial quantum number. The application of microwaves in non-resonant conditions may affect the charge transport characteristics. In the multi-photon regime, both virtual states in the electrodes and excited states within the QD can contribute to assist the tunneling process.[2]

Here we investigate single-electron tunneling in hard-wall InP/InAs nanowires in the presence of an off-resonant microwave drive. For source-drain bias up to few mV, Coulomb diamonds spread with increasing intensity as a function of microwave power and they also present multiple current polarity reversals. This behavior can be modeled in terms of multi-photon processes and evidences features that depend on the type of QD orbitals involved in the tunneling process. In particular, we focused on a Coulomb peak located at the threshold between manifolds with different longitudinal quantum numbers. Here we studied the effects of the microwave field on both ground state (radial wavefunction) and excited state (axial wavefunction). The experimental results are supported by simulations, which have been carried out by means of a simple model that clearly accounts for the experimental trends.[3]

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#138 - ELECTROLYTE GATING OF III-V SEMICONDUCTOR NANOWIRE-BASED DEVICES: IONTRONICS FOR ENERGY HARVESTING

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The electrostatic control of semiconductor nanodevices by exploiting the field effect is ubiquitous in nanoscience and technology and traditionally follows the metal-oxide-semiconductor approach [1]. In parallel to the MOSFET approach, we have explored different routes for achieving higher degree of field-effect manipulation in nanoscale semiconductor devices. One routes envisions the use of metallic finger gates to exploit the quantum confined Stark effect. This allowed us to achieve full control of individual charge and spin degrees of freedom in nanowire quantum dot systems and to investigate the tunneling rates [2].

A second route, with a true paradigm change, envisions the use of soft-matter as the gate medium for applying impressively high static electric fields to semiconductors. This route exploits the way of *iontronics* to electrostatic gating, using the movement and arrangement of ions to build up an electric double layer that is the ultimate responsible for the electrostatic gating. Applied first to 2D materials, this approach is currently rising great promise for application also with other types of semiconductor nanostructures such as nanowires. Recently we proposed the use of ionic liquids as gate media for III-V semiconductor nanowire-based devices, demonstrating unprecedented gating efficiency and gate-induced change of the temperature behavior in the device [3]. We investigate the ionic liquid dynamics with atomistic simulations, correlating the hysteretic features to the microscopic parameters of the ionic liquid. Based on these results, we develop innovative device architectures exploiting the electric double layer gating for thermal management and energy harvesting at the nanoscale, towards the full benchmark of the thermoelectric figure of merit resorting to substrate-unbound nanowire-based device architectures [4].

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#139 - FARADAY-LIKE SCREENING BY TWO-DIMENSIONAL NANOMATERIALS: A SCALE-DEPENDENT TUNABLE EFFECT

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The modulation of electric fields by mono- or few-layer two-dimensional (2D) nanomaterials embodies a major challenge through vast technological areas, including 2D nanoscale electronics, ultrathin cable shielding, and nanostructured battery/supercapacitor electrodes. By a quantum-mechanical analysis of Faraday-like electrostatic screening due to diverse 2D nanolayers we demonstrate that electric field screening is triggered by charge response non-locality. The effective screening factor is not only influenced by average polarizability, but further exhibits non-trivial scalings with respect to surface distance: while ideal 2D metallic systems cause complete Faraday-cage screening, semi-metallic graphene yields a finite, roughly scale-independent field reduction factor. Conversely, screening by finite-gap MoS$_2$ appears most effective in the vicinity of the surface, gradually vanishing in the long-distance limit due to the intrinsic finiteness of the charge-response length scale. The variability of screening effects and of their scaling laws with respect to accessible physical parameters opens novel pathways for experimental modulation of electric fields, ionic interactions, and adsorption of charged/polar moieties.

#140 - ELECTROSPUN TRANSITION METAL OXIDE/CARBON FIBRES FOR WATER DESALINATION VIA CAPACITIVE DEIONISATION

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In the latest years, several water desalination methods have been developed in order to cope with the growing demand for freshwater. Among them, the capacitive de-ionization (CDI) is the most attractive one by virtue of its simplicity, efficiency, ecofriendliness and low operating voltage (0.8–1.2 V), which enables its use in remote areas.

Hierarchical porosity, large specific surface area, no secondary emission of contaminant agents, possibility to regenerate the electrode after its saturation, are the main requirements needed for the electrodes materials utilised to fabricate the CDI cell. Therefore, a great variety of nanocarbons (such as activated carbons, C nanotubes, electrospun C nanofibers, C aerogel and graphene) have been successfully employed as electrode materials in CDI cells. However, nanocarbons that store ions through electrostatic interactions at their surface generally exhibit limited salt adsorption capacities.

Very recently, it has been demonstrated that electrospun N-doped carbon fibres (N-CNFs with ~20 wt% of N) are able to remove relevant amounts of NaCl from a salty solution (17 mg/g for an initial concentration of 585 mg/L). The electrosorption capacity outstandingly increases (up to ~28 mg/g) if the N-CNFs are enriched with graphene (GN-CNFs) [1].

Transition metal oxides (TMOs) are redox-active materials featured by great abundance on earth, low cost and environmental friendliness. They store ions through the Faradic processes involving reversible redox reactions at or near to their surface and generally exhibit high capacitance.

Improved adsorption capacity is expected to derive from combining hierarchical porosity and large specific surface area of the (G)N-CNFs with high capacitance of the TMOs.

This contribution deals with the synthesis, via electrospinning, and the thorough characterisation, by means of several techniques, of hybrid TMO/(G)N-CNFs. Their morphology depends on the transition metal (Mn, Fe, Ti or Zn). Together with the relative amount of the surface species (N and C-bonded O) and the specific micropore volume,it has strong impact on the effective areal capacitance (1.2-6.0 F/m^2, at 5 mV/s) of the CDI electrodes. Since ion storage in the hybrid fibres occurs via a mixed capacitive/pseudocapacitive process, increasing their TMOcontent partly compensates for the growing hindrance to diffusion encountered by the ions as the scan rate increases from 5 to 100 mV/s.

[1] Y. Belaustegui et al, Desalination 428 (2018) 40.

#141 - NORMALLY-OFF GAN POWER DEVICE

Ferdinando Iucolano (I) - STMicroelectronics

Gallium nitride (GaN) power devices are an emerging technology that enables the design of power converters at higher switching frequencies and efficencies respect to conventional Silicon (Si) devices. Indeed, GaN technology adresses the compelling demand for high density and high efficency power electronics thanks to its excellent physical characteristics in term of: a)higher electron mobility, which allows lower on-resistances ad lower conduction losses; b)higher breakdown electric field, which allows higher voltage devices; c) higher saturation velocity.

Firstly, the presentation willshow the application map and the market scenario for Wide Band-Gap (WBG) devices, explaining why wide bandgap technologies such as Gallium Nitrdea Silicn Carbide, have becoming more admore commercially successful.

It will be explained the strucutre of the AlGaN/GaN HoghElectron Mobility Transistor (HEMT) device, enlightening how the heterojunction structure provides a vry low channel on-resistance called two-dimensional electron gas (2-DEG) and extremely low parasitic capacitances, which are fundamental for high current and high speed power devices.

Moreover, it will be reviewed te mot important techniques to implement normally-off (the natural HEMT transistor is a normal -ON). A common technique is to cascode the normally-on power device with a low voltage MOSFET, but it is acomplex solution and introduces parasitic. P-Gate and recessed solutions are preferable because they physically deplete the 2-DEG channel, implementing the normally-off device.

It will showed same challenges in GaN HEMTdevices. One issue is the breakdown, worsend by high density of dislocations and uncrotrolled impurities in GN layers. Another importat issue in GaN devices is the degradationof dynam performnce due to the shallow energy traps, which results in a temporary (tha is, reversible) increase on the dain-source on resistance ad in the current collapse.

At the end, it will be exhibited same measured performance of GaN power device designed by the R&D GaN deviceGRoup of STMicroelectronics. The measured Figure-of-Merit (FOM) and efficency in application show superior perfomance of GaN devices respect tothe other products based on silicon super-junction, GaN cascose and SiC. A brief comparison between GaN and SiC technologies will be showed.

#142 - TUNGSTEN CARBIDE (WC) CONTACTS FOR CMOS COMPATIBLE GAN HEMT TECHNOLOGY

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AlGaN/GaN heterostructures are excellent systems for the next generation of high-power and high-frequency devices. In particular, the formation of a two-dimensional electron gas (2DEG) at the AlGaN/GaN interface enables fabrication of high electron mobility transistors (HEMTs). Recently, notable progresses have been recorded in GaN-on-Si HEMT technology, where the elimination of gold (Au) represents a big challenge for the development of GaN devices within the Si fabs (CMOS compatibility).

In this context, great efforts have been devoted to develop Au-free metallizations. The use of a Au uppermost layer in Ohmic and Schottky metallizations is aimed to prevent the metal surface oxidation and to the reduce the overall metal resistivity. Conventional Schottky contacts consists in the use of Ni/Au layer.

In this work, we propose tungsten carbide (WC) has a novel solution for Schottky contacts on AlGaN/GaN heterostructures. This carbide has been previously described as a stable Schottky contact on other wide band gap semiconductors (SiC and diamond). The as deposited WC layer on AlGAN/GaN heterostructures showed a very flat morphology (RMS=1.34 nm in 5x5 region), which resembled the morphology of the AlGaN. No changes of the WC surface morphology were detected after annealing at 400°C. Then, the temperature dependence of current-voltage (I-V) characteristics of WC/AlGaN/GaN Schottky contact have been investigated. The forward I-V characteristics indicated a thermionic emission mechanism, with a F_B that increases from 0.74 eV to 0.91 eV with increasing the temperature from 25°C to 125 °C. The ideality factor decreases from 1.84 to 1.52 moving from 25°C to 125°C. Indeed, the coexistence of different mechanisms cannot be excluded. In reverse bias configuration, the I-V curves showed an increase of the current with increasing temperature. The behavior has been explained by a Poole-Frenkel emission mechanism. Finally, using a WC gate contact and Au-free Ti/Al/Ti source-drain Ohmic contacts, fully CMOS compatible HEMTs have been fabricated. Then, WC based HEMTs shows a low gate leakage transfer characteristics with a I_{ON}/I_{OFF} ratio about $2x10^8$ and anextrinsic transconductance $g_m=dI_{DS}/dV_G$ which reach a peak of 80 mS/mm around $V_G=+1$ V.

#143 - DEVELOPMENT OF THERMAL AND ELECTRICAL NUMERICAL MODEL FOR THE DESIGN OPTIMIZATION OF GAN-HEMT DEVICES AND CIRCUITS

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The AlGaN/GaN High Electron Mobility Transistors (HEMTs) show very promising characteristics for high-power microwave applications. Indeed the high energy gap and the presence of spontaneous and piezoelectric polarization charges that induces the two-dimensional electron gas at the AlGaN/GaN heterojunction allow to achieve high electrical performance, including high sheet carrier density, high breakdown voltage, high velocity saturation and carrier mobility. In these devices the operating temperature of the active region is an extremely important parameter. Indeed, under high power operating conditions, self-heating occurs increasing the device temperature and affecting the device performance and reliability. The exact knowledge of the channel temperature distribution is therefore an essential element for the design of the systems based on these components. In this work, we will show the development of an accurate electro-thermal model for the optimization the device and circuit design and the improvement of their performance and reliability. The electro-thermal model includes a compact electrical model, based on Angelov-Stoffels model, and the numerical simulation of the device thermal behaviour carried out by the COMSOL Multiphysics software. The actual device structure was included in the simulation directly importing the GDS layout. The electrical compact model parameters were extracted by fitting the electrical characteristics of the state of art GaN-HEMT, with 0.25 µm of gate length, on SiC substrates, manufactured by Leonardo. The transfer and output electrical characteristics of the devices were measured at different temperatures (from 300K to 450 K) in pulsed mode to make negligible self-heating effect during the measurements. The electrical compact model was used to calculate the device current in the thermal numerical simulations. Each of the ten fingers that form the multi-finger gate were split in ten sub-gates along the direction of the channel width. In each of the sub-gates it is assumed that the working temperature is constant and the current flowing in it is independently computed by the electrical compact model. The corresponding power dissipations in each of the sub-gates are used by the COMSOL Multiphysics software in order to self-consistently compute the overall temperature distribution in the whole device region. In order to validate simulation results, a thermography technique based on Raman spectroscopy has been developed and applied to measure the temperature distribution with sub-micrometric spatial resolution (~ 1 µm), without contact, and in a non-invasive way and under device operating conditions. The results of the Raman thermal analysis have been directly and successfully compared with the thermal simulation results.

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#144 - LOW TEMPERATURE PLASMA-ENHANCED ALD PROCESS FOR THE GROWTH OF EPITAXIAL ALN FILMS ON GAN SUBSTRATES

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Aluminum nitride (AlN) is a material of great interest due to its intrinsic properties, such as a wide direct band gap, piezoelectric effect and good thermal stability in optoelectronic and electronic devices. In particular, almost recently the high mobility two-dimensional electron gas at AlN/GaN interface has attracted much attention for applications in high-electron mobility transistors [1]. High quality epitaxial AlN films on GaN substrates are typically grown at high temperatures (>700°C) by MOCVD or MBE deposition techniques. However, the principal drawback of these procedures is the cracking of the AlN films due to the thermal expansion coefficient and lattice mismatches between AlN films and GaN substrates, especially for thickness above 6-7 nm [1]. In this context, plasma-enhanced atomic layer deposition (PE-ALD) performed at reduced temperature (300°C) [2] can represent a more convenient approach.

In this work, AlN films with different thickness values, from 5 to 15 nm, have been deposited by PE-ALD onto GaN on sapphire substrates. The morphological and structural properties have been extensively investigated by several techniques such as atomic force microscopy, High-Resolution X-Ray Diffraction and high-resolution transmission electron microscopy. All the investigated AlN films, show crystalline structure and quite good epitaxial relationship with respect to the GaN substrate. In fact, they demonstrated to possess an almost perfect *c*-axis orientation and also a quite good in-plane orientation. In particular, the initial layers of the AlN films perfectly matches the hexagonal stacking of GaN, nevertheless by increasing the film thicknesses some stacking faults have been detected due to stress relaxation processes.Finally, electrical characterization has been perfomed by contactless sheet resistance measurements on as-deposited samples. The Hg-probe measurements showed very low current leakage across these layers and the presence of a high density two-dimensional electron gas ($>2\times10^{13}$ cm^{-2}) at the AlN/GaN interface. Furthermore, the evolution of the morphological, structural and electrical properties of these films upon subsequent thermal treatments have been investigated [3].

The PE-ALD deposited AlN developed in this work can find important applications in GaN technology, such as a gate insulator on the recessed GaN channel for normally-off AlGaN/GaN MIS-HEMTs, or as a passivating layer for GaN surface.

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#145 - AL2O3 AS CHARGE-TRAP LAYER TO OBTAIN NORMALLY-OFF GAN MIS-HEMT DEVICES

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Aluminum oxide (Al_2O_3) thin layer, grown by Plasma Enhanced-Atomic Layer Deposition (PE-ALD) on AlGaN/GaN heterostructures has been investigated as charge-trap layer to control the threshold voltage and to obtain non-recessed normally-off MISHEMT devices. The morphology and structural features of the dielectric material were monitored by atomic force microscopy (AFM), high-resolution transmission electron microscopy (HR-TEM) and electron energy-loss spectroscopy (EELS), and correlated to the electrical performance of MISHEMTs.The deposited amorphous Al_2O_3 films were uniform and with a thickness of 30 nm. However, EELS spectra of aluminum $L_{2\text{-}3}$-edge demonstrated the occurrence of locally low coordinated aluminum cations, which can be associated to local oxygen deficiency. C-V measurements on Al_2O_3/AlGaN/GaN MIS capacitors revelaed that these defects acts as electron traps. In particular, under appropriate positive bias stress, the oxygen-relateddefects (N_{OT}= $5x10^{12}$ cm^{-2}) can be filled with electrons spilled from the 2DEG of AlGaN/GaN heterostructure. In this way, the 2DEG is depleted (pinch-off) and the normally-off condition is reached. The transcharacteristics (I_D-V_G) of HEMT devices employing Al_2O_3 dielectric, showed a positive pinch-off voltage (V_{PO}) of +1.5V after an appropriate positive bias applied to charge the insulator traps. The effectiveness and stability of the process have been been demonstrated also under negative stress bias (V_G = - 20 V) at 100° C.

#146 - STUDY OF METAL/SEMICONDUCTOR CURRENT TRANSPORT MECHANISM OF TI- AND TA- “AU-FREE” OHMIC CONTACTS ON ALGAN/GAN HETEROSTRUCTURES

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Gallium Nitride (GaN) is a promising material for high-power and high-frequency electronics. In particular, good quality Ohmic contacts are important both in GaN and in AlGaN/GaN heterostructures. GaN-on-Si technology requires “Au-free” metallizations, to enable the device fabrication inside Si fabs. The most straightforward approach to obtain Au-free Ohmic contacts is to employ low work-function metals in contact with (Al)GaN, in order to obtain a low Schottky barrier. In this context, while Ti/Al- and Ta/Al-based contacts have been already reported, a systematic comparison of these systems on non-recessed heterostructures was not presented yet.

In this work, we studied the electrical and structural behavior of Ti/Al/Ti and Ta/Al/Ta trilayers, deposited onto AlGaN/GaN heterostructures. With increasing the annealing temperature an increase of the current was observed in TLM structures, leading all the systems into an Ohmic condition at 600°C, with values of the specific contact resistance in the order of 10^{-4} Ωcm^2. During annealing, an increase of the surface roughness was observed, which was associated to the formation of new phases in the stack (e.g., $TiAl_3$, $TaAl_3$…) and metal/AlGaN reactions. Interestingly, a thin TiN layer was observed in the Ti/Al/Ti samples, showing the lowest contact resistance. On the other hand, Ta-based contacts exhibited a better surface morphology, most probably owing to the higher stability of the Ta upper layer under high temperature annealing.

A quantitative description of the carriers transport mechanism through the metal/AlGaN interfaces has been obtained by monitoring the temperature dependence of the electrical parameters. The sheet resistance R_{SH} follows a power-law relation, typically used to describe the temperature dependence of 2DEG mobility. The behavior of R_{SH} is consistent with the prevalence of the optical phonon scattering mechanism.The temperature dependence of the specific contact resistance allowed to establish a thermionic field emission of the carriers over the barrier (with barrier height values in the range 0.5-0.6eV). Moreover, $\rho_C$has been studied as a function of the AlGaN thickness (d_{AlGaN}) using the TFE-2DEG model. The experimental values of ρ_C are in agreement with those predicted by the model and the calculated curves suggest that a further improvement of ρ_C can be achieved by a reduction of the AlGaN barrier layer thickness.

This result was correlated with the structural composition of the interface.

#147 - ASSISTED SELF-ASSEMBLING OF MONOCRYSTALLINE SILICON WIRES ON SOI SUBSTRATES

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Semiconductor nanowires exhibit superior and configurable electronic and optical properties with respect to their bulk counterparts. Their growth has been tackled with a plethora of techniques challenging the production of controlled, ultra-long structures matching the needs of high yield production and scalability. Several bottom-up, self-assembly methods can be employed to obtain high-quality parallel wires. On the other side, lithographic top-down methods can be used to precisely prepare a substrate for further engineering as, for instance shown for the cases of controlled wetting or nano-imprint lithography. However, their fabrication over large scales often requires demanding procedures and are hardly scalable. Here we synthesize arrays of parallel ultra-long (up to 0.75 mm), monocrystalline, silicon-based nano-wires and complex, connected circuits exploiting electron beam lithography and dewetting process of commercial thin silicon films on insulator. We demonstrate the ultimate control of UT-SOI dewetting for the precise formation of complex nano-architectures featuring extremely reduced fluctuations of size, shape and positioning (a few %) over hundreds of repetitions and on large scales [1]. The solid state dewetting initiated at the edges of the patterns controllably creates the ordering of wires with *ad hoc* placement and periodicity [2]. Phase field simulations benchmark the experimental results considering anisotropic surface diffusion limited kinetics and show the role played by surface energy anisotropy leading to crystal faceting and stabilizing the wires against breaking. Wires splittings, interconnections and direction are independently managed by engineering the dewetting fronts and exploiting the spontaneous formation of kinks. Finally, we show the use of the wires as FET transistors. Beyond the first experimental evidence of controlled dewetting of patches featuring a record aspect ratio of∼1/60000 and self-assembled ∼mm long nano-wires, our method constitutes a distinct approach for the deterministic implementation of atomically-smooth, mono-crystalline electronic and photonic circuits.

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#148 - OPTOMECHANICAL SYSTEMS FOR QUANTUM TECHNOLOGIES

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Recent progress in the fabrication oRecent progress in the fabrication of nanomechanical resonators has enabled their operation in the quantum regime, that is, selected vibrational modes of nanostrings and nanomembranes have been prepared and detected in quantum states such as squeezed or entangled states. These mechanical elements offer unique opportunities for interfacing different degrees of freedom and different radiation wavelengths and are essential tools within a quantum network also due the possibility to integrate them within silicon-based platforms. We discuss here briefly three possible applications of optomechanical systems, that is, nanomechanical resonators controlled by a driven optical cavity field by means of the radiation pressure interaction. As a first example we discuss how a reversible optical-to-microwave interface is realized by a metalized nanomembrane placed within a cavity and capacitively coupled to a high resonant LC circuit. Such a converter can be operated in the quantum regime at cryogenic temperatures and allows the optical transfer of quantum states between distant superconducting solid-state based quantum computers which are currently operated and controlled with microwave fields. A further interesting configuration is the one obtained by placing a stack of two or more membranes within the cavity; in this case collective and interference effects allows to significantly enhance the optomechanical coupling and reach a regime where a single vibrational phonon is able to shift the cavity frequency by more than its bandwidth. In this regime single photon/phonon routing can be achieved and at the same time the device could be operated as a quantum sensor of weak forces. In fact in this regime electrical, magnetical and inertial force acting on the membranes could be detected with quantum-limited sensitivity.

#149 - A NOVEL QUANTUM COMPUTING MODEL FOR AN ARTIFICIAL NEURON

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Artificial neural networks are the heart of machine learning algorithms and artificial intelligence protocols. Historically, the simplest implementation of an artificial neuron traces back to the classical Rosenblatt’s “perceptron”, but its long term practical applications may be hindered by the fast scaling up of computational complexity, especially relevant for the training of multilayered perceptron networks. We introduce a quantum information-based algorithm implementing the quantum computer version of a perceptron, which shows exponential advantage in encoding resources over alternative realizations. We present an experimental test of a few qubits version of this model on an actual small-scale quantum processor, which gives remarkably good answers against the expected results. We show that this quantum model of a perceptron can be used as an elementary nonlinear classifier of simple patterns, as a first step towards practical training of artificial quantum neural networks to be efficiently implemented on near-term quantum processing hardware.

#150 - COMPLEXITY OF QUANTUM MOTION, ENTANGLEMENT, AND SCRAMBLING: A PHASE-SPACE APPROACH

Giuliano Benenti - Univ. Insubria - INFN

Measuring complexity has been a major and long quest in both quantum and classical dynamics. While there exists a direct connection between chaos and algorithmic complexity of trajectories in classical physics, the problem is particularly elusive for quantum mechanics, where the notion of trajectory is forbidden by the Heisenberg uncertainty principle and complexity can be attributed not only to the lack of integrability but also to the tensor-product structure of the Hilbert space, that is, to entanglement.

The phase space representation of quantum mechanics is a very convenient framework to investigate quantum complexity, in that one can compare classical and quantum dynamical evolutions of distributions in phase space.

We measure complexity by means of either the number of harmonics or the separability entropy of the Wigner distribution. Both quantities, as well as scrambling, characterized by the growth rate of the square commutator between two observables, in the semiclassical limit are determined by the Lyapunov exponent of the underlying classical dynamics. Our results are illustrated in a model of two coupled nonlinear oscillators, both in the chaotic and in the integrable regime.

#151 - QUANTUM DECAY AT SHORT, INTERMEDIATE, AND LONG TIMES AND ITS OBSERVATION IN INTEGRATED PHOTONICS

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The decay of an unstable system is usually described by an exponential law. However, quantum mechanics predicts strong deviations of the survival probability from the exponential: under very general assumptions, the decay is quadratic at short times (the “Zeno region”), while at very large times it follows a power law, with superimposed oscillations. The latter regime is particularly elusive and difficult to observe. Here, we discuss a next-to-nearest-neighbor hopping model on a semi-infinite one-dimensional lattice, and analyze the time evolution of an initial state in which a particle is created in the first site of the chain. By varying the model parameters, we find cases in which the decay is predominantly exponential, cases in which corrections at short and long times become dominant, and even cases in which the initial state becomes stable. We describe the implementation of the discussed class of models in arrays of single-mode optical waveguides, where the transverse optical modes correspond to distinct quantum states and the temporal evolution is mapped into the spatial propagation coordinate. By injecting coherent light in the fabricated photonic structures and by measuring a small scattered fraction of such light, we are able to experimentally observe not only the exponential decay regime, but also the quadratic Zeno region and the power-law decay at long evolution times.

#152 - SUPERCRITICAL ENTANGLEMENT, VIOLATION OF CLUSTER DECOMPOSITION AND ANOMALOUS DYNAMICS IN SOME LOCAL QUANTUM SPIN MODELS

Luca Dell'Anna - University of Padova

We compute exactly some correlation functions and peculiar entanglement properties for two classes of local integer and half-integer spin chains whose non-degenerate ground states can be expressed in terms of uniform superpositions of Motzkin and Dyck paths. Surprisingly we find a violation of the cluster decomposition property for the correlation functions, a large deviation from the area law for the entanglement entropy and an extremely fast propagation of the excitations after a quantum quench.

#153 - INTERACTION OF MECHANICAL OSCILLATORS MEDIATED BY THE EXCHANGE OF VIRTUAL PHOTONS

Alessio Settineri - Università di Messina

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Effective interactions able to coherently couple spatially separated qubits are highly desirable for any quantum computer architecture. Recently, it has been shown that the exchange of virtual photons between artificial atoms can give rise to effective interactions of multiple spatially separated atoms,opening the way to vacuum nonlinear optics. Moreover, systems where virtual photons can be created and annihilated can be used to realize many nonlinear optical processes with qubits. Given these results, one may wonder whether it is possible for spatially separated mesoscopic or macroscopic bodies to interact at a quantum level by means of the vacuum fluctuations of the electromagnetic fireld.

Owing to quantum fluctuations, the electromagnetic vacuum is able, in principle, to affect the motion of objects through it, like a complex fluid Here we consider an optomechanical system consisting of two vibrating mirrors coupled to a detuned optical resonator . We find a noticeable coupling rate between the two spatially-separated vibrating mirrors determined by the motional forces. Furthermore, by tuning the

two mechanical oscillators into resonance, we demonstrate that mechanical quantum excitations can be coherently transferred among spatially-separated mechanical oscillators through a dissipation-less quantum bus, thanks to the exchange of virtual photon pairs originating from the dynamical Casimir effect (DCE) .

The processes here proposed demonstrate that the electromagnetic quantum vacuum is able to transfer mechanical energy acting like an ordinary fluid. It would be as if the vibration of a string (mechanical oscillator 1) could be transferred to the membrane of a microphone

(mechanical oscillator 2) in the absence of air or of any medium filling the gap. This puzzling result opens up exciting possibilities of applying ideas from fluid dynamics to the study of the electromagnetic quantum vacuum. Furthermore, we show that this system can operate as a mechanical parametric down-converter even in the very low excitations regime. This effect can also be used as an indirect probe

(not aected by the problem of thermal photons) of the DCE.

In conclusion the obtained results show that the DCE in high frequency optomechanical systems can be a versatile and powerful new resource

for the development of quantum optomechanical technologies. If, in the future, it will be possible to control the interaction time (as currently realized in superconducting artificial atoms), e.g., changing rapidly the resonance frequencies of mechanical oscillators the interaction scheme proposed here would represent an attractive architecture for quantum information processing with optomechanical systems.

#154 - WITNESSING QUANTUM CORRELATIONS IN QUANTUM OPTICS VIA LARGE DEVIATION FUNCTIONS

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The standard way to investigate quantum effects in optics relies on the properties of certain observables associated with light-matter systems, or on the characterization of the output of a given optical circuit, providing the inputs are properly specified. The former approach often neglects the complete features of the emission, the latter deals with the output states without considering the dynamics of the sources. In this work we provide a link between the two methodologies by exploiting the thermodynamics of quantum trajectories for a given measurement setup. This procedure enables the investigation of the quantum properties of the photon fields emerging from a generic quantum optical experiment, when the dynamical properties of the sources are fully taken into account. The methodologies here presented are relevant for practical experimental modelling, in particular when a long-time collection of statistical data is required.

#155 - MULTI-MODAL IN VIVO IMAGING OF CORTICAL PLASTICITY AFTER STROKE

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Optics is a formidable tool to investigate brain rewiring in vivo. Here, we combined several optical imaging and manipulation tools to investigate cortical remodeling in a mouse model of stroke. Two-photon fluorescence imaging in vivo revealed that the instability of synaptic contacts induced by stroke is recovered by rehabilitation. By using a combination of in vivo and ex vivo imaging we showed that the vascular 3D maps, profoundly modified by rehabilitation after stroke, are associated with transiently altered permeability. Furthermore, wide-field functional imaging during motor training showed how different therapies might act differently on the temporal and spatial features of cortical activation in the peri-infarct area. An all-optical approach that combines optogenetics manipulation and calcium imaging allowed revealing altered inter-hemispheric connectivity induced by rehabilitation after stroke. The same combination of tools was used to test optogenetic stimulation as a plasticizing treatment and monitor the associated cortical functional remapping. The present work provides the first evidence that rehabilitation promotes the combined recovery of structural and functional features distinctive of healthy neuronal networks.

#156 - METAL COATED SILICON NANOWIRES AS SMART INTERFACE FOR INVESTIGATING ASTROCYTES PHYSIOLOGY AND EVALUATE THEIR EXTRACELLULAR ACTIVITY IN VITRO

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The use of nanostructures in neuroscience is a key strategy to interface living matter and investigate mechanisms underlying cells differentiation and their interactions *in vitro*. Indeed, nanostructures can resemble a nano/micro-environment allowing cells to grow and promote *in vivo like* behaviours. This aspect is crucial in identifying molecular, biophysical and chemical factors that drive cell polarization/differentiation process. Among different nanostructures, disordered metal-coated silicon nanowires offer several advantages: low mechanical stress, peculiar optical properties and facile surface functionalization, resulting in a low-cost and high scalable material that can be easily integrated with conventional electronics and/or polymeric substrate. Moreover, this nanostructure allowsto shrinkage pad dimensions preserving low-noise and low-impedance in high-density recording making this tool a major candidate to investigate and define new models for understanding the central nervous system and its components such as astrocytes.

Astrocytes represent the bulk of the brain and they are key players in brain physiology and pathology supporting neurons in their activity. Their star-like shape is not generally preserved when astrocytes are seeded in cultures, thus reducing the validity of the findings in vitro. Conversely, we demonstrate that gold-coated silicon nanowires (Au/SiNWs) enable the expression of *in-vivo*-like morphological and functional phenotype of astrocytes. In this work, we show how Au/SiNWspromote astrocytes adhesion and growth without need for additional coating and result crucial in inducing proper cell arborisation of processes. Fluorescent imaging, SEM and AFM reveal that astrocytes respond to the substrate topography by morphological differentiation and 3D growth with elongation sprouting from the cell body. GFAP analyses reveal that cellular differentiation is not due to gliotic reaction, confirming the differentiation capability of astrocytes in the proposed model. Finally, we report extracellular recording of astrocytes culture grown on Au/SiNWs based electrode array, implementing a new model for investigating glial interactions.

In conclusions,our results validate Au/SiNWsas novel glial interface that promote the growth, differentiation of astrocytes *in vitro*, enabling also extracellular recording to offer new perspective in glia physiology. This work was supported by AFOSR projects ASTROMAT and ASTRONIR.

#157 - TAPERED OPTICAL FIBRES FOR MULTIFUNCTIONAL OPTICAL NEURAL INTERFACES

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In vivo optical interfaces with in deep structures of the mouse brain are still limited by the use of flat-cleaved optical fibers, whose illumination and light collection performances is restricted to a small and fixed volume close to fiber facet [1,2]. If two-photon microscopy has allowed multipoint stimulation and monitoring of neural activity for almost the whole cortical depth, last 5 years have seen the development of several technological approaches to reach sub-cortical regions with improved spatial resolution, including μLEDs, GRIN lenses, Indium Thin Oxide-based probes and tapered optical fibers [3-10].
After a review of the state-of-the-art in this field, this presentation will focus on the engineering and use of tapered optical fibers to control and monitor neural activity using only one optical waveguide with reduced invasiveness. The technology exploits mode-division demultiplexing operated by a millimeters-long taper that allows to redirect and/or collect light over different brain regions and subregions. Exploting micro and nanotechnologies to structure the highgly curve surface of the fiber taper, it is possible to engineer the stimulation and the collection volume, as well as to realize multiple electrodes for extracellular electrophysiology along the taper.
The simplicity of this technique, together with its versatility, reduced invasiveness and compatibility with both laser and LED sources, indicate this approach can greatly complement the set of existing methods for optical neural interfaces with deep brain regions.

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#158 - ADVANTAGES OF THE USE OF SILICON PHOTOMULTIPLIERS FOR CONTINUOUS WAVE FUNCTIONAL NEAR-INFRARED SPECTROSCOPY OF THE HUMAN BRAIN CORTEX

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Silicon Photomultiplier (SiPM) detectors provide very promising characteristicsfor human brain cortex monitoring through Continuous Wave Functional Near Infrared Spectroscopy (CW-fNIRS). The positive characteristics of SiPMs in CW-fNIRS arise from a high gain (of the order of vacuum photomultiplier tubes, PMTs, $\sim 10^7$), low operation voltage, small size, robustness ,reliability and low cost.

The fNIRS technique relies on the transparency of human tissues within the near infrared (NIR) spectrum. In this range, the light absorption is mainly due to the oxygenated (O_2Hb) and de-oxygenated (HHb) hemoglobin in blood. In fNIRS, the information is encoded in the amount of back-scattered photons and it is related to the changes in O_2Hb and HHb concentrations, providing relevant markers of hemodynamic and metabolic changes associated with neural activity in the brain. CW-fNIRS mapping relies on cyclic measurements of light diffusion from the brain cortex at multiple source-detector couples with at least two wavelengths in the 700-950 nm range. In each clock cycle, each optode couple (detector – optical source pair) performs a measurement of the O_2Hb and HHb concentrations in a specific region of the brain cortex defined by the optodes position on the scalp and the relative distances between the detector and the light source (SDS, Source Detector Separation). Importantly, different SDSs provide different depth sensitivities from the investigation surface. We investigated some major characteristics and issues when using Silicon Photomultiplier (SiPM) detectors in CW-fNIRS. We analyzed the after-pulsing effect, proposing the physical mechanism causing it, and determining its relevance for CW-fNIRS. Moreover, we studied the SiPM transients occurring as the SiPM device goes from the dark (LED switchd off) to the illumination (LED switched on) conditions, and vice-versa. We studied the SiPM Signal to Noise Ratio (SNR) in standard CW-fNIRS operation and after that, we successfully integrated SiPMs in a 6 channels fNIRS prototype. We reported an in vivo comparison of the system with a commercial system relying on laser diodes, PMTs, and optical fibers for light probing and detection. Our prototype showed excellent performances providing a correct estimation of brain hemodynamics similar to those obtained with the commercial fNIRS system that employed far more complex and expensive hardware. Finally, by taking into account all the characteristics, issues and performances of SiPMs for CW-fNIRS, we designed and built a 120-channel system with excellent SNR, employing multiple and particularly large SDSs. In the talk we discuss the developed fNIRS devices focusing on the advantages of SiPMs usage with comparison to the state of art fNIRS systems based on other types of photodetectors. This study has been performed in the framework of the EU Project ASTONISH.

#159 - NON THERMAL EFFECTS OF RADIOFREQUENCY ELECTROMAGNETIC FIELD EXPOSURE ON NEURAL CELLS

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The non-thermal mechanisms, underlying the damage induced on human cells by radiofrequency electromagnetic fields (RF-EMFs), are still unclear and only few studies reported about the effect of RF-EMFs on self-renewal of neural progenitor cells. In this research, we investigated the influence of low intensity RF-EMFs on Olfactory Ensheathing Cell (OEC) cultures, typical glia cells showing characteristics of stem cells. Cell cultures were exposed, in far field condition,at 900 MHz continuous and amplitude modulated EMFs for 10, 15 and 20 min at 37°C. The expression of OEC marker (S-100), stem cell marker (Nestin), cytoskeletal proteins (GFAP and Vimentin), apoptotic pathway activation by Caspase-3 cleavage and cell viability, were evaluated. Surprisingly 20 min of exposure to continuous or amplitude modulated 900 MHz EMF induced a different and significant decrease in cell viability, diverse dynamic changes in the expression of the analysed markers and in the activation of apoptotic pathway.

#160 - UNDERSTANDING THE EFFECT OF PATHOGENIC MUTATIONS ON THE STRUCTURE AND FUNCTION OF THE VOLTAGE-GATED POTASSIUM CHANNEL KV4.3

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The voltage-gated potassium channel Kv4.3 plays a vital role in shaping the timing, frequency, and backpropagation of electrical signals in the brain and heart by generating fast transient currents at subthreshold membrane potentials in repetitively firing neurons. In recent years, an increasing number of inherited and de novo mutations on Kv4.3 channel have been identified and, in the case of the brain, linked to the spinocerebellar ataxia type 19/22. However, how these mutations affect the channel function at the molecular level remains to be elucidated. Here, we chose a mild and a severe pathogenic single mutant of Kv4.3, namely M373I and S390N, and systematically studied their effect on the functioning of the ion channel and its modulation by an auxiliary Kv channel-interacting protein. By employing electrophysiology, homology modelling, and molecular dynamics simulations, we could link functional abnormalities to the structural changes induced by each mutation at the molecular level. Our findings show that the pathogenic mutations not only affect the channel structure and function but also interfere with their modulation by cell-specific interacting partners.

#161 - FAST-DEMAGNETIZATION AND FOUR WAVE MIXING PROCESSES WITNESSED USING FERMI SEEDED-FEL.

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Free Electron Lasers (FELs) offer unprecedented opportunity for exploiting ultrafast dynamics with chemical sensitivity. Using appropriate seeding methods combined with pulse tunability, multiple polarization and multi- single or two color pulse schemes have enabled studies of dynamical responses in complex systems, by assessing how specific excitations develop and/or propagate among different sites.

Another great advantage of seeded-FELs, as FERMI@Elettra, is that they have also opened the route to X-ray coherent non-linear experiments for exploiting, among other, electronic correlations and charge transfer between different atomic constituents in the sample.

This presentation will overview different class of experiments performed at the DiProI end-station [1] taking advantage of the unique characteristics of the FERMI seeded-FEL [2]. Particular emphasis will be on novel schemes used to study magnetic dynamics after optical excitation at different absorptions edges in time coincidence, taking advantage of two-colors emission of FERMI FELs both in real space by means of time resolved holography [3] or using Fresnel zone plate to stretch the incoming X-ray pulse keeping an angular encoding of the arrival time [4]. The second part will report on the first four wave mixing (FWM) experiments in EUV/soft X-ray regime [5], based on 3rd order coherent non-linear light matter interactions, which has paved the road to other recent transient grating (TG) and coherent anti stokes Raman scattering (CARS) experiments [6]. They demonstrate the unique prospects to exploit the dynamics and coupling between “low-energy” modes, such as vibration and valence electronic states, and “high-energy” excitation involving core levels.

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#162 - NANOSCALE DYNAMICS ACROSS THE MOTT TRANSITION IN V2O3

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The phase diagrams of 3*d* metal oxides provide rich landscapes to explore the non-equilibrium degrees of freedoms during an insulator-to-metal transition (IMT). In these materials, the dynamics of nano-textured insulating and metallic phases is characterized by an unexplored complexity than enables manipulation of phase separation to control the properties of quantum materials on ultrafast timescales. Here, we combine X-ray photoemission electron microscopy and non-equilibrium optical spectroscopy to link the temporal and spatial dynamics of the IMT in the Mott insulator V_2O_3. Our experiments show that the low-temperature monoclinic antiferromag- netic insulating phase is characterized by the spontaneous formation of striped polydomains, with different lattice distortions. The insulating domain boundaries accommodate the birth of metallic nano-droplets, whose non-equilibrium expansion can be triggered by the photo-induced change of the 3***d***-orbital occupation. We address the relation between the spontaneous nanotexture of the Mott insulating phase in V_2O_3 and the timescale of the metallic seeds growth. We speculate that the photoinduced metallic growth can proceed along a non-thermal pathway in which the monoclinic lattice symmetry of the insulating phase is partially retained.

#163 - ATTOSECOND CORE EXCITON DYNAMICS IN MGF2

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The investigation of ultrafast dynamics of core excitons in solids is of crucial importance from the theoretical viewpoint and for the exploitation of excitonic properties in technological applications. So far ultrafast exciton dynamics were investigated only on thin nanofilms using attosecond transient absorption spectroscopy [1]. This technique has two main drawbacks: heat exchange in a very thin sample is not efficient and usually it is not possible to produce free-standing monocrystalline samples with nanometric thickness. In this work we report on the investigation of ultrafast dynamics in a crystalline MgF_2 sample by employing attosecond transient reflectivity spectroscopy (ATRS).

Attosecond pulses with photon energy ranging between 30 eV and 64 eV were focused on a single-crystal sample together with an opportunely delayed infrared (IR) 8-fs pulse. The spectrum of the reflected attosecond radiation was collected by an extreme-ultraviolet (EUV) spectrometer, while scanning the temporal delay between EUV and IR pulses. We applied this technique for the first time on a crystalline MgF_2 sample since static reflectivity results show a very clear excitonic feature around 54.6 eV photon energy [2], corresponding to the Mg $2p^{++} \rightarrow \Gamma_1$ transition. We used a two foci pump-probe configuration [3]. In the first focus we placed a Time-Of-Flight (TOF) electron spectrometer. A Neon photoelectron trace was recorded in order to precisely calibrate the pump-probe temporal axis and retrieve the temporal behaviour of the IR electric field. A [001] MgF_2 sample was located in the second focus, where an ATRS trace was simultaneously recorded.

The experimental results showed femtosecond dynamics around the excitonic peak that can be used to extract information about exciton formation and lifetime [1]. Furthermore, we observed clear oscillations of the reflected radiation at twice the IR frequency (2ω) in the bottom region of the conduction band (above 56 eV). These features can be explained in the framework of the dynamical Franz-Keldysh effect [4]. 2ω-oscillations in the ATRS trace were also observed in the valence band (below 43.2 eV) during the pump-probe temporal overlap, which could be originated from the ultrafast microscopic current initiated by the pump pulse in the sample. These experimental results, together with theoretical support will give an unprecedented insight in the core exciton excitation and relaxation dynamics in crystalline insulators.

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#164 - PROBING THE ULTRAFAST DYNAMICS WITH A SUB-NANOMETRIC AND SUB-PICOSECOND SPATIO-TEMPORAL RESOLUTION: ULTRAFAST ELECTRON MICROSCOPY

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Electron Microscopy (EM) is a powerful and versatile technique allowing to obtain morphological, structural, chemical and field information of specimens at the nanoscale[1]. Nevertheless, despite the implementation of fastest cameras, the investigation of the material dynamics is limited to the millisecond timescale. Ultrafast EM overcomes this limitation. Combining the excellent temporal properties of ultrafast lasers or ultrafast electrostatic beam blankers it is possible to trigger a pulsed electron beam with ultrashort electron pulses and push the temporal resolution of the instrument to the picosecond timescale and beyond.
Several strategies to investigate material dynamics at the nanoscale with a sub-picosecond time resolution will be presented, in both Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). Ultrafast Scanning Electron Microscopy (USEM), firstly developed in CALTECH[2] has been improved in AMOLF afterwards, allowing Time-Resolved Cathodoluminescence (TR-CL) spectroscopy to acquire CL decay traces and the autocorrelation function g(2) of the CL signal[3]. The first Ultrafast Transmission Electron Microscope based on a Cold FEG emission source, recently developed at CEMES-CNRS[4], allows to perform time-resolved ultrafast pump-probe TEM experiment exploiting a high coherent ultrafast electron beam[5]. We will show the performances of such an instrument as well as the first experimental results obtained by Electron Energy Gain Spectroscopy (EEGS). Some outlooks on future applications will be given.

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#165 - ULTRAFAST OPTICAL STUDIES OF SINGLE LAYER TRANSITION METAL DICHALCOGENIDES AND RELATED HETEROSTRUCTURES

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Transition metal dichalcogenides (TMD) are semiconductors exhibiting a transition from indirect to direct bang gap structure when are thinned to a single layer (1L). This property combined with a strong light matter interaction, enhanced by many-body effects, make semiconducting 1L-TMDs forefront materials in the field of electronics, optoelectronics, photonics and energy harvesting research. In addition to that, 1L-TMDs are an ideal platform to study exciton physics even at room temperature: the strong quantum confinement effect and the reduced Coulomb screening, have a deep impact on the 1L-TMD optical response which is dominated by excitons characterized by large binding energy. Moreover, the lower energy excitons are formed at *K* and *K'* valley at the edge of the

Brillouin zone and they can be optically addressed by circular polarized light opening up tantalizing possibilities for valleytronics and spintronics applications. In my talk, I will study the non-equilibrium optical response of 1L-TMDs by optical pump-probe spectroscopy. I will show that the non-linear optical response of such materials exhibits strong signature of many body interactions such as band-gap renormalization process. By using time-resolved Faraday rotation and circular dichroism techniques, I will also give an overview of the inter and intravalley relaxation processes occurring in 1L-TMDs. In the last part of the talk, I will show recent results on charge transfer and spin/vally dynamics occurring in TMD heterostructures.

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#166 - ACCESSING TEMPERATURE WAVES IN QUANTUM CORRELATED MATERIALS

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In order to account for non-Fourier heat transport, occurring on short time and length scales, the often-praised Dual-Phase-Lag (DPL) model was conceived, introducing a causality relation between the onset of heat flux and the temperature gradient. The most prominent aspect of the first-order DPL model is the prediction of wave-like temperature propagation, the detection of which still remains elusive. Among the challenges to make further progress is the capability to disentangle the intertwining of the parameters affecting wave-like behaviour. This work contributes to the quest, providing a straightforward, easy-to-adopt, analytical mean to inspect the optimal conditions to observe temperature wave oscillations. The complex-valued dispersion relation for the temperature scalar field is investigated for the case of a localised temperature pulse in space, and for the case of a forced temperature oscillation in time. A modal quality factor is introduced showing that, for the case of the temperature gradient preceding the heat flux, the material acts as a bandpass filter for the temperature wave. The bandpass filter characteristics are accessed in terms of the relevant delay times entering the DPL model. The optimal region in parameters space is discussed in a variety of systems, covering nine and twelve decades in space and time-scale respectively. The here presented approach is of interest for the design of nanoscale thermal devices operating on ultra-fast and ultra-short time scales, a scenario here addressed for the case of quantum materials.

#167 - HIERARCHICAL APPROACH TO REDUCED TRANSPORT MODELS IN FUSION PLASMAS

Matteo Valerio Falessi (I) - ENEA

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A framework to validate reduced particle and energy transport models based on the theory of phase space zonal structures is proposed. The motivation of the present work is two-fold: (i) extending first-principle-based gyrokinetic simulations to long time scales is extremely demanding from a computational resource point of view; and (ii), the relevant physics processes can be illuminated and extracted from complex simulations by means of reduced models. Consequently, in our work, particle and energy transport equations are formulated first, and then solved within three levels of increasing simplification based respectively on: the weak-amplitude expansion, i.e. $\delta \equiv |\delta B \perp |/B 0 << 1$; the assumption that the parallel mode structure is set by linear theory, i.e. $\tau N L \sim \gamma L -1 >> |\omega| -1$; and, finally, the quasi-linear description. The systematic comparison of these levels of approximation against nonlinear gyrokinetic simulation results yield a verified reduced description retaining only the essential physics ingredients. Although completely general, this framework is particularly relevant for energetic particle (EP) transport and nonlinear dynamics in fusion plasmas. In particular, the hierarchy of verified reduced descriptions, discussed in this work, may be adopted for systematic analyses of the role of EPs as mediators of cross-scale couplings. Accordingly, simplifying assumptions in their governing equations must be strictly and systematically validated in realistic scenarios. Experiments with a set of dimensionless parameters relevant for burning plasma studies such as the Divertor Tokamak Test facility (DTT), are the ideal testbed for the further validation process.

#168 - SCIENTIFIC OBJECTIVES OF THE DIVERTOR TOKAMAK TEST (DTT) FACILITY

Gustavo Granucci (I) - ISTP-CNR Milano

Appropriate disposal of the non-neutronic energy and particle exhaust in a reactor is universally recognized as one of the high priority challenges for the exploitation of fusion as an energy source. The new Divertor Tokamak Test (DTT) facility, which will be built in Italy, is a tool to address that challenge in high-field, high performance tokamak with complete integration between core and edge plasma scenarios. The DTT plasma condition will be relevant for DEMO (the european DEMOstration power plant) with condition of power flow to the divertor of 15 MW/m, where 17 MW/m is the expected level for a reactor. DTT is a superconducting tokamak with 6 T of on-axis maximum toroidal magnetic field carrying plasma current up to 5.5 MA, in pulses with length up to 100s. The D-shaped device is up- down symmetric, with major radius R=2.14 m, minor radius a=0.64 m and an average triangularity of 0.3.The auxiliary heating power, coupled to the plasma at maximum performance, is 45 MW, shared between ECH (Electron Cyclotron Heating, ICH (Ion Cyclotron Heating) and NNBI (Negative Neutral Beam Injectors).

Many aspects relevant for the physics of magnetic fusion will be addressed. Fast particles up to 700 KeV (simulating the alfa generated by nuclear fusion reaction) will be generated through the ICH power while the chosen energy of NNBI (400 KeV) allows to have a super-Alfvenic population to study fast particle collective transport. A strong relevance will be given also the physics of plasma heating in different scheme and configuration, having DTT the possibility to use all the three main heating systems used in ITER and foreseen in DEMO. The physics of the divertor will be addressed exploiting the possibilities to use DTT as a test bed of new divertor materials (including liquid metals), while preliminary electromagnetic studies confirm the possibility of producing a variety of divertor magnetic topologies.

This presentation will discuss the state of the art of the project, illustrating its scientific background, the expected plasma scenarios - in particular as far as plasma exhaust is concerned – and the main technology choices so far. Emphasis will be given to highlight the effort to design an experimental tool, which will be a device not only for plasma exhaust studies, but also for the advancement of fusion science in the grand sense.

#169 - COLLISIONLESS SHOCKS AND NON-EQUILIBRIUM PHENOMENA IN ASTROPHYSICAL PLASMA: THE CASE OF SUPERNOVA REMNANTS

Marco Miceli (I) - Università di Palermo

Astrophysical shocks at all scales, from those in the solar system up to cosmological shock waves, are typically ‘collisionless’, because the thickness of their jump region is much shorter than the collisional mean free path. Collisionless shocks behave differently than collisional shocks (like those observed on Earth), because collective effects (electro-magnetic fluctuations and plasma waves) provide the viscous dissipation and the jump conditions at the shock front. Moreover, the sudden heating of the plasma induces a underionization of the post-shock flows and ions reach the equilibrium of ionization on much longer timescales.

Supernova remnants are ideal targets to study astrophysical shocks because of their bright post-shock elecromagnetic emission (on a wide range of wavelengths) and fast blast waves. I here review the recent findings related to the collisionless shock heating of heavy ions and to the post-shock conditions of non-equilibrium in supernova remnants.

#170 - PHASE-SPACE CASCADE IN TURBULENT PLASMAS: OBSERVATIONS AND THEORY

Sergio Servidio (I) - University of Calabria

Other Authors: University of Calabria

Plasma turbulence has been investigated using unprecedented high-resolution ion velocity distribution measurements by the Magnetospheric Multiscale mission (MMS) in the Earth’s magnetosheath. These novel observations of highly structured particle distribution suggests a cascade process in velocity space [1-2]. This complex velocity space structure has been investigated using a three-dimensional Hermite transform, revealing, for the first time in observational data, a power-law distribution of moments. In analogy to hydrodynamics, a Kolmogorov approach leads directly to a range of predictions for this phase-space transport. The scaling theory is found to be in agreement with observations and new simulations [3-4]. The combined use of state-of-the-art MMS data sets, novel implementation of a Hermite transform method, scaling theory of the velocity cascade and kinetic simulations opens new pathways to the understanding of plasma turbulence and the crucial velocity space features that lead to dissipation in plasmas.

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#171 - HELICAL MAGNETIC SELF-ORGANIZATION OF PLASMAS IN TOROIDAL PINCHES WITH TRANSPORT BARRIER FORMATION

Marco Veranda (I) - Consorzio RFX (CNR, ENEA, INFN, Università di Padova, Acciaierie Venete SpA)

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Nonlinear MHD modeling of toroidal pinch configurations (reversed-field pinch and tokamak) for hot plasma confinement describes several features of the helical self-organization, observed in both reversed-field pinches and tokamaks. It can also give a hint on why transport barriers are formed, by far one of the more interesting observations in experiments.

The research work will be summarized in two points.

The first one regards the recent successful technique to “channel” reversed-field pinches into a chosen macroscopic helical shape through the use of small edge magnetic perturbations. Helical self-organization is predicted in nonlinear MHD modeling, successfully tested in RFX-mod experiment in Padova and awaits further exploration in the updated device RFX-mod2. The upgraded machine, soon starting operation, is characterized by a shell-plasma proximity reduction, likely improving feedback coils action, thus favoring the study of the beneficial properties of helical states built upon helixes not resonating with the safety factor profile.

The second point regards the MHD description of the process of formation of transport barriers by macroscopic magnetic chaos healing, which allows the emergence of hidden Lagrangian structures acting as barriers to the transport. The radial position of such structures is observed to correspond to higher gradients of magnetic field lines connection length to the edge and to higher temperature gradients, computed by numerically solving the anisotropic heat flow equation. Comparison with thermal measurements in RFX-mod will also be offered.

#172 - MEV RANGE BREMSSTRAHLUNG MEASUREMENTS OF THE RUNAWAY ELECTRON DISTRIBUTION FUNCTION IN MID AND LARGE SIZE TOKAMAKS

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The mitigation of runaway electrons (RE) that may be generated in disruptions is among the key priorities for the safe operation of a tokamak based reactor. The most pursued mitigation techniques are currently based on the injection of a high Z impurity in the plasma (predominantly Argon) as a way to achieve RE dissipation. Examples are experiments based on Massive Gas Injection (MGI) or, more recently, Shattered Pellet Injection (SPI), which are presently conducted in tokamaks worldwide. In both cases, the aim of the experiments is to gain detailed physics insight on the mechanisms that drive the RE mitigation, which is achieved by comparing data from a broad range of RE diagnostics to currently available codes. The goal is to possibly validate the theoretical models so that the results of present experiments can be reliably extrapolated to machines of the next generation.

The RE distribution function is one of the most interesting parameters for validation, but this has also remained elusive for a large range of experimental scenarios. Recently, advancements in the development of gamma-ray spectrometers with MHz counting rate capabilities and, hence, millisecond time resolution have made spectral measurements of the hard x-ray (HXR) emission from REs at typical energies in the MeV range possible. These in turn depends on the RE distribution function, so that changes of the HXR spectrum reveal modifications of the velocity space dynamics of the REs.

In this contribution we present an overview of measurements of the RE distribution function by the detection of bremsstrahlung spectra in the MeV range in MGI and SPI experiments in mid and large size tokamaks. The measurements are obtained by observing the plasma with gamma-ray spectrometers displaced along multiple collimated sightlines which, in some cases, allow access to the spatial profile of the HXR emission, besides its energy spectrum.

We further discuss the deconvolution methods that are used to obtain the RE distribution function from the hard x-ray measurements and, in particular, to retrieve the maximum energy E_{max} of the RE beam and its evolution in the post-disruption phase. Finally, we compare the time evolution of E_{max} with a one-dimensional model that, albeit simplified, is capable to capture the gross features of our experimental findings for a number of scenarios.

#173 - ADVANCED COMPUTATIONAL METHODS: THE RELATIVISTIC LATTICE BOLTZMANN METHOD

Alessandro Gabbana (I) - University of Ferrara and INFN-Ferrara

Relativistic kinetic theory and relativistic fluid dynamics play an increasingly important role in several fields of modern physics, finding application both at large scales, in the realm of astrophysics, at atomic scales (e.g. in the study of the flow of electrons in graphene) and further down to subnuclear scales, in the realm of quark-gluon plasmas. This motivates the quest for powerful and efficient computational methods, able to accurately study fluid dynamics in the relativistic regime and seamlessly bridge the gap between relativistic and low-speed non-relativistic fluid regimes.

Recently, numerical schemes based on the Lattice Boltzmann Method (LBM) have emerged as a promising tool for the study of dissipative relativistic hydrodynamics.
The Lattice Boltzmann Method (LBM) is a class of computational fluid dynamics solver which has attracted much interest in the past three decades for the solution of the Navier-Stokes equations.
The method stems from the kinetic level and consists of a quadrature-based discretization of the Boltzmann equation on regular grids, in turn offering a large amount of easily identified parallelism;
LBM algorithms are therefore ideally suited for implementations using massively parallel codes, running on modern many-core HPC systems.

In this talk we give an overview of the algorithmic derivation of the relativistic Lattice Boltzmann Method, with special focus on computational related aspects. We also present the results of a detailed study on the transport coefficients connecting the mesoscopic parameters to the transport parameters of the associated dissipative hydrodynamic equations, which will serve as a solid basis for accurately calibrated computational studies of relativistic dissipative flows.

#174 - DISCONTINUOUS GALERKIN APPROACH FOR THE SIMULATION OF CHARGE TRANSPORT IN GRAPHENE

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In the last years an increasing interest has been devoted to graphene field effect transistors (GFETs) as potential candidates for high-speed analog electronics, where transistor current gain is more important than ratio current ON/current OFF [1]. Several types of GFETs have been considered in the literature [2]: top-gated graphene based transistors, obtained synthesizing graphene on silicon dioxide wafer, and double gate GFETs.
The current-voltage curves present a behaviour different from that of devices made of classical semiconductors, like Si or GaAs, because of the zero gap in monolayer graphene. The current is no longer a monotone function of the gate voltage but there exists an inversion gate voltage corresponding to which the type of majority carriers changes. This introduces a certain degree of uncertainty in the determination of the current-off regime which requires a rather well tuning of the

gate-source voltage.

Usually the considered type of devices are investigated by adopting reduced one dimensional models with some averaging procedure [3,4] and by describing the charge transport with drift-diffusion models, e.g. that proposed in [5].

Here we solve directly the semiclassical Boltzmann equation for electrons in graphene by using a discontinuous Galerkin (DG) method [6-9].

Numerical solutions of GFETs will be presented.

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#175 - COUPLED MOLECULAR DYNAMICS AND FINITE ELEMENT METHOD SIMULATIONS FOR THE KINETICS OF PARTICLES SUBJECTED TO FIELD MEDIATED FORCES

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A computational approach that couples Molecular Dynamics (MD) and the Finite Element Method (FEM) technique is here proposed for the theoretical study of the dynamics of particles subjected to electromechanical forces. The system consists of spherical or ellipsoidal particles (modeled as micrometric rigid bodies with proper densities and dielectric functions) suspended in a colloidal solution, which flows in a microfluidic channel in the presence of a generic non-uniform variable electric field generated by electrodes. The particles are subjected to external forces (e.g. drag or gravity) which satisfy a particle-like formulation that is typical of the MD approach, along with an electromechanical force that, in turn, requires the three-dimensional self-consistent solutions of correct continuum field equations during the integration of the equations of motion. In the MD-FEM method used in this work, the Finite Element Method is applied to solve the continuum field equations while the MD technique (both standard and rotational Verlet's schemes) is used for the stepwise explicit integration of the equations of motion. Our work shows the potential of coupled MD-FEM simulations for the study of electromechanical particles and opens a double perspective for implementing (a) MD away from the field of atomistic simulations and (b) the continuum/particle approach to cases where the conventional force evaluation used in MD is not applicable.

#176 - A SELF-CONSISTENT ARTIFICIAL NEURAL NETWORK INTER-ATOMIC POTENTIAL FOR LI/C SYSTEMS

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AThe increasing demand for high energy density lithium ion batteries motivates a search for alternative electrode materials. Experimentally obtained graphene-based structures have been suggested to replace the state-of-the-art graphitic anode[1]. In a recent work, we studied Li adsorption on single layer graphene at finite temperature via Monte Carlo with a site-based inter-atomic potential[2]. While the site-based potential successfully sheds light to Li clustering on graphene, a more flexible and accurate potential is needed to study Li/C interaction in battery environment. Here, we present a self-consistent approach to construct Li/C interaction potential where evolutionary phase space exploration[3] and accurate ***ab-initio*** energetics and forces [4] are integrated with Artificial Neural Network potentials within the PANNA code[5]. The performance of this potential is then assessed on a wide range of Li intercalated Carbon allotropes.

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#177 - MULTISCALE AB-INITIO/MONTE CARLO MODELLING FOR THE GROWTH KINETICS OF SIC SUBSTRATES AND NANO-PARTICLES

Giuseppe Fisicaro - Consiglio Nazionale delle Ricerche Istituto per la Microelettronica e Microsistemi (CNR-IMM)

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The growth of high-quality Silicon Carbide (SiC) substrates and nanoparticles is a topic of extreme technological interest due to the importance of this material for current and future technologies. Concurrently, such growth process is challenging due to the meta-stability of different crystal symmetries (polytypes) in the usual growth conditions. We report a multiscale theoretical analysis designed to study at an atomic resolution the growth kinetics of compounds characterized by the sp3-type bonding symmetry. First we explored the configurational space of cleaved and defective (adatoms and vacancies) surfaces with ab-initio structure predictions algorithms at density functional theory level. Then the atomistic configurations and energetics are input of a kinetic superlattice Monte Carlo code which simulates the growth kinetics of SiC substrates and nanoparticles. We explored several calibration paradigms starting from the ab-initio data. Formalization and implementation details are presented for the particular case of the 3C-SiC material. A key feature of this numerical tool is the ability to simulate the evolution of both point-like and extended defects. We focus on the evolution of antiphase boundary and stacking-fault defects for planar (100) substrates and nanoparticles. The growth of inverted pyramids on the (100) surface is also explored. Quantitative predictions of the microstructural evolution of the studied systems can be readily compared with the structural characterization of actual processed samples.

#178 - PHONON TRANSPORT CORRECTIONS IN THERMAL SIMULATIONS OF NANOSTRUCTURES DURING LASER ANNEALING

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Laser thermal annealing (LTA), with nanosecond range pulses, is the reference annealing technique in micro- and nano- electronics when strongly confined heating is needed in the semiconductor device manufacturing flows. The application of the process in future electronic device generations is hindered by the difficulties in the process control. LTA process is highly influenced by the interaction between electromagnetic (EM) field and complex device structures. Models of laser annealing process have been developed by for specific applications and implemented in academic or commercial packages. However, several limitations remain, in the previous modeling approaches for the general application in future devices, characterized by complex structures with nm wide elements made of different materials/phases, which currently hinders its applicability to realistic use cases. In this context we try to integrate phonon transport corrections to our existing simulation tool, LIAB (LASSE Innovation Application Booster) that will help us to reproduce experimental data and predict behavior of semiconductor structures upon laser annealing. In the work we present we are using the finite element methods (FEM) to solve Fourier’s Law (FL), and then to derive corrections to FL using the Chapman Enskog expansion of the Boltzmann’s Transport Equation (BTE) for phonons, knowing that bulk corrections follow the Fourier’s Law but boundary conditions are shown to be of temperature jump type. We simulated thermal transport induced by conventional and laser annealing in various structures like Si infinite nanowires and a Ge telescopic nanowire comparing the results in which standard conditions and corrections were applied, noticing that there is a discrepancy between standard and corrected solutions. This difference is greatly enhanced when we reduce the size of the structure, highlighting the fact that apparent thermal conductivity is size dependent. The code we developed uses the FEniCS computing platform for solving Maxwell Equations and FL and Gmsh as 3D finite element mesh generator.

#179 - NEW PERSPECTIVES IN BIOPHYSICS: SPATIOTEMPORAL CORRELATION SPECTROSCOPY OF DYNAMIC SUBCELLULAR NANOSTRUCTURES

Francesco Cardarelli (I) - Scuola Normale Superiore

Nanoscopic, dynamic, sub-cellular structures, such as synaptic vesicles, endo-/exo-cytotic vesicles, organelles, or entire cellular protrusions, are receiving increasing attention asessential intracellular platforms for signal transduction and, consequently, as a due target for a new era of *theranostic* strategies. Yet, a satisfactory understanding of living-matter physiopathology at this level remains one of the lingering challenges in molecular biophysics. This bottleneck can be now tackled by a straightforward combination of new imaging technologies and analytical approaches. This will be discussed by illustrating a number of recent/ongoing applications to paramount biological processes, including: the study of metabolism in small organelles, the vesicle-mediated intracellular transport of nanocarriers, the mechanism by which Insulin is packed into nanoscopic granules and secreted by pancreatic β-cells.

#180 - FROM EUKARYOTIC CHROMOSOMES TO THE PHYSICS OF CRUMPLED RING POLYMERS

Angelo Rosa (I) - Scuola Internazionale Superiore di Studi Avanzati (SISSA)

Other Authors: Ralf Everaers (Ecole Normale Supérieure de Lyon, Lyon, France)

In this talk, I will first introduce the audience to the relevant phenomenology of chromosome organization inside the nuclei of eukaryotic cells. Then, by employing simple and generic physical arguments, I will discuss how chromosome folding can be understood based on the analogy to unknotted and unlinked ring polymers which adopt "crumpled" conformations in dense solutions. The explanation of this analogy will offer the opportunity to discuss in detail the rich phenomenology of ring polymers: in particular, I will report about recent theoretical and computational work addressing the debated connection between ring polymers and melts of branched polymers.

#181 - MEMBRANE TENSION AS A REGULATOR OF MALARIA PARASITE INVASION IN RED BLOOD CELLS.

Pietro Cicuta (I) - University of Cambridge

Malaria has had a major effect on the human genome, with many protective polymorphisms such as sickle cell trait having been selected to high frequencies in malaria endemic regions. A novel blood group variant, Dantu, was recently shown to provide 74% protection against all forms of severe malariain homozygous individuals. This is a similar degree of protection to sickle cell trait and considerably greater than the most advanced malaria vaccine but, until now, the mechanism has been unknown. In the current study, we demonstrate a significant impact of Dantu on the ability of *Plasmodium falciparum* to invade RBCsobtained from children inKenya. The Dantu variant was associated with extensive changes to the RBC surface protein repertoire, but unexpectedly the malaria protective effect did not correlate with specific RBC-parasite receptor-ligand interactions. By following invasion using video microscopy, we found a strong link between RBC tension and parasite invasion. In fact even in non-Dantu RBCs we discovered that there is a tension threshold above which RBC invasion did not occur. Dantu RBCs had higher average tension, meaning that a higher proportion of Dantu RBCs could not be invaded. These findings not only provide an explanation for the protective effect of Dantu against severe malaria, but also provide fresh insights into the essential process of *P. falciparum* parasiteinvasion, and how invasion efficiency varies across the heterogenous populations of RBCs that are present both within and between single individuals. The talk will focus on the contributions to this work from Pietro Cicuta's lab, where automated microscopy and video

analysis techniques enabled live imaging, measurement of membrane tension and phenotyping of invasion events at the single cell level.

#182 - EXPLOITING THE TUNABILITY OF STIMULATED EMISSION DEPLETION (STED) MICROSCOPY FOR SUPER-RESOLUTION IMAGING

Luca Lanzano' - Istituto Italiano di Tecnologia

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Optical super-resolution is generally achieved by switching on-off the fluorophores by stochastic or targeted approaches [1]. For instance, in stimulated emission depletion (STED) microscopy, excited fluorophores located on the periphery of the Point Spread Function (PSF) are completely switched off by a doughnut-shaped beam, producing an effective PSF of smaller size. Recently, we have introduced an alternative strategy for super-resolution imaging, called separation of photons by lifetime tuning (SPLIT), based on the separation of the position-dependent fluorophore dynamics rather than fluorophore switching [2]. We demonstrated that the phasor-based analysis of lifetime variations generated in a CW-STED microscope produces a tunable, subdiffraction PSF that can be used for imaging subcellular structures [2].

Here we show that the SPLIT method is not limited to the analysis of lifetime variations generated in a CW-STED microscope but has a more general applicability in super-resolution microscopy. First of all, we show that the same principle can be applied to STED-Fluorescence Correlation Spectroscopy (FCS) for measuring molecular diffusion at tunable subdiffraction spatial scales [3]. Then, we present a method to enhance the spatial resolution of a STED microscope based only on the modulation of the STED intensity during the acquisition of a STED image [4]. Finally, the application of SPLIT to another popular targeted superresolution methods, Structured Illumination Microscopy (SIM), is discussed.

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#183 - BIOCOMPATIBLE LUMINESCENT SILICON NANOSTRUCTURES FOR LABEL-FREE TIME-GATED IN VIVO IMAGING IN HYDRA VULGARIS

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Luminescent porous silicon nanostructures have gained great attention as label-free probes for bioimaging and even theranostic applications in the last years, thanks to the demonstrated biocompatibility, easily tunable surface chemistry, high surface-to-volume ratio and peculiar optical properties[1]. In this regard, they constitute a promising alternative to highly toxic heavy metal-based semiconductor quantum dots[2].

In the present work, we present an *in vivo* study exploiting highly luminescent biocompatible porous silicon nanoparticles (PSiNPs) as label-free probes. To stabilize the emissive nanocrystals in biological conditions, a thermal treatment with undecylenic acid (UA) has been carried out to

passivate the NPs surface. Previous characterizations have shown bright photoluminescence (PL quantum yield >10%), effective preservation of all the relevant photonic properties (steady-state PL intensity; wavelength-dependent PL lifetime >30 μs at maximum emission) and morphological stability for up to 6 h incubation in physiological medium (at pH = 7.4) after UA capping, thus preventing the otherwise uncontrolled oxidation of the material[3].
Hydra vulgaris is used as *in vivo* model for internalisation studies by virtue of its tissue-like structural complexity: it basically consists of a tube made up of two connected epithelial cell layers, namely ectoderm and endoderm. Therefore, it is simpler than vertebrates, with specific apparatuses, but more complex than cultured cells. Moreover, the degree of morphological damage of *Hydra* can be quantified and correlated to the toxicity of the surrounding environment. Indeed, both organic and inorganic compounds may induce behavioural response and cause severe tissue damages[4]. Hereof, the morphological preservation of *Hydra* after 72 h exposure at high concentrations of UA-modified PSiNPs, which is a long term period compared to the animal life cycle, has been verified by direct microscope observation, demonstrating the biosafety of the material.
To conclude, the peculiarly bright tissue autofluorescence can be bypassed by exploiting the long PL lifetime of UA-modified PSiNPs, making them prone to the use of the time-gated imaging technique[5]. Therefore, we show that we can effectively pursue a temporal discrimination of the signals, getting rid of the undesired ns-lived endogenous fluorescence component, and quite rapidly achieve (at ~1 Hz sampling rate) a dynamic framing of the motion of *Hydra* as well as the probe internalization mechanisms *in vivo*.

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#184 - SEQUENCE AND STRUCTURAL PATTERNS DETECTED IN ENTANGLED PROTEINS REVEAL THE IMPORTANCE OF CO-TRANSLATIONAL FOLDING

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Proteins must fold quickly to acquire their biologically functional three-dimensional native structures. Hence, these are mainly stabilized by local contacts, while intricate topologies such as knots are rare. Here, we reveal the existence of specific patterns adopted by protein sequences and structures to deal with backbone self-entanglement. A large scale analysis of the Protein Data Bank shows that loops significantly intertwined with another chain portion are typically closed by weakly bound amino acids. Why is this energetic frustration maintained? A possible picture is that entangled loops are formed only toward the end of the folding process to avoid kinetic traps. Consistently, these loops are more frequently found to be wrapped around a portion of the chain on their N-terminal side, the one translated earlier at the ribosome. Finally, these motifs are less abundant in natural native states than in simulated protein-like structures, yet they appear in 32% of proteins, which in some cases display an amazingly complex intertwining.

#185 - TRANSLOCATION, BIOLOGICAL FATE AND TRANSFORMATION OF NANOMATERIALS IN BIOLOGICAL MATRIXES

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Tracing nanomaterials (NMs) in biological matrixes and moreover, determining the intracellular or organ dose of NMs pose several challenges since NMs are not easy to visualize and to quantify once in a biological environment. However, NMs dose at cell and body level and NMs fate and translocation are fundamental aspects regarding the application of NMs in biomedicine and for understanding toxicological end points of NMs.   In this presentation NMs fate *in vitro* and*in vivo* will be discussed mainly in relation with their quantification and stability.. Cell uptake and intracellular fate of NMs will be followed by Confocal Raman Microscopy, Ion Beam Microscopy and Confocal Laser Scanning Microscopy. The interaction of NMs with biomolecules, protein corona formation and the aggregation behavior of nanoparticles will be investigated by means of Fluorescence Correlation Spectroscopy (FCS) in cell culture media and in live cells. Fluorescence Cross Correlation Spectroscopy (FCCS) will be applied to study the intracellular stability of protein corona.

The bio distribution, organ accumulation and fate of radiolabelled NMs will be studied in animal models by means of Positron Emission Tomography (PET) and Single-Photon Emission Computerised Tomography (SPECT). A dual radiolabelling strategy of nanoparticle core and coating will be presented using gamma emitters with non overlapping emission bands. After intravenous administration into rats, energy-discriminant resolve each radioisotope independently revealing different fate in vivo for the core and coating, which will be used to evaluate NP integrity.

#186 - 3D NANOMETRIC PARTICLE TRACKING OVER TUNABLE AXIAL RANGES

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The precise localization of nanometric objects in three dimensions is essential to identify functional diffusion mechanisms in complex systems at the cellular or molecular level. However, most optical methods can achieve high temporal resolution and high localization precision only in two dimensions or over a limited axial range. Here we develop a novel wide-field detection system based on an electrically tunable lens that can track multiple individual nanoscale emitters in three dimensions over a tunable axial range with nanometric localization precision. The optical principle of the technique is based on the simultaneous acquisition of two images with an extended depth of field while encoding the axial position of the emitters via a lateral shift between images. We provide a theoretical framework for this approach and demonstrate tracking of free diffusing beads and GABAA receptors in live neurons. This approach allows getting nanometric localization precision up to an axial range above 10 μm with a high numerical aperture lens. Synchronization or complex fitting procedures are not requested here, which leads to a suitable architecture for localizing single molecules in four dimensions, namely, three dimensions in real-time.

#187 - COLLAGEN FIBRILLOGENESIS INVESTIGATED BY MOLECULAR DYNAMICS AND UV SPECTROSCOPY TECHNIQUES

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Collagen is a fibrous protein representing the main constituent of connective tissue in mammals, with a basic structural unit called tropocollagen that is a triple helix consisting of Gly-Xaa-Yaa repetitions, in which one-thirds of the X and Y residues are either prolines or hydroxyprolines. Collagen triple helices associate in fibrils, where tropocollagens are staggered side-by-side with a shift of 67 nm (234 residues) between two neighbours.

To investigate the assembly mechanisms, collagen aggregation was studied by means MD simulations both at physiological conditions and at low ionic strength.

Two tropocollagen fragments with different hydropathic profiles were chosen and built from ***Rattus norvegicus*** type I collagen sequence. Other fragments were selected from the same sequence with a shift of 234 residues upstream and downstream of it. Repeated MD simulations suggest that tropocollagens prefer to associate in pairs, with first approach between hydrophobic regions, suggesting that the mechanism is mainly driven by hydrophobic effect and mediated by hydroxyprolines. Association of two, three or four fragments shows that the amino-acidic composition of the triple helices strongly influences their assembly propensity: poorly charged (PC) segments easily associate at 0.1 M salt concentration, contrary to highly charged (HC) ones. As expected, HC fragments are more suited to self-assembly at low ionic strength.

Collagen self-assembly was monitored *in vitro* by measuring the turbidity changes of the solution as observed from the increase in absorbance at 310 nm. Rat tail tendon collagen was prepared at low temperature and at different pH. Curves of aggregate fractions vs time display a sigmoid profile, indicating, according with literature, a cooperative process with a lag phase whose length depends on the solution pH.

#188 - KINETIC BOUNDS FOR NONEQUILIBRIUM SYSTEMS

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Many stochastic processes at the mesoscale level are expected to work properly and efficiently for producing a specific result. Circadian clocks should oscillate regularly despite of the noise due to the environment and the stochasticity of small systems; as another example, molecular machines need to pull cargoes with a regular speed by exploiting the ATP fuel in order to beat not only the external load but also stochastic fluctuations [1].

We show that in the typical far-from-equilibrium stochastic regimes there exists a limitation to the performances that is of kinetic rather than thermodynamic origin [1,2]. The expectation that a dissipation of more resources allows a better battle against randomness, thus improving performances, is often not met. The reason is that the dynamical activity of the system determines other limiting constraints when far from equilibrium. The dynamical activity, or frenesy, is a time-symmetric non-dissipative aspect of the dynamics that quantifies the degree of agitation of a stochastic system. This quantity is needed in successful descriptions of nonequilibrium systems, in addition to the notion of entropy production.

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#189 - DYNAMICS OF LARGE DEVIATIONS

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We consider systems with a non-trivial probability distribution of an observable O exhibiting a a singularity in O_c. Fluctuations with O>O_c are characterized by a condensation phenomenon: whenever O>O_c the system populates a narrow region of phase-space and a single mode grows macroscopic, similarly to what happens in the usual Bose-Einstein condensation. We consider the evolution of a rare fluctuation from an initial state without condensation to a final one where consensation occurs. The problem is studied analitically in solvable paradigmatic models of statistical mechanics. We show that the dynamics in this case is non trivial as due to the build up of the mode contributing macroscopically, and resembles that of a system brought across a phase-transition.

#190 - THERMODYNAMIC UNCERTAINTY RELATION VIA SECOND LAW OF THERMODYNAMICS

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We consider a Brownian particle in harmonic confinement of stiffness k, in one dimension in the underdamped regime. The whole setup is immersed in a heat bath at temperature T. The center of the harmonic trap is dragged under any arbitrary protocol $\lambda(t)$ starting from $\lambda(0)=0$. The thermodynamic uncertainty relation for both position of the particle and the current at time t are obtained using the second law of thermodynamics for both underdamped and overdamped cases.

#191 - DYNAMICAL PHASE DIAGRAM OF A QUANTUM ISING CHAIN WITH LONG RANGE INTERACTIONS

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We investigate the effect of short-range correlations on the dynamical phase diagram of quantum many-body systems with long-range interactions. Focusing on Ising spin chains with power-law decaying interactions and accounting for short-range correlations by a cluster mean field theory we show that short-range correlations are responsible for the emergence of a chaotic dynamical region. Analyzing the fine details of the phase diagram, we show that the resulting chaotic dynamics bears close analogies with that of a tossed coin.

#192 - QUENCH DYNAMICS OF THE ORDER-PARAMETER STATISTICS

Mario Collura - Padova University

One of the paradigms of quantum mechanics is the statistical nature of measurements: the result of measurements is indeed described by a probability distribution function (PDF), and measuring the same observable in identical systems will give different outcomes in accordance with this distribution. The PDF carries very detailed information about the system, going much beyond the simple average. Here we exploit the Matrix Product Operator representation of the Generating Functions to efficiently perform local measurements in one-dimensional spin systems using Tensor Network Methods, both in and out-of-equilibrium. We study this process for the paradigmatic case of the spin-1/2 Heisenberg XXZ chain and the transverse field Isign quantum chain. We determine the full quantum mechanical distribution function of the local order-parameter as a function of time after a quantum quench from a fully ordered state. This provides a detailed picture of how the order melts and reveals the existence of an interesting regime where the stationary order-parameter statistics is indeed related to that of the ground state.

#193 - PHASE DIAGRAM OF ACTIVE DISKS IN TWO DIMENSIONS

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We study the phase diagram of active disks interacting by short range repulsion [1]. At small activity, we find that the 2D melting behavior of passive hard disks still holds with a continuous Halperin-Nelson transition between the solid and hexatic phases, and a first order transition between the hexatic and liquid phases, when density or packing fraction are decreased at constant temperature.
By increasing activity, hexatic-liquid coexistence reduces to a critical line that reaches at high activity another coexistence region where clusters and a dilute phase are observed. We study the role of defects in the different transitions. We also show the differences with the phase diagram of active dumbbells where the coexistence region continuously extend from the passive limit to high activity [2].

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#194 - A LONG-RANGE CONTACT PROCESS FOR THE EPIGENETICS SPREADING

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Other Authors: Davide Marenduzzo (University of Edinburgh), Davide Michieletto (University of Edinburgh)

Several kinds of the so-called ``contact-process" model have been proposed over the past years to rationalise critical behaviours in the presence of absorbing states. Different realizations of the contact-process can fall in the celebrated universality class of Directed Percolation (DP), which is the paradigm for non-equilibrium phase transitions with a single absorbing state. Nevertheless, real systems which can be described by DP are very rare. Additionally, changing the nature of the absorbing states in a subtle way can lead into a totally different universality class.

In our work we propose a 1D contact-process with two absorbing states, to study the competition between epigenetic writers and erasers of methylation marks on chromatin in living cells. Our model displays a nonequilibrium transition between an unmethylated and a methylated state, as well as a spinodal line separating a regime with bistability from one without. When the spreading of epigenetic marks is short-range, our model belongs to the Compact Directed Percolation (CDP) universality class. When the spreading process is long-range, and modelled by a Levy flight (which constitutes a more realistic hypothesis biologically), the behaviour at the transition changes dramatically. We find that the survival probability exponent depends continuously on the contact exponent, and displays a crossover between an exponential and a power-law decay regime as system parameters vary. Our simple model also provides a possible mechanism for the stochastic spreading of epigenetic marks in populations of genetically identical yeast cell.

#195 - PHOTOCATALYTIC SYNTHESES: GREEN CHEMISTRY APPLICATIONS FOR A SUSTAINABLE DEVELOPMENT

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Photocatalytic syntheses: Green chemistry applications for a sustainable development

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Heterogeneous photocatalysis is a promising technology based on the capability of semiconducting materials to generate charges upon irradiation of suitable energy. The photogenerated electrons and holes induce redox reactions involving species adsorbed on the surface of the photocatalyst giving rise to chemical transformations. The presence of oxidizing radicals thereby generated made photocatalysis long believed as an unselective oxidation process. In fact, it has found hitherto applications in the field of environmental remediation as a tool to degrade pollutants. However, it is possible to perform highly selective synthetic reactions by carefully tailoring crystallinity, surface and structural properties of the photocatalyst, and its interaction with the substrates [1]. This is testified by the increasing number of photocatalytic syntheses published so far, such as selective partial oxidations, reduction reactions, coupling reactions, and fuels production [1,2 and references therein]. Moreover, it is possible to perform these reactions under mild operating conditions, by using cheap and abundant solar light, and in full compliance with the "green chemistry" requirements described by Anastas and Werner [3] in 1998. Due to these features, photocatalysis can compete with the traditional synthetic routes, which generally require drastic experimental conditions. The efficiency of photocatalytic organic syntheses can be further improved by acting on parameters related to the engineering of the reaction system and by coupling photocatalysis with other advanced oxidation processes and membrane separation units.

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#196 - CELLULOSE ACETATE/SNO2: ULTRAFINE FIBROUS MATS FOR THE PHOTO-CATALYTIC DEGRADATION OF ORGANIC DYES

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The rapid growth of the population and industrialization in combination with the limited availability of water resources, results nowadays in the enhanced demand for efficient treatment of industrial and urban wastewaters. This, in combination with the fact that the conventional treatment processes are often not effective due to the presence of a continuously growing number of substances classified as harmful contaminants, raises the need for the development of new, innovative, and sustainable materials and methods for efficient remediation processes (1).

In such scheme, in the last decades, semiconductor nanoparticles (NPs) based photocatalytic processes are among the most promising technologies for the removal of organic pollutants from aquatic environments (2)(3). The embedding of NPs in the polymeric matrix can overpass the limitation limitation of the powder based photocatalysts, and therefore to minimize the post-treatment steps and the costs of the purification procedure.

In this work, the preparation of Cellulose Acetate (CA) fibrous mats consisted of two steps, the electrospinning of polymer/tin salt solution and the consequent ***In Situ*** thermally activated conversion of salt in SnO_2 directly in the solid fibrous matrix. The morphological characterization (HR-SEM, TEM and XRD analysis) confirm the presence of NPs; these are directly grown on the surface of the ultrafine fibers, are highly reactive and guarantee the oxidation role in the photocatalytic process under UV light.

In particular, the photo-catalytic properties of the developed material are tested in the presence of methyl orange and methylene blue, proving that the mats are able to photodegrade both dyes with efficiency higher than 90%. The LC-MS characterization of the treated solutions confirm that the dyes are degraded in other species.

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#197 - NEW STRATEGIES BASED ON MULECULAR IMPRINTED POLYMERS FOR WATER REMEDIATION

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The presence of pharmaceuticals, such as non-steroidal anti-inflammatory drugs (NSAIDs) and antibiotics in the aquatic environment, represents a worldwide threat. These drugs are indeed considered “emerging contaminants” of water since the traditional methods are not designed to efficiently remove them. Aiming to overcome the limits of the conventional wastewater treatment plants, we propose molecularly imprinted polymers (MIPs) as valid materials for selective adsorption and removal of these drugs from water. MIPs are synthesized by polymerization of cross-linking and functional monomers in the presence of a target analyte, which acts as a molecular template. Following the polymerization, the template is removed to leave cavities with molecular memory for the analyte, allowing the polymer to rebind the analyte with a very high specificity.

In particular, we have prepared a polymeric powder for the selective removal of diclofenac, one of the most common NSAIDs, by a simple bulk polymerization process. After an extensive characterization, the adsorption abilities of the synthesized polymer were evaluated and compared with those of a corresponding non-imprinted polymer used as reference. Thanks to the imprinting effect, the prepared MIP adsorbs with extreme selectivity its template molecule, i.e. the diclofenac. This effect was evaluated by testing the adsorption abilities towards several organic pollutants.

Another promising approach, that we have undertaken consists in the realization of a selective adsorbent by the surface molecular imprinting technique. In this method the MIP is grafted on a surface of a material, e.g. Fe_3O_4 particles. The outside layer of the resulting core-shell microspheres is formed by the MIP and acts as the selective adsorbent of water contaminants. Instead, the magnetic core facilitates the recovery of the powders after water treatment. Such peculiarity, that represents the novelty of this work, opens the route for the application of the MIP materials for water treatment on a large scale.

#198 - FORMULATION OF NICKEL-FREE 3D GRAPHENE FOR VISIBLE-LIGHT PHOTOCATALYSIS

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One of the most persistent problem affecting the twenty-first century is the environmental pollution and the insufficient access to clean and sanitized water. The visible-light photocatalysis (VLP) represents one of the promising environmental-friendly technology, taking advantage in the use of solar-light as clean and renewable source. In this context, the combination of organic photosensitizers with graphene can improve the photocatalytic activity by boosting the separation and transfer of photo-generated charges. We formulated a freestanding material combining polymer porphyrins by π-π interaction with 3D-graphene (3DG) via a time-saving etching procedure to remove Nickel substrate [1,2]. The latter, could constitute a critical issue being released as Ni^{2+} in water during the purification step. Moreover, its removal can determine higher graphene surface exposure to the light irradiation improving the photocatalytic process. The photocatalytic activity of the novel hybrid composite was evaluated by photo-degradation of Methylene Blue. Photoluminescence measurements were performed as well as free-radical and hole scavenging measurements. Finally, we propose a photocatalytic mechanism, reporting for the first time the HOMO and LUMO energy levels of poly-porphyrins calculated by electrochemical study.

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#199 - SINGLE ATOM CATALYST: H2 DISSOCIATION ON SINGLE NOBLE METAL AT CERIUM OXIDE (111) SURFACE

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Single atom catalyst (SAC) is the new frontier of heterogenous catalysis: where the cat- alyst consists of single metal atoms dispersed on a support [1]. This is the most efficient way to exploit every single metal atom, but the role of the atom in the catalysis is cur- rently unclear [2]. To clarify this aspect, we have studied the effect of the SAC in the activation of the Hydrogen molecule on the CeO2 (111) surface. The oxidation of H2 is a very important process because it is the reaction occurring at the anodes of proton ex- change membrane fuel cells (PEMFC), which could represent the next generation power sources [3] or a step in the synthesize of chemical products [4].

We have focused on single Ag catalysts, and compared them to Cu and Au. For all the noble metals we have considered different configurations: atom adsorbed on the surface, atom substituting a Ce on both the stoichiometric and the reduced CeO2(111).

Density functional calculations (DFT) have been carried out using the Quantum Espresso Package [5],[6]. The Hubbard correction has been added on the f orbitals of the cerium atoms due to the strong electron correlation in these orbitals. The potential energy pro- files along the Minimum Energy Pathway (MEP) have been obtained using the CI-NEB [7].

We have found that when a single nobel metal atom is adsorbed on CeO2, the activa- tion energies drop with respect to those of pure ceria, and in particular they are slightly lower for Ag than Au and Cu. Instead, when the noble metals substitutes a Ce atom, we have calculated that only for Ag a significative decrease of the barrier energy occurs. If an Oxygen vacancy is present on the surface then both Ag and Au are good catalysts, whereas the activation energy for the reaction is larger for Cu.

Charge transfers play a key role in determing the catalytic noble metal behavior: the noble metal facilitates the oxidation of H2 if, following the breaking of the molecule, it could reach its favorite oxidation state by acquiring the H2 electrons.

Thus, Ag is the best single atom catalyst in the activation of H2 on the CeO2(111) sur- face: indeed, for all the examined configurations of Ag on the (111) ceria surface, the H2activation energy is remarkably lowered.

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#200 - LOW-COST SYNTHESIS OF NIO NANOFOAM FOR SELECTIVE NO2 DETECTION AT ROOM TEMPERATURE

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Gas sensing is receiving increasing attention driven by the need to ensure human safety by monitoring pollutant gases in the atmosphere such as NO_2. Gas sensors based on metal oxides operating at room temperature are of great interest due to their energy saving and cost effective characteristics. Among the different materials investigated so far there is NiO, even if there are only a few reports regarding the low-cost fabrication of high-performance NiO-based sensors. In this work, we designed and fabricated a novel NiO nanofoam by a low-cost approach and applied it for the detection of NO_2 at room temperature. $Ni(OH)_2$ nanowalls were directly synthesized onto interdigitated contacts by chemical bath deposition and converted into a 3D network of NiO nanoparticles (30-50 nm in size) through thermal annealing. Sensing tests showed a high response to NO_2 at room temperature even for the lowest concentration of 140 ppb. In addition, the sensor presented an excellent selectivity at room temperature vs high concentrations of acetone, methane, CO, CO_2, H_2. A model is presented to explain the improved NO_2 sensing performances at room temperature. The unique characteristics of the NiO nanofoam make it a potential candidate also for other applications such as electrochemical (bio)sensing, catalysis, energy storage.

#201 - INVESTIGATION OF ZNO-DECORATED CNTS FOR UV LIGHT DETECTION APPLICATIONS

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UV sensor technology has shown to be suitable for applications in many important fields including agriculture, medical diagnostics, healthcare, space & climate research and environmental monitoring. Various UV-sensitive materials and detectors have been reported in the last decade, which include silicon and silicon carbide or sensors based on ZnO, TiO_2, GaN and Ga_2O_3 [1,2]. Among all these sensor materials, the Metal Oxide Semiconductor materials are the most developed because of high sensitivity, relative low price and other superiority characteristic. On the other hand the main drawbacks of these materials are the high operation temperature and high power consume [3]. Today, innovative UV sensors with high sensing properties operating at room temperature and simultaneously with low power consume and high thermal and electronical stability is strongly required. An attractive method to achieve that goal is to couple ZnO with carbon nanotubes, in order to form a hybrid system having the properties of both components. Moreover, such hybrid layer could attract considerable attention due to high degree of flexibility on bendable substrates [3,4]. In this work we report the preparation of multi-walled carbon nanotubes (CNTs) decorated with zinc oxide nanoparticles (ZnO NPs), with different weight ratios, in isopropanol solution by a simple and room temperature process. The nanocomposites were characterized from structural, morphological, electronic and optical points of view. A strong interaction between ZnO and CNTs is fully confirmed by all the characterization techniques. The combination between CNTs and metal oxide provides the electrical transduction element and the sensitive material, respectively. ZnO NPs-CNTs nanocomposites were deposited as a dense layer between two electrodes, in order to investigate the electrical behaviour. The electrical response of the nanocomposite layers to UV light irradiation was recorded, for a fixed voltage: as the device is exposed to the UV lamp, a sharp current drop takes place and then an increase is observed as the irradiation is stopped. The effect can be explained by oxygen adsorption and desorption phenomena taking place on the ZnO nanoparticle surface under irradiation and by charge transfer between ZnO and CNTs, thanks to the strong interaction between the two nanomaterials. The nanocomposite material shows good sensitivity and fast response to UV irradiation. Room temperature and low cost processes used for the device preparation,compatible with low cost plastic substrates, combined with room temperature and low voltage operational conditions make this methodology very promising for large scale UV detectors applications.

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#202 - FREESTANDING OXIDE HETEROSTRUCTURE MEMBRANES PRODUCED BY DISRUPTIVE STRAIN RELAXATION

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Two-dimensional electron gases (2DEGs) at oxide interfaces, as $LaAlO_3/SrTiO_3$ (LAO/STO) and its several variants, show multiple functional properties of major physical interest, including a high low-temperature mobility, superconductivity, a large Rashba spin-orbit coupling, an exceptionally large spin-to-charge conversion efficiency and a yet controversial magnetic ground state. Such properties are tunable under external control parameters, as electric field effect. In a number of experiments briefly described in the talk, we will first show the capability of tailoring unexpected samples properties by pushing growth control of our crystalline interfaces to the highest level. We will then focus on the control of strain relaxation, selecting the conditions in which an epitaxially strained state is retained much above the expected critical thickness. In this regime, strain relaxation is highly disruptive and surprisingly causes the formation of freestanding LAO/STO membranes, which preserve the metallic properties of macroscopic LAO/STO samples. Such membranes can be manipulated, contacted and employed as elements of microscopic circuits on a generic surface.

#203 - STRAIN RELAXATION MECHANISMS IN INAS/INP/GASB CORE-MULTISHELL NANOWIRES

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InAs/GaSb core-shell nanowires (NWs) have attracted great attention because of very low lattice mismatch (0.6%), broken-gap band alignment (type-II) and small effective masses of electrons and holes in InAs and GaSb regions, respectively. Electronic devices fabricated with these heterostructures combine closely-spaced n-type and p-type conductors, and can display negative differential resistance due to transport across the broken gap junction [1]. Further interesting electronic configurations can be achieved if carriers in the InAs core and GaSb shell are decoupled [2]. To this end, in the present work we have inserted a thin InP barrier of different thicknesses in between InAs core and GaSb shell. Since InP is lattice mismatched with InAs and GaSb, understanding the strain relaxation in this system is crucial in view of its applications in NW-based electronic devices. Catalyst-free InAs/InP/GaSb core-multishell NWs are grown by chemical beam epitaxy on Si (111) substrates. Detailed morphological, structural and compositional studies of the NWs as a function of growth parameters are carried out by scanning and transmission electron microscopy and energy-dispersive x-ray spectroscopy.

Furthermore, by combining the application STEM-Moiré technique with geometric phase analysis (GPA), we have derived the residual strain in this system.The results reveal that in InAs/InP/GaSb core-multishell NWs with 1 nm thick InP barrier few defects were established at all {112} side facets, and no defects are found in {110} side facets. When the InP layer thickness is increased to 8 nm, defects were distributed along {110} side facets while the {112} side facets are defect-free. Finally using core-multishell NWs with InP thickness exceeding 9 nm, we fabricated nanowire-based electronic devices. We performed two-probes DC transport experiments, in the temperature range from 300 K down to 4.2 K, measuring the electrical current as a function of the applied source-drain bias and the back gate voltage applied to the SiO_2/Si++ substrate. Preliminary results indicate effective suppression of nonlinear features in the I-V characteristics of the shell-shell contact geometry.

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#204 - POLYMER NANOCOMPOSITES BASED ON SI NANOSTRUCTURES COUPLED WITH C NANOTUBES

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Polymer nanocomposites constitute an emerging class of versatile materials where the inclusion of appropriate nanofillers is intended to enhance or modify the polymer matrix properties. Such nanocomposite materials are conceived for multiple applications, spanning from agile mechanical materials or devices to drug delivery systems to sensors. In this work, composite films are prepared using polyEthilene-co-Vinyl Acetate (EVA) as the polymer matrix, and both Silicon NanoStructures (SiNSs) and Multi Walled Carbon Nanotubes (MWCNTs) as nanofillers. The SiNSs are used to investigate the optoelectronic properties of the nanocomposite films while the MWCNTs are incorporated to improve their electrical conductivity. A two steps process is used for the film preparation, namely ball milling of the powder followed by their film casting via hot-pressing. The structural, electrical and optical properties of the different nanocomposite films were systematically investigated as a function of the different SiNWs and MWCNTs loadings. In particular, the loading of 15% w/w MWCNTs improved the nanocomposite electrical conductivity of several orders of magnitude, making it highly conductive. In conclusion, our study demonstrates that the easy processing of polymers associated with the peculiar properties of Si based nanostructures and MWCNTs, could give rise to a variety of novel nanocomposites which can be exploited for future applications in flexible optoelectronics.

#205 - STRUCTURAL AND ELECTRONIC PROPERTIES OF METALLO-PORPHYRINES ADSORBED ON FE(001)-P(1X1)O

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Chemisorption of a single atomic layer of oxygen on the Fe(001) surface yields a highly ordered and reproducible benchmark substrate [1] for experimental and for theoretical studies, and for the epitaxial growth of metal oxides and hybrid interfaces [2] with foreseen applications, e.g., in organic spintronics. Within this realm, we focus on self-assembled monolayers of porphyrin molecules, whose surface chemistry finds various scientific and technological applications [3], adsorbed on the Fe(001)-p(1x1)O surface.

We combine experimental studies by scanning tunneling microscopy, low-energy electron diffraction, and electron spectroscopies, with theoretical simulations based on density functional theory with a dispersion-corrected functional. We describe the adsorption properties of simple flat metallo (Me)-porphine and of Me-tetra-phenyl-porphyrin (MeTPP, with Co,Ni,Zn) in the experimentally observed square lattice. The adsorbed MeTPPs exhibit a significant distortion with flattening of phenyl rings and saddle deformation of the porphine structure. We then focus on the electronic and magnetic properties, finding that the magnetic character of the substrate acts markedly different in the three MeTPP considered, ranging from the antiferromagnetic coupling of spin-polarized CoTPP to a mild influence for ZnTPP (as found in our previous investigation of C_{60} on the same substrate [4]), while NiTPP sets at an intermediate stage, despite its non-magnetic character as a free molecule.

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#206 - ARE GOOD QUALITY SIMULATIONS OF WATER-CARBON INTERFACES POSSIBLE WITH MODERN COMPUTATIONAL TECHNIQUES?

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The adsorption of water on carbon nanostructures, such as graphene and carbon nanotubes, is of great scientific and technological interest. It is a widespread system involved in numerous applications like filtration, desalinisation, or lubrication. Experiments provide useful insight but struggles at yielding a molecular level understanding, and lack of knowledge limits the progress of emerging technologies. Computational approaches are asked to provide the missing information. This poses a big challenge to the present methodologies, where classical potentials lack the required accuracy and electronic structure approaches are asked for a very careful evaluation of electron correlation effects.

Even for the most fundamental system, a single water molecule interacting with graphene, the nature of the interaction has been long debated and only recently a definitive answer has been given through an extensive set of complementary state-of-the-art computer simulations on some of the world's largest supercomputers [1].

Here we characterize the nature of water-carbon interfaces via several highly accurate evaluations of interaction energies obtained deploying reference electronic structure methods like coupled cluster (CC) and diffusion quantum Monte Carlo (DMC).

As CC and DMC are computationally too expensive to be employed in long molecular dynamics simulations, we compare the reference evaluations with predictions from more affordable approaches. The comparison highlights the level of confidence of available methods. Modern vdW corrections to density functional theory prove promising and significantly improved over their precursors. Machine learning potentials could be the ultimate approach, allowing to scale up in system size without compromising the accuracy.

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#207 - HOPG ELECTROCHEMICAL EXFOLIATION STUDIED BY LOW-ENERGY ION BOMBARDMENT IN A COMBINED TOF-SIMS/SPM TOOL

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Graphene has been intensively studied due to its powerful mechanical, optical, thermal and electronic properties. The present crucial development of graphene research is, besides the insight of the fundamental aspects, being able to synthesize high-quality graphene on large-scale and control over its production phases.Graphene sheets are naturally stacked inside Highly Oriented Pyrolytic Graphite (HOPG) and its exfoliation into one-atom-thin sheets can be electrochemically achieved in electrolytic solutions. The final preservation of graphene properties is closely dependent to the changes that occur in the graphitic matrix during such electrochemical routines. Currently, complete knowledge of the chemical and physical processes at the base of such changes has not been experimentally explained yet. In this work, we describe from a chemical point of view, by using a new approach combining ToF-SIMS under low-energy ion sputter beam conditions and *in-situ* SPM, the effects of the ions intercalation on the HOPG surface and bulk. We will show, with molecular accuracy, the structural connection between the surface defects and the spatial arrangement of the molecular groups from the solvent. Furthermore, a new picture of the ion intercalation process, based on the results of low-energy ion beam depth profiling experiments, will be proposed.

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#208 - A MULTI-SCALE APPROACH TO LASER-INDUCED EFFECTS ON ZNO NANORODS FOR BIOSENSING APPLICATIONS

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In the development of nanostructured devices, Zinc oxide (ZnO) represents an appealing choice among the several metal oxides because of its easy growth process, biocompatibility, wide bandgap (3.4 eV), tuneable resistivity, etc.

The electrical properties of devices based on ZnO thin films are heavily affected by the surface morphology [1]. Hence, by properly tuning the surface morphology, it is possible to optimise the material properties.

In the case of ZnO nanorods (ZnO-NRs), excellent candidates for biosensing applications, the surface morphology can be tuned by means of the local heating induced by excimer laser: upon irradiation, the nanorods are either partially melted or even completely ablated, depending on the laser fluence [2]. Such effect can be exploited to tailor the ZnO-NRs conductivity, modifying the response of the final sensing device. However, a fine understanding of the specific chemical and physical mechanisms determining the sensing phenomena on the local and on the macroscopic scale is still missing and it is fundamental for optimal performances.

Such a challenging task requires the use of a versatile, non-destructive probe capable of investigating not only the structural, electronic, and chemical properties of the ZnO-NRs but also their complex interplay. Synchrotron radiation (SR), thanks to the high penetration depth and tunability, is the perfect tool to perform similar multi-scale investigations yielding complementary information on the properties of the system.

In this work, SR X-ray Photoemission Spectroscopy (XPS), Ultraviolet Photoemission Spectroscopy (UPS), and X-Ray Diffraction (XRD) were employed to probe the ZnO-NRs local structure, their long-range crystalline order, and their electronic properties. The complex picture emerging from these techniques provides details on the laser-induced effects in terms of nanorods morphology and homogeneity, crystalline arrangement, chemical state, and electronic structure. Furthermore, the outcome of this combined analysis was interpreted taking into account the evolution of the system morphology and electrical response probed by laboratory techniques. Our results provide the key to enhance the sensor properties as well as to increase the device selectivity and sensitivity.

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#209 - ELECTRONIC PROPERTIES AND MAGNETIC COUPLING OF HIGHLY ORDERED CO TETRA PHENYL PORPHYRIN LAYERS ON OXYGEN-PASSIVATED FE(001)

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Ultra-thin films of magnetic molecules grown on a magnetic substrate are promising candidates for future hybrid electronic devices such as memories or other components where they are used as coupling layers or spin filters [1,2]. A key point for the development of such systems is the understanding of the complex chemical and electronic interactions occurring at the interface with the substrate. Magnetic substrates such as transition metals are characterized by very reactive surfaces and therefore strongly modify the physical and chemical properties of chemisorbed molecules, making it difficult to predict and control the actual behavior of such hybrid systems [3]. For the technologically relevant Fe(001) substrate, a high degree of electronic decoupling and structural order can be achieved by using a specific class of organic molecules, namely tetra-phenyl-porphyrins (TPP) and by properly modifying the metal surface. This was first demonstrated by the authors for a single layer of ZnTPP grown on the oxygen-passivated Fe(001)-*p*(1x1)O surface [4,5].

In the present communication, we extend our investigation to the magnetic CoTPP molecule. Our results, obtained by means of spin resolved photoemission and inverse photoemission spectroscopy techniques (PES and IPES), unequivocally demonstrate the magnetic ordering of CoTPP molecules on Fe(001)-*p*(1x1)O at room temperature. As observed with ZnTPP, an ordered molecular arrangement is detected at the monolayer coverage by low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). Finally, the details of molecular interaction with the substrate (molecular conformation, charge transfer, modifications in the electronic structure) are investigated by Near edge X-ray adsorption fine structure spectroscopy (NEXAFS), PES and X-ray photoemission spectroscopy (XPS) aided by theoretical simulations based on Density Functional Theory with a dispersion-corrected functional.

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#210 - NANOSCALE ELECTRICAL CHARACTERIZATION OF SIC INTERFACES AND DEVICES

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Owing to its superior physical properties (wide bandgap, high critical electric field, high thermal conductivity) and its rich polytypism (4H, 6H, 3C,…), SiC is a material of choice for many applications. In particular, 4H-SiC emerged in the last years as the key material in power electronics [1]. Although several 4H-SiC based devices (like Schottky diodes, JBS and MOSFETs) are already industrially produced, their performances are still below the theoretical expectations, due to some scientific and technological open issues mainly related to surfaces and interfaces [2,3]. In this context, high resolution electrical characterizations based on scanning probe microscopy (SPM) are crucial for better understanding of the nanoscale current transport mechanisms at metal/SiC contacts (Ohmic or Schottky) or at dielectric/SiC interfaces. A nanoscale correlation between material defects and current transport at interfaces is even more critical in the case of less mature polytypes (i.e., 3C-SiC), where device applications are still hindered by the lower material quality.

This invited talk will review applications of electrical SPM techniques to several critical surface and interface issues related to SiC devices fabrication and operation [4]. This will include:

(i) The characterization of electrically active extended defects in homoepitaxial 4H-SiC layers and heteroepitaxial 3C films on Silicon by CAFM.

(ii) The evaluation of lateral homogeneity of Schottky and MOS interfaces by CAFM.

(iii) The determination of electrically active dopant profiles in 4H-SiC by SCM and SSRM. Besides providing 2D maps of carrier distribution in SiC devices, these techniques allowed to evaluate the electrical activation of P and Al implanted SiC after high temperature annealing. Furthermore, due to their high spatial resolution, SCM and SSRM have been employed to investigate the electrical modifications (counter-doping) of the SiO2/4H-SiC interface in the channel of MOSFETs after N2O annealing typically employed to passivate interface traps and to improve channel mobility.

Nanoscale electrical SPM, combined with atomic resolution structural/chemical analyses (STEM-EELS) and transient current and capacitance measurements of 4H-SiC MOSFETs, allowed to shed light on the origin of some critical issues affecting state-of-the-art 4H-SiC transistors, such as threshold voltage instability and low inversion channel mobility

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#211 - INTERFACE DENSITY OF STATES AND CARRIER BAND MOBILITY INTERPLAY IN SILICON CARBIDE PLANAR MOSFETS DEVICES

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Silicon carbide (SiC) technology has gained considerable interest in recent years due to its unique combination of physical properties that are desirable for developing power electronics applications. However, due to the presence of carbon impurity, the SiC/SiO_2 interface quality in MOS structures has a very high defect density that could be responsible of reduced field-effect mobilities (μ_{FE}) with respect to the bulk mobility.

In this work, the effect of the Density of States (DOS) at SiC/SiO_2 interface is investigated by

analyzing the transfer and output electrical characteristics of planar MOSFET devices. The devices exhibit μ_{FE}, as deduced from transconductance measurements, of the order of 4 - 5 cm^2/Vs at room temperature that increases to ~ 10 cm^2/Vs at T = 150 °C. The increase of the μ_{FE} with temperature has been attributed by some authors to a dominance of the Coulomb scattering mechanism at interface due to the presence of a high amount of interface states.
The experimental transfer characteristics have been reproduced by using a one-dimensional model that determines the electrostatic potential distribution and the carrier density along the depth of the active layer, taking into account the presence of an interfacial DOS at semiconductor/insulator interface and a doping profile in the semiconductor, while the output characteristics have been computed by using a commercial two-dimensional semiconductor numerical simulation software ("Sentaurus" by Synopsys Inc.). The model determines the interface DOS and the carrier band mobility (μ_b) by fitting the experimental transfer characteristics at low drain bias. The extracted interface DOS is similar to the one determined with the Gp/omega method and the μ_b has the same order of magnitude and temperature dependence of μ_{FE}.
In order to further check the hypothesis of a Coulomb scattering dominance, the electrical characteristics have been also reproduced by assuming a high μ_b, much closer to the SiC bulk mobility. It is found that also in the high μ_b case the electrical characteristics can be reproduced assuming an interface DOS with very high band tails near the conduction band edge, located in an energy region that is not accessible by the Gp/omega method.
In order to discriminate between these two scenarios (low and high μ_b) we propose a combined analysis of capacitance-voltage and current-voltage characteristics. Coupling C-V and I-V characteristics has been already demonstrated to be a powerful tool to extract interface state density and bulk defect density in amorphous and polycrystalline silicon thin film transistors. The results of the combined analysis of the C-V and I-V characteristics will be presented at the conference.

Acknowledgments: this work has been made in the framework of the ECSEL project WinSiC4AP (Wide band gap Innovative SiC for Advanced Power), grant agreement N. 737483.

#212 - 3C-SIC BULK GROWTH: EFFECT OF GROWTH RATE AND DOPING ON DEFECTS AND STRESS

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Many attractive mechanical and electrical properties make silicon carbide (SiC) a material of interest in both electronic devices and sensors for nowadays technology Silicon carbide exists in nature in several crystalline structures, called polytypes, differentiated by the stacking sequence of the Tetrahedrially bonded Si-C bilayers. Different polytypes have widely ranging physical properties. For instance, 3C-SiC shows the highest electron mobility and saturation velocity, because of the reduced phonon scattering resulting from a higher symmetry, while its band gap energy is the lowest (2.3 eV).
In this work we will show the effect of the growth rate and of the doping on the stress and the defect density of a 3C-SiC bulk layer grown at low temperature on a silicon substrate. After the growth process, the silicon substrate was melt inside the CVD reactor used for the deposition and then the intrinsic stress could be measured by measuring the curvature of the wafer without influence of the thermal stress between silicon and 3C-SiC. The average defect density was measured by XRD, m-Raman and KOH etch. Several conclusions can be reported on the effect of the growth process on the stress and the defects density.
With a process with three different growth rate a thick layer of about 60 mm has been grown. Subsequently the temperature was increased above the melting point of silicon and the substrate was

completely melted inside the CVD reactor. Finally the temperature was decreased until room temperature and the different 4 inches wafers were characterized.

In the experiment can be observed that a considerable increase of the curvature is observed increasing the doping of the layer. The average stress is compressive and then produces a convex bow. At the same time, the average quality of the grown material deteriorates increasing the doping concentration. Using m-Raman measurement is cross-section of the 3C-SiC grown samples, it is possible to observe the dependence of the stress and of the quality of the material as a function of the thickness and of the growth rate, due to the variation of the growth rate during the process. From these analyses it is possible to observe that the increase of the growth rate produces both an increase of the stress and a decrease of the material quality. Furthermore, the increase of the doping concentration produces both an increase of the stress and a further deterioration of the crystal quality.

#213 - 2D EXTENDED DEFECTS INTERACTION: THE CASE OF GRAIN BOUNDARY AND STACKING FAULTS IN 3C-SIC

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Cubic silicon carbide (3C-SiC) is posed to open new industrial markets pending the fabrication of high quality material. 3C-SiC has a highly symmetric structure, which leads to good electron mobility and saturation velocity. With respect to other SiC polytypes, the lower band gap of 3C-SiC means less semiconductor/oxide interfacial defects density, which is benefit for the development of MOSFET devices. Exploiting these desirable properties depends first on the development of high quality 3C-SiC, meaning that the defect density must be reduced. 3C-SiC growth on Si has been under development for roughly the past three decades. Although actually point defects (0D) can be controlled acting on the growth parameters, the control of dislocation defects (1D) and 2D defects such as stacking faults (SF) and grain boundary (GB) remains an open point. Elimination of SFs and GBs is the key to reduce the leakage current in the 3C-SiC diodes and for the use of 3C-SiC in industry.

The presence of 2D defect, in 3C-SiC grown on Si, seems to be strictly related to residual stress in the hetero epitaxial film. 3C-SiC and Si have different thermal expansion coefficients and different lattice constants leading to the formation of high stress region near interface. The formation of stacking faults and steps together with mosaic and anti-phase domains seems to be structures able to relax the stress.

In the present paper, we have performed scanning transmission electron microscopy (STEM) analysis both in high and low resolution in order to characterize the 2D defects such as grain boundaries and stacking faults and have more insight in their interaction.

3C-SiC samples are grown hetero-epitaxially on Si using chemical vapour deposition (CVD), at the LPE industry. The CVD growth process is performed at low pressure and a temperature of 1370° C. The gases used during the growth are trichlorosilane, ethyene and Hydrogen as silicon and carbon precursors and gas carrier respectively The material was analysed using a JEOL 2010F transmission electron microscope in scanning mode configuration.

During the conference, several images showing different kind of interaction between SFs and GB will be presented. In particular we will present both generation, annihilation of SF from a GB and some example of structural modification of the GB after the interaction with SF. Considerations on the stress and how the SF and GB contribute to the reduction of the wafer stress will be also reported.

#214 - LASER ANNEALING OF P AND AL 4H-SIC IMPLANTED EPITAXIAL LAYERS

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Through new improvements in SiC crystal growth and processed technology, the manufacturing of powered metal-oxide-semiconductor field-effect transistors (MOSFETs) has begun. Source and body regions in MOSFETs are achieved by ion implantation and subsequent mandatory thermal annealing at T > 1600 °C. However, in this temperature regime generation of C interstitial-vacancies couples is registered along the whole epitaxial layer, affecting carriers mobility and lifetime in channel region. Particularly, carbon vacancies have been found to be the origin of the so called $Z_{1/2}$ and EH_7 deep energy levels: the main carrier lifetime killer in 4H-SiC. In addition, a network of dislocation loops is also produced in the implant projected range together with low dopant activation rates.

To work around this issue, pulsed-laser-based methods have been applied for post-implant annealing of P and Al doped 4H–SiC epitaxial layers in order to recover the crystal structure and to electrically activate the doping species. Experimental activity was conducted on wafers with a 6 mm epitaxial layer. Source P ion implantation was performed at 500 °C with energies between 30 and 200 KeV and fluences ranging from 10^{13} to 10^{14} cm^{-2} in order to obtain an almost uniform doped layer, 200 nm thick, with a concentration of 10^{20} cm^{-3}. Laser treatments on implanted area were carried out through a Lambda Physics LPX 300 XeCl pulsed eccimer laser (l=308 nm) with 40 Hz pulse and 1000 shots/point. The sample camera temperature was setted at 580 °C and a mobile stage allowed to implement an irradiation process from 1 to 1000 shots/point. For comparison, 1 h isochronical thermal annealings at 1650,1700 and 1750 °C were performed on the same implanted samples.The effectiveness of laser treatment was verified by micro Raman and photoluminescence (Pl) analysis conducted with a He-Cd laser source (l= 325 nm) and a Horiba Jovin Yvon LabRAM HR spectrofluorimeter with a 1800 l/mm grating. Zeiss SEM was used for surface characterization, while a further structural investigation was performed using TEM microscopy on a 2010F Jeol apparatus.

Pl analysis shows crystal recovery proportional to the laser energy density investing the sample up to the phase separation threshold at 0.6 J/cm^2 and a lower density of point defects.

During the conference dopant activation will be shown to prove the viability of L.A. as future candidate for conventional post implant thermal treatments.

#215 - SILICON CARBIDE DETECTORS FOR HIGH ENERGY IONS AND NEUTRONS

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The wide band-gap of silicon carbide reduces significantly the rate of thermally generated charge carriers reducing the noise level. Also the radiation damage can affect various properties of a detector; phenomena connected with the alteration of these properties are the increase of the leakage current, the decrease of charge collection efficiency (CCE) and the removal of free carriers from the conductive regions of the device. Radiation hardness is the inertness of these device parameters to high doses of particle irradiation. SiC, due to its wide gap and strength of its chemical bonds, has been seriously considered as a valid alternative to silicon for the production of radiation hard ionizing particle detectors. A further important aspect, in connection with the large band-gap, is the SiC insensitivity to photons in the visible range. Such fundamental property makes of SiC devices very promising for neutrons and charged particles detection in a plasma environment.

Two detectors with 10 mm and 100 mm has been mounted in a telescope configuration. In order to avoid dead layers between the first and the second stage of the telescope, the first stage is reverse mounted while the second is front mounted. The ΔE-E correlation obtained from the first two stages of telescope shows different ridges corresponding to different atomic numbers of the impinging fragments.

The Silicon Carbide detector produced within the SiCILIA project has been tested at FNG by using 14.1 MeV neutrons. The detector, featuring an active area of 25 mm^2 and an epitaxial thickness of

100 µm, showed good efficiency values thus demonstrating the improvements made in the growing procedures.
During the conference both the performance and the radiation hardness of these detectors will be shown in detail.

#216 - 3C-SIC GROWTH ON ISP SUBSTRATES: EFFECTS OF SUBSTRATE GEOMETRY ON VOID FORMATION AND GROWTH RATE

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Cubic Silicon Carbide (3C-SiC) is regarded as a very promising candidate for high power and high frequency device applications since 3C-SiC allows for a higher speed of electron transport within the crystal. Actually, the main limitation for device realization on such a material comes from the wafer fabrication. Furthermore the defect density that is very high with respect to the α-SiC counterpart limits the development of 3C-SiC-based electronics. Crystallographic defects are extended from the interface up to the film surface, with micro twins and anti-phase boundaries (APBs) observed as vanishing defects in thicker films. The main limitation of 3C-SiC comes from stacking faults since their propagation throughout the epitaxial film causes device failure and their linear density at the film surface is still high (ρ_{SF}~10^4 cm^{-1}). In 2013 we have presented a new approach using a new patterned substrate (Inverted Silicon Pyramid or ISP) that improve the quality of the grown material reducing the density of stacking faults even after low thickness. In this work, we will present the effect of substrate geometry on the void formation inside the material and on the growth rate on the (111) and (100) surfaces that are present in the structure.
The growth of the 3C-SiC layers was obtained using a classical process using silane and propane gases as silicon and carbon precursors and hydrogen as gas carrier. Different parameters of the growth has been varied (growth temperature, C/Si ratio, growth rate, …) to understand the influence of these parameters on the growth. The samples have been analyzed by TEM cross-sections, SEM cross-sections, XRD, Raman to determine the quality of the hetero-epitaxial material grown and the morphology.
From TEM cross-section of the 3C-SiC layer grown on ISP structure it is possible to see the main defects present in this material: stacking faults, grain boundary and voids. The stacking faults are starting from the silicon interface. The (111) surfaces of the ISP structure help in the reduction of these defects aiding the annihilation process. It is possible to see also the presence of grain boundary starting essentially from the (100) surface between the ISP structures. Finally, several voids are observed inside the ISP structures. This last defect has been observed that depends on the dimension of the ISP. Furthermore, the growth rate has also a large effect on these voids.

#217 - ION IMPLANTATION IN 4H-SIC: DEFECTS AND DOPANT ACTIVATION

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Silicon Carbide (SiC) is a material that is currently widely used in the semiconductor industry, for its potential applications in high power, high frequency and high temperature electronic devices. The realization of semiconductor devices requires various processes and among these a fundamental step is the selective doping, that in the case of SiC, due to the low diffusion coefficients of the doping species, it is achieved by ion-implantation. However, the drawback of ion-implantation is the induced damage, and to minimize this effect the implants are generally performed at high temperature (500 °C). Subsequently, high-temperature annealing processes (> 1600 ° C) are required to restore the crystalline structure and electrically activate the implanted ions.

The aim of this paper is a detailed investigation of Al implants on 4H-SiC and the subsequent high-temperature treatment in order to optimize the concentration of active implanted species.

Hall effect measurements were performed to determine the active dopant concentration and carrier mobility. These measurements require special preparation of the samples which must have 4 symmetrical contacts. The contacts were created by depositing 100 nm of Ni followed by a thermal process at 900 ° C for 30 min to produce 200 nm of nickel silicide (Ni_2Si). Photoluminescence (PL) measurements were performed to obtain information on the type of defects, using an excitation wavelength of 340 nm.

The Al implants, with a total dose of $3.3x10^{15}cm^{-2}$, were performed at 500 ° C and at various energies and doses in order to obtain a 250-nm-deep box profile. Then the samples were thermally treated at various temperatures: 1675 °C, 1775 °C and 1825 °C for 15 min.

The Hall measurements indicate that the active dopant concentration increases with increasing temperature up to 1750 ° C and then a small decrease is observed, while the mobility is almost constant with temperature. The annealing temperature of 1750 ° C would seem to be the one that produces the best results. However, even at this temperature the maximum fraction of measured active doping is 3.7%. This is due to the presence of residual defects after the thermal process and to the incomplete ionization of the carriers at the measurement temperature (room temperature).

Photoluminescence measurements performed on the same samples show the presence of two contributions associated with two different stacking faults (2SSF and 4SSF). These defects are not present in the post-implantation sample but originate after thermal treatment. Moreover, their concentration is lower for the sample at 1775 ° C, while at higher temperature clusterization of point defects occurs, highlighting once again that the annealing temperature of 1775 ° C is the one that leads to satisfactory results.

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#218 - CAN UNCONVENTIONAL JOSEPHSON JUNCTIONS OFFER ALTERNATIVE ROOTS TO BE COUPLED TO OTHER QUANTUM SY

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Josephson junctions (JJs) are undoubtedly the key elements of superconducting electronics and of superconducting qubits. Al- and Nb-based JJs guarantee extremely high quality and standards in terms of junction performances and are commonly used for most of the cutting-edge applications and for all types of superconducting qubits. The more profound knowledge of the behaviour of a Cooper pair box inside a resonant circuit has in principle given the possibility to use a wider range of JJs because of the beneficial effect of the circuit in reducing the dissipative effects originated in the junction. Based on our expertise on unconventional JJs and on the possibility of controlling them through different physical means, we are exploring different solutions to drive a junction in unconventional manners. This goes towards the development of an integrated quantum device that is expected to be better than the sum of its ingredients. We refer to the capability of an all-RF drive of ferromagnetic Josephson junctions [1], which is expected to allow novel tuning mechanisms that are not susceptible to flux noise, and permit alternative control schemes. These may open up new avenues in coupling schemes between the qubit processor and SC waveguide cavities. Measurements of switching current distributions allow to identify different transport mechanisms and to classify dissipation regimes [2-3]. These studies provide an electrodynamic characterization required to evaluate the possible use of these systems in more complex circuits, as cryogenic memories or spintronic devices, and suggest new solutions of hybrid JJs in superconducting qubits.

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#219 - COHERENT PROBING OF ULTRASTRONG LIGHT-MATTER INTERACTION

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Non-perturbative light-matter interaction is a fundamental building block for the emerging quantum technologies, such as quantum simulators and quantum memories. In the last decade, the solid state devices allowed the exploration of the so-called ultrastrong coupling (USC) regime, where the coupling strength is comparable to the energies of the uncoupled systems[1-3]. In this regime of interaction, several intriguing phenomena can occur, such as quantum phase transitions, ground state entanglement or generation of correlated excitations [4-6]. So far, a direct evidence of the USC is provided by standard spectroscopy. Here we present a different approach, whose aim is to probe the USC via dynamical detection of the virtual photon pairs in the dressed eigenstates, i.e. the non-conservation of the total number of excitations induced by the counter-rotating terms in the light-matter coupling [7,8]. In particular, by exploiting superconducting quantum circuits, such photon production channel can be coherently amplified by Stimulated Raman Adiabatic Passage (STIRAP), that provides a suitable tool for an unambiguous dynamical detection of USC in present state-of-art quantum technology.

Finally, we also show that STIRAP-like protocol within USC regime can be exploited in order to realize an almost perfect quantum state transfer among different nodes in a quantum network [9].

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#220 - STUDY OF DISSIPATION IN FERROMAGNETIC JOSEPHSON JUNCTIONS TOWARDS QUANTUM DEVICES

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Josephson coupling between superconducting (S) and ferromagnetic (F) layers is driving new fundamental physics and innovative applications for superconducting electronics and quantum circuits [1]. We will report on transport measurements down to mK temperatures, providing clear fingerprints of different dissipation sources in Josephson junctions (JJs) composed by pure metallic ferromagnetic layers (SFS) [2], by an insulating barrier and a ferromagnetic layer (SIFS) [3], and by a ferromagnetic-insulator barrier (SI$_F$S) [4,5], respectively. These fingerprints and the self-consistent reconstruction of the electrodynamics [2,5,6], give strong indications on the presence of triplet correlations, show the capability to tune the scaling energies through different means and point out new routes for superconducting qubits based on tunnel-ferromagnetic JJs.

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#221 - SET UP OF AN EXPERIMENT FOR AXION SEARCH WITH SINGLE MICROWAVE PHOTON JOSEPHSON JUNCTION DETECTORS

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The detection of single photons in the microwave range is interesting for different applications, for example for the search of Axions (hypothetical elementary particles, possible candidates as cold dark matter) and Axion like particles. This is a difficult task because of the low energies involved but it can be effectively achieved, for example by using Josephson junctions as switching detector activated by the absorption of single photons with tuned frequencies. The SIMP project is developing an appropriate experimental setup for the direct conversion of Axions in microwave photons and the detection of them thanks to the coupling of a suited Josephson junction detector. We present the SIMP project and the developed setup and discuss issues and perspectives of this experiment.

#222 - MEASURING NONCLASSICALITY WITH SILICON PHOTOMULTIPLIERS

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The search for optimal receivers endowed with photon-number-resolving capability has led us to consider Silicon photomultipliers (SiPMs) for quantum optics experiments. Despite their low quantum efficiency (up to 60%), an unprecedented photon-number resolution, together with a proper minimization of their drawbacks, allows for a fair reconstruction of light statistics [1]. Moreover, due to their compactness and cheapness, SiPMs can be embedded in portable systems.

Our research focused on testing this class of photodetectors for measurements of nonclassicality. We exploited the nonclassical features of mesoscopic twin-beam (TWB) states generated by pumping a BBO crystal with the fourth harmonic of a pulsed Nd:YLF laser regeneratively amplified at 500 Hz. By adopting an optimization procedure [2] in order to reduce the effects of optical cross-talk, we succeeded in detecting nonclassical correlations between the two parties of TWB states and in obtaining subPoissonian conditional states [3,4].

These results put SiPMs forward for the implementation of quantum communication protocols.

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#223 - REALISTIC PULSE SEQUENCES FOR SINGLE QUBIT OPERATIONS IN SEMICONDUCTOR SPIN QUBITS

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Spin qubit architectures represent a promising platform for quantum computation and simulation applications. In the last decades, they have been deeply investigated from a theoretical point of view and realized at least on the scale of few devices in the laboratories. In semiconductor materials two main directions for the realization of spin qubits can be identified: qubits realized defining the logical states of the spin of electrons in electrostatically defined quantum dots (QDs), and qubits which uses the spin of electrons or nuclei of impurity atoms in the semiconducting host material (donors). The two approaches can be used to create different implementations: single electron spin qubits, singlet-triplet spin qubits, or three electrons architecture, e.g. the hybrid qubit.

In this work, we study five qubit types, namely the quantum dot spin qubit, the double quantum dot singlet-triplet qubit, the double quantum dot hybrid qubit, the donor qubit and the quantum dot spin-donor qubit. For each one, we derived analytical time sequences to drive single qubit rotations along the principal axis of Bloch sphere.

However, in this analysis it is mandatory to include the non-idealities of the control signals. The realistic transients of the control voltage pulses are obtained by adopting an appropriate filter function and the effect of the input disturbances is taken into account by using a Gaussian noise model. This study provides a comparison of the gate fidelities for the different qubit implementations highlighting which one is the most robust with respect to the considered control noises.

#224 - ULTRAFAST CHARGE INJECTION AT COMPLEX INTERFACES: ORGANIC-ORGANIC, ORGANIC-INORGANIC AND ORGANIC-GRAPHENE

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Interface processes strongly affect the performances and efficiency of organic based devices. The integration of 2D materials like graphene in organic devices (for example as electrodes) is expected to improve the overall device performances. To reach this goal a deeper understanding and control of interfaces between organic films, graphene and metals and related charge transfer (CT) processes is critical. Charge injection across molecular junctions can occur at the femtosecond time scale or even shorter. In most cases this time frame is still out of reach of the pump probe spectroscopies. Here we use X-ray spectroscopies to investigate charge injection in complex hetero-structures that include organic molecules, graphene and metallic substrates. We show that the Core hole clock implementation of the Resonant Photoemission spectroscopy (RESPES) allows us to determine charge dynamics in both directions (to/from the molecule) at these interfaces and can give clues on the interface parameters that can increase/decrease the charge transfer efficiency. Examples of model systems will be discussed.

It will be shown how RPES allows us to elucidate the role of inter-molecular interaction on through-space charge transfer characteristics in π-stacked molecular systems [1], the electronic coupling, morphology and charge transfer rates at the donor-acceptor (D/A) interfaces between C60 and either flat- or contorted hexabenzocorones (HBC) [2] and the relation with improved internal (IQE) and external (EQE) quantum efficiency of devices based on these shape-matched molecular systems. The case of ammine and pyridine terminated organic overlayers will be discussed in connection with recent results of break junction experiments [3]. In this case we show how core-hole clock spectroscopy can be used to measure charge transfer through noncovalent interactions and map charge delocalization times from carbon and nitrogen sites on the molecules. Comparison of charge transfer rates between different substrates (metal, graphene and graphene nanoribbons) will be discussed elucidating the role of the local density of states of these materials and the level alignment in the charge transfer process [4].

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#225 - VIBRATIONS AND ELASTIC RESPONSE AT THE NANOSCALE IN COMPLEX MATERIALS

Stefano Mossa - CEA Grenoble- IRIG

In a recent series of papers [1-5] we have described extensive numerical work focusing on the concept of elastic heterogeneity in disordered solids. The fundamental idea is quite simple: glasses and even (complex) crystals with defects show inhomogeneous mechanical response at the nanoscale, which does not conform to the macroscopic limit predictions. This property can be demonstrated to strongly influence vibrational and thermal properties of the materials, and could ultimately lie at the bottom of puzzling anomalous features like boson peak, Raleigh-like strong scattering, or temperature dependence of thermal conductivity.

We have investigated the above issues systematically and in great details by classical Molecular Dynamics simulation. On one side, we have employed different toy models including monodisperse

Lennard Jones nanoparticles, and soft spheres with particles size disorder. On the other, we have considered multiple phases with variable amount of disorder, ranging from glassy configurations, to crystals with defects and superlattices. In all cases, we have monitored independently mechanical response, collective excitations, and heat transfer features, establishing precise correlations among the heterogeneous local mechanical response, the nature of the vibrational states, and the variation of thermal conductivity.

In the talk I will discuss some of our findings and put them in perspective, also with reference to advanced spectroscopy measurements with X-Rays. I will also show how information of this nature can be exploited to engineer interfaces, devising metamaterials with tailored functions.

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2. H. Mizuno, S. Mossa, and J.-L. Barrat, Relation of vibrational excitations and thermal conductivity to elastic heterogeneities in disordered solids, Phys. Rev. B 94, 144303 (2016) [10.1103/PhysRevB.94.144303]

3. H. Mizuno, S. Mossa, and J.-L. Barrat, Beating the amorphous limit in thermal conductivity by superlattices design, Sci. Rep. 5, 14116 (2015) [10.1038/srep14116]

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#226 - INVESTIGATING SIMULTANEOUSLY ENERGY (HEAT) EXCHANGE AND SURFACE PHYSICS ON SAMPLES AT THE NANO-SCALE

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The family of devices at the micro- or nanoscale is exponentially growing in the last decades, pushing research to develop new experimental techniques to characterise them. In particular, a general method for the direct evaluation of the energy balance of such systems is not available at present. Calorimetry usually requires samples having mass in the 10-100 mg range, while nano-devices range in the ng-mg. Here we report on the development of an original experimental setup able to detect temperature variations as low as 10 mK in a sample of ~10 ng, using a sensitive gold film thermometerwith physical dimensions of 5x5 mm^2 [1]. We have used this technique to measure the enthalpy release during the adsorption process of D_2on a titanium decorated monolayer graphene sample. Ti-MLG has been extensively investigated for application in the hydrogen storage field [2-6], which makes this system a benchmark and a reference.The sensitivity of this thermometer allows to detect a hydrogen uptake of ~10^{-10} moles, corresponding to ~0.2 ng, with a temperature increase of ΔT=0.065 K and an

enthalpy release of ~23 μJ. A limitation of the thermometer is the surface roughness, which does not allow atomic resolution with the STM probe. Therefore, we have developed an upgraded version.
Here we present the fabrication, characterization, and calibration of an atomically flat, monocrystalline gold film thermometer on mica substrate [7]. Gold re-crystallization is obtained inside the STM chamber, allowing the successive investigation of the thermometer surface by LEED and with STM imaging. Large gold terraces allow achieving a resolution comparable with atomic dimensions during STM imaging of the surface. Moreover, the gold-on-mica thermometer performs about 10 times better than the previous sensor based on a Si substrate. This work opens the possibility to investigate simultaneously energy (heat) exchange mechanisms and surface physics with the same physical support, opening a unique perspective in understanding physics and chemistry at the nanoscale.

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#227 - NANOPOROUS GOLD PARTICLES: FABRICATION AND CHARACTERIZATION

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Nanoporous Au attracts great technological interest as a promising candidate for optical and electrochemical sensors [1]. The present literature is, mainly, focused on fabrication, characterization, and application of nanoporous Au leafs and films [1-3]. Recently, however, large interest was attracted by nanoporous Au micro- and nano-structures due to much higher surface-to-volume ratio than bulk nanoporous Au leafs and films [4, 5].
In this work we report on the development of simple, versatile, cost-effective approaches for the production of nanoporous Au micro- and nano-structures directly on surfaces. In particular, the following procedures were developed: nanoscale-thick Au/Ag bilayers (being, respectively, x_{Au} and x_{Ag} the thicknesses of the Au and Ag layers) were deposited on SiO_2 or FTO (fluorine-doped tin oxide) substrates; then, the alloying and dewetting processes of the bilayers were induced by furnace annealing treatments of the bilayers on SiO_2 or by nanosecond-pulsed laser irradiations of the bilayers on FTO. The alloying and dewetting processes were observed to produce the formation of Au_xAg_y sub-micrometric alloy particles being x and y tunable by x_{Au} and x_{Ag}; finally, the Au_xAg_y alloy particles were dealloyed in HNO_3 solution to selectively etch Ag. Thus, the formation of nanoporous sub-micrometric Au particles on the substrates was observed to occur. The morphological characteristics of these nanoporous particles were analyzed by scanning electron microscopy and we report and discuss the following results: a) the dependence of size and shape of the particles on the type of the dewetting process (solid-state dewetting on SiO_2, molten-state dewetting on FTO); b) the dependence of particles porosity on the type of the alloying process (~32% for the particles fabricated by the furnace annealing at temperature of 900 °C, ~45% for the particles fabricated by the laser irradiation at fluence of 0.5 J/cm^2). Perspectives on the exploitation of these systems in plasmonic-based sensors are, finally, outlined.

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#228 - MODELING THE POROUS SILICON - EUMELANIN INTERFACE: OPTICAL PROPERTIES OF SI(001)-ADSORBED EUMELANIN

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Eumelanin is a photoprotective pigment, widely present in living organisms: it is interesting both for its biological role and in view of possible applications, e.g. as a photoactive layer in hybrid solar cells.

Porous silicon (PSi) – eumelanin interfaces are interesting systems for photovoltaic applications, due to (a) the large surface-to-volume ratio of the porous substrate, (b) the peculiar broadband UV-vis absorption spectrum of the pigment, and its biocompatibility and biodegradability. Indeed the ability of eumelanin functionalization to extend the absorption range of PSi towards longer wavelengths has been demonstrated [1,2].
The basic building blocks of eumelanin are 5,6-dihydroxyindole (DHI) – like molecules. Although the detailed 3D structure of the pigment is not known, a wealth of experimental measurements suggest the presence of locally ordered π-stacked arrangements of relatively small oligomers (like tetramers or pentamers) of DHI-like molecules, and the role of stacking and oligomerization in the emergence of the broadband eumelanin spectrum is actively studied [e.g. 3,4].
Computational investigations have been reported on the energetics, adhesion properties, electronic properties, interface stability of simplified models of the PSi-eumelanin interface, consisting of tetramers of DHI-like molecules interacting with the Silicon(001) surface [5,6].
Clearly, a theoretical understanding of the effects of eumelanin on the optical properties of the substrate in these hybrid systems is of paramount importance. First principles calculations on organically functionalized surfaces are able to yield valuable information in this respect (e.g. [7]). In this work we investigate, by plane wave density functional theory, the absorption spectra and Reflection Anisotropy Spectra (RAS), of the DHI-like tetramer - functionalized Si(001) surface, focusing on the effect of molecule adsorption, the sensitivity to the type of adsorbed molecule and to its adsorption configuration.

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#229 - INNOVATIVE SMART NANOCOMPOSITES OF CHITOSAN NANOPARTICLES CONTAINING METAL OXIDE

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Recently hybrid organic-inorganic nanocomposites received a great interest from scientific comunity, specially the combination of inorganic nanoparticles and polymers. Indeed, organic biopolymers can be used as coating for other materials such as metal oxide (MOx) nanoparticles to improve their biocompatibility and extend their range of applications in biosensing, gas sensing, treatment of heavy metal water contaminants, biomedical device and drug delivery, and nanofertilization in agricolture. In our work, we propose innovative smart nanocomposites of chitosan (CS) nanoparticles containing MOx. CS has been selected for its well-known biodegradable, antimicrobial, antimycotic properties [1,2]. Furthermore, the primary amine groups in CS are responsible for various properties such as cationic nature, controlled drug release, in situ gelation, antimicrobial and permeation enhancement. These peculiarities make CS an interesting host for nanofillers by allowing controlled drug delivery and smart release of nanofillers in response to external stimuli, such as pH and chelating agents [1]. As nanofillers, we have chosen MOx nanoparticles of Copper and Cerium Oxides because they are interesting for sensing application [3] and as growth stimulator of many plants in agricoluture [4]. We have prepared the hybrid nanocomposites by polyelectrolite complexation, an environmentally friendly chemical preparation [4]. The polymeric coating of the MOx nanoparticles is driven by the electrostastic interactions between ammine groups and MOx charged surface. By strategical adjustments of synthesis conditions, i.e. pH and polymer/cross-linker ratio, we obtained an accurate control of the density and size of the nanocomposites. Their morphology and size distribution has been accurately studied by Scanning Electron Microscopy images. The mean size has been compared with the hydrodinamic radii obtained by Dynamic Light Scattering. Moreover we have demonstrated the efficacy of MOx encapsulation inside the CS nanoparticles by Energy Dispersive X-Ray Spectrometry (EDX) maps. The EDX images demonstrate the effective metal distribution inside the nanocomposite with nanometric resolution. UV-vis absorption and photoluminescence have been also performed to evaluate the influence of polymer on the optical properties and the eventual effect of its degradation under proper stimuli, i.e. pH and light. The results demonstrate that the synthesized hybrid nanocomposites has great potentiality for developing carriers delivery and smart release systems. [1] A. Ali and S. Ahmed, Int. J. Biol. Macromol. 109, 273, (2018). [2] S.A. Agnihotri et al., J. Control. Release 100, 5, (2004). [3] Panpan Guan, Yongjian Li, Nanomaterials, 6, 159(2016) [4] M. Kah, Nat. Nanotechnol. 13, 677, (2018).

#230 - LIGHT EMITTING POROUS SILICON MICROPARTICLES: FROM SYNTHESIS TO SURFACE FUNCTIONALIZATION

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Nanostructured light emitting porous silicon is obtained by electrochemical etching of crystalline silicon wafer in HF solution. A successive sonication treatment allows to obtain porous silicon light emitting microparticles that, due to their properties could be traced by imaging techniques and used as carrier for drug loading and release. After a functionalization to introduce negative (COOH) or positive (NH_2) groups at the microparticles surface, this material was proved to be optically stable for years in ethanol.

Since this top-down approach leads to a very broad size distribution, we developed a post-functionalization procedure to reduce the average microparticle size and to narrow the size distribution. Aiming at this, we optimized an ultrasonic (US) treatment, by varying the microparticles concentration, the US duration and its power density. This simple procedure is effective in reducing the average size and the size distribution, without affecting the functionalization, the optical properties and the porous structure of the material.

To test the biocompatibility with in-vitro test, we need to disperse the microparticles in an aqueous solution (i.e. PBS – Phosphate Buffered Saline), but a fast quenching of the optical properties, caused by the oxidation of the material, is observed. Hence, we coated the pSi microparticles either by organic polymers (i.e. PEG and chitosan) or by an inorganic layer of titanium dioxide.

The organic polymers were covalently attached to the porous silicon surface; the microparticles were negatively charged after the PEG coating, while positive in the case of chitosan. The optical properties were proved to be stable for long time, in particular for PEG coating, by fluorescence spectroscopy. To overcome the problem of silicon pores occlusion by the attached polymers thickness, we deposited thin inorganic layers obtained by ALD (Atomic Layer Deposition), which allows a uniform layer deposition with tuneable thickness. We choose titanium dioxide in perspective of using this material for biomedical application, since TiO_2 is a biocompatible and widely used material in the field. We investigated this process, where the surface of the microparticles is firstly exposed to a precursor of titanium, then to water and this is repeated for several cycles, to obtain the desired TiO_2 layer thickness. The procedure was optimized by considering long or short Ti precursor exposure time and then we focused on the exposure to water, since it was found to be crucial in the optical stabilization. Therefore, we obtained pSi microparticles that are stable in aqueous solution, both optically and structurally, giving the chance to this material to be used as drug delivery carrier, for its porosity, and traceable by imaging techniques, due to its photoluminescence.

#231 - PHOTOLUMINESCENCE CHANGES INDUCED BY HIGH TEMPERATURE ANNEALING UNDER NITROGEN ATMOSPHERE OF SILICON NANOSTRUCTURES

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Other Authors: Sonia Freddi (1,2,3), Filippo Fabbri (4), Simona Boninelli (5), Annalisa Cannizzaro (5), Marta Agati (5), Richard Dolbec (6), My Ali El Khakani (3) and Paola Castrucci (1) (1) Dipartimento di Fisica, Università di Roma "Tor Vergata", 00133 Roma, Italy (2) I-Lamp and Dipartimento di Matematica e Fisica, Università Cattolica del Sacro Cuore, Via Musei 41, Brescia, Italy. (3) Institut national de la recherche scientifique (INRS), Centre-Énergie, Matériaux et Télécommunications, Varennes QC-J3X 1S2, Canada (4) Center for Nanotechnology Innovation @NEST, Italian Institute of Technology, Pisa, Italy (5) CNR-IMM, Via Santa Sofia 64, 95123, Catania, Italy (6) Tekna Plasma Systems Inc., 2935 Industrial Blvd., Sherbrooke, QC, J1L 2T9, Canada nanometer-sized silicon oxide shell. This assortment of SiNS, obtained as a Si nanopowder using an inductively coupled plasma -torch technique, comprises nanowires (with diameters in the nm range and lengths of up to several microns) and silicon spheres with diameters ranging from about 10 nm to few μm. The nanowires consist of a crystalline nanocore embedded in a SiOx outer-shell and are of three main different types, namely silicon nanowires (SiNWs) with a continuous core, nanowires with a "chaplet-like" core, and nanowires of which core is made up of disconnected spherical Si nanocrystals. Statistical analysis carried out on several transmission electron microscopy images show the presence of a high percentage of SiNS with diameter below 5 nm (i.e. the Si exciton Bohr radius) and revealed changes in SiNS morphology and size occurring upon annealing. Electron energy loss, x-ray photoelectron and infrared Fourier transform spectroscopies indicate the formation of silicon nitrides and/or silicon oxynitrides. Interpretations about the origin of the observed PL changes are given.

Silicon nanostructures (SiNS), namely nanocrystals and nanowires, have attracted an ever increasing of interest in all scientific and technological fields due to their unique properties and their potential to be used for disparate applications. Several decades after the first evidence of the photoluminescence (PL) from porous silicon, light emission and amplification in SiNS-based devices, though extensively explored, still remain a fascinating challange. Here, we report on PL changes in drop-castes films of as-grown (AG) and 1200°C annealed in N2 flux. The films consisted of multisize SiNS embedded in a few nanometer.-sized silicon oxide shell. This assortment of SiNS, obtained as a Si nanopowder using an inductively coupled plasma torch technique, comprises nanowires (with diameter in the nm range and lengths of up to several microns) and silicon spheres with diameter ranging from about 10nm to few micrometer. The nanowires constist of a crystallinfe nanocore embedded in a SiOx outer-shell and are of three main different types, namely, silicon nanowires (SiNWs) with a continuous cilindrical core, nanowires with a chaptle-like core and nanowires of which core is made up of disconnected spherical Si nanocrystals. Statistical analysis carried out on several transmission electron microscopy images show the presence of a high percentage of SiNS with diameter below 5nm (i.e. the Si exciton Bohr radius) and revealed changes in SiNS morphology and size occurring upon annealing. Electron energy loss, x-ray photoelectron and infrared Fourier transform spectroscopies indicate the formation of silicon nitrides and/or silicon oxynitrides. Interpretations about the origin of the observed PL for AG sample are given in terms of excitonic recombinations in SiNCs and band tail recombinations for oxides while for 1200C the PL spectra are mostly attributed to band tail recombination of oxides and nitrides.

#232 - MAGNETIC NANOPARTICLE PRODUCED BY PULSED LASER ABLATION

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SmCo is a permanent magnetic material having peculiar characteristics.The SmCo Nanoparticles can be used in different application fields like sensors and biosensors for environmental and biological measurements. SmCo nanoparticles could be applied for temperature treatments of the cancer in medicine. Hyperthermia is the physic procedure that permits increasing the local temperature in human body using radio frequency magnetic fields. When a cancer culture cell is exposed to temperature in range 40- 43°C, a cell apoptosis occurs. The number of cancer cells is reduced and using also chemotherapy treatment the cancer disruption could be obtained . Hyperthermia is the physic procedure that permits increasing the local temperature in human body using radio frequency magnetic fields.The number of cancer cells is reduced and using also chemotherapy treatment the cancer disruption could be obtained . In this paper, we present preliminary experimental results and we discuss both Transmission Electron Microscopy and the SmCo NPs thermal data to hyperthermia.

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#233 - CHARGE DENSITY WAVES IN CUPRATES OUTSIDE THE PSEUDOGAP REGIME

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It is commonly accepted that charge density waves (CDW) are present in all high Tc superconducting cuprates in the underdoped regime. Their importance is due to their interplay with superconductivity, as competing and/or intertwined phenomena. Resonant soft x-ray scattering is probably the most direct and sensitive experimental method for their observation, and has been providing the core of the systematic information on them, including temperature dependence and onset temperature that are used to delimitate the CDW region in the phase diagram. The picture is nonetheless still fragmented, also because other techniques have been bringing results not easy to reconcile, eg the influence of magnetic fields on c-axis correlation and the role of discommensuration.
We have exploited the superior sensitivity of the ERIXS instrument of the beam line ID32 of the ESRF to take a deeper look at the CDW phenomenon. We could thus observe the existence of Charge Density Fluctuations (CDF) aside the already known CDW in the 123 family [1] Combined with the discovery of charge order in overdoped Bi2201 [2] and with the observation of high temperature CDW in LBCO [3], are going to stimulate a revision of the current understanding of the CDW phenomenon in cuprates. The discovery of CDF can provide a phenomenological explanation of the Marginal Fermi Liquid behavior of cuprates in the normal state [4].

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#234 - DYNAMICAL CHARGE DENSITY FLUCTUATIONS PERVADE THE PHASE DIAGRAM OF CUPRATES

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It is commonly accepted that charge density waves (CDW) are present in all high Tc superconducting cuprates in the underdoped regime. Their importance is due to their interplay with superconductivity, as competing and/or intertwined phenomena. Resonant soft x-ray scattering is probably the most direct and sensitive experimental method for their observation, and has been providing the core of the systematic information on them, including temperature dependence and onset temperature that are used to delimitate the CDW region in the phase diagram. The picture is nonetheless still fragmented, also because other techniques have been bringing results not easy to reconcile, e.g. the influence of magnetic fields on c-axis correlation and the role of discommensuration.
We have exploited the superior sensitivity of the ERIXS instrument of the beam line ID32 of the ESRF to take a deeper look at the CDW phenomenon. We could thus observe the existence of short-ranged Charge Density Fluctuations (CDF) aside the already known CDW in the 123 family [1]. They persist up to well above the pseudogap temperature T*, are dynamical, i.e. characterized by energies of few meV, and pervade a large area of the phase diagram: their discovery is going therefore to stimulate a revision of the current understanding of the charge order phenomenon in cuprates.

Remarkably, we found that CDF may explain the linear ***T*** dependence of the resistance above ***T****, indicating that they are likely the long-sought excitations underlying the anomalous Marginal Fermi Liquid behavior of HTS [2].

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#235 - INFLUENCE OF HYDROSTATIC PRESSURE AND OF EU/BI SUBSTITUTION ON THE MAGNETIC PROPERTIES OF EU2IR2O7

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The arrangement of magnetic moments at the vertices of a pyrochlore lattice leads to a great variety of electronic ground states for $R_2M_2O_7$ materials. One important finding common to several families of these oxides is that changes in r_I, the ionic radius of the rare-earth ion R^{3+}, gradually tune the local crystalline environment around the transition metal ion M^{4+} and the overall electronic behavior of the compound in turn. For M = Ir, the characteristic temperature T_{MI} for the development of a metal-to-insulator transition is directly controlled by the average value r_I related to a gradual chemical substitution. Moreover, the metal-to-insulator transition in $R_2Ir_2O_7$ is associated with a dramatic change in the magnetic behavior as well.

Here, we report on the magnetic properties of $Eu_2Ir_2O_7$ under pressure, both from dc magnetometry and μ^+SR [1]. The absence of a localized magnetic moment from *f* shells in $Eu_2Ir_2O_7$ is a great advantage in the study of the intrinsic magnetic properties of the Ir sublattice. We deduce a markedly nonmonotonic P-dependence of the critical transition temperature to the antiferromagnetic state (T_N) hinting at its departure from T_{MI}. The behavior recently reported for T_N from relativistic LDA+DMFT calculations closely reproduces our data under the assumption that P influences the U/W ratio (U and W representing the Coulombic repulsion and electronic bandwidth, respectively). Our μ+SR data confirm that the Ir^{4+}magnetic moment and/or the local magnetic configuration are only weakly perturbed by pressure in the P < 24 kbar range. Accordingly, our measurements strongly support the preservation of a 4-in/4-out ground state.

We also report on our recent study of the pyrochlore series $(Eu_{1-x}Bi_x)_2Ir_2O_7$ for polycrystalline samples for $0 \leq x \leq 1$ [2]. We show that the lattice undergoes an anomalous contraction for $x \leq 0.05$ but that the magnetic all-in/all-out state remains robust in that limit of chemical dilutions. For small x values, the resistivity approaches a 1/T dependence at low temperatures, suggesting a proximity to the Weyl semimetallic phase, as predicted theoretically. At x = 0.1 a qualitatively new ground state emerges, which is characterized by a metalllic behaviour and absence of magnetic ordering at least down to 20 mK. For higher Bi-doping values, the resistivity remains metallic and it evolves gradually from T-like to T^2-like and, eventually, to $T^{3/2}$-like, suggesting the possibility of a variety of novel exotic phases.

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#236 - TUNING SPIN-CHARGE INTERCONVERSION WITH CONFINEMENT IN ULTRATHIN BI/GE(111) FILMS

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Spin-charge interconversion (SCI) phenomena have attracted a large interest in nowadays spintronics, since they represent an essential step towards the design and engineering of spintronic devices. In this respect, the scalability down to the nanometer scale and the integrability with opto-electronic and spintronic devices are important features that drive the choice of the SCI platform. Here, we investigate SCI in ultrathin Bi films epitaxially grown on Ge(111) as a function of the Bi thickness t. We use x-ray diffraction and scanning tunneling microscopy to obtain a clear picture of the morphology and crystallography of the system. Through spin- and angle-resolved photoemission we show that spin-polarized surface states crossing the Fermi level are present. Then, we directly probe the charge-to-spin conversion by detecting with magneto-optical Kerr effect the electrically-induced spin accumulation in Bi, and the spin-to-charge conversion by generating a spin current in the system with either optical or ferromagnetic resonance-driven spin injection. We recover large SCI signals in the thickness range ($1 < t < 3$ nm) characterized by the presence of small Bi nanocrystals.We observe that the conversion efficiency drastically decreases as t increases, when the Bi islands start to percolate. Since bulk SCI is small, the conversion is mainly related to the Rashba-Edelstein effect associated with electron transport in the spin-polarized surface states. In this frame, we tentatively explain the observed thickness dependence of SCI by reminding that the Bi conductivity can be strongly affected by quantum confinement effects. In the high confinement conditions realized in the Bi nano-islands obtained for $1 < t < 3$ nm, the bulk resistivity is assumed to be high enough to electrically disentangle the upper and lower Bi surfaces, which otherwise would give rise to opposite contributions to SCI conversion that tends to cancel out, drastically decreasing the net SCI signal. Our results indicate that quantum size effects might be exploited as a tool to tune SCI and investigate a very rich spin-physics.

#237 - ELECTRON DOPING IN BA2NAXCA1-XOSO6 SPIN – ORBIT QUANTUM OXIDES: A LOCAL STRUCTURAL STUDY

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Spin-orbit oxides belong to the novel class of *quantum materials*, the physical properties of which are greatly influenced by the quantum mechanical nature of interactions between constituent electrons. In this context we study the local atomic and electronic structure of Osmium-based double perovskites (DPs) which exhibit a combination of strong spin-orbit coupling (SOC) and anisotropic exchange interactions. In this system SOC is of similar magnitude to crystal field and electron correlation effects (Hubbard U), making the prediction of properties more complex than for DP containing more well known 3*d* cations. We have studied the evolution of the properties of $Ba_2Na_xCa_{1-x}OsO_6$ by substituting monovalent Na with divalent Ca cations. Muon spin spectroscopy and magnetization measurements indicate that the magnetic ground state changes from FM-canted for x=1 to AFM for x=0 with a monotonic increase of the magnetic transition temperature from 5 to 40 K.

Here we present astudy of the changes of the material’s local atomic and electronic structure in $Ba_2Na_xCa_{1-x}OsO_6$, using a combination of XAFS and ***ab-initio*** simulations. XAFS is the method of choice to determine local atomic and electronic structure simultaneously; its combination with ab-initio simulations is particularly powerful. XAFS measurements at the Ca, Na, Os and Ba edges have been recorded and analyzed. The ab-initio calculations, performed with the Vienna Ab initio Simulation Package (VASP) within the non-collinear DFT+U+SOC scheme, provide support to the experimental evidences by delivering independent structural and electronic properties and allowing for a detailed microscopic interpretation of the results.

The extended range (EXAFS) data indicates that the local structure is the expected DP one, with a random distribution of Ca and Na and no anti-site defects; interatomic distances vary linearly with concentration. The Os L_3 near edge spectra (XANES) exhibit no shift with x, indicating that the net local charge on this cation does not change, despite the substitution of a monovalent cation with a divalent one. This indicates a delocalized distribution of the excess charge associated with an increased hybridization between Os-d and O-p states. The intensity of transitions to t_{2g} orbitals increases with x with respect to that relative to transitions to e_g ones. These experimental results are compared to the local electronic structure derived from *ab-initio* electronic structure simulations.

#238 - MANIPULATING THE GROUND STATE IN NICKELATES USING PROXIMITY WITH MAGNETIC LAYERS

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Transition metal oxides (TMO) are a class of materials where the charge, orbital, magnetic, and spin degrees of freedom are mutually connected. Interfacing different TMOs offers the possibility to act on each of these degrees of freedom, tailoring new materials with desired properties. In this work, we investigate the effect of the presence of a magnetic proximity layer on the ground state of neodymium nickelate (NNO) interfacing thin NNO films with ferro- and antiferromagnetic manganite layers (strontium and calcium doped lanthanum manganite – LSMO and LCMO) grown *via*pulsed laser deposition (PLD). Angle resolved photoemission spectroscopy (ARPES) and X-ray magnetic circular dichroism (XMCD), supported by momentum-resolved density fluctuation (MRDF) theory, revealed the suppression of the PM metal – AFM insulator transition in NNO thin films, and the emergence of a new FM metal ground state. This work paves the way for tailoring magnetic properties in different oxides, where already existing magnetic ordering can be tuned using proximity effects.

#239 - METALLIC AND INSULATING STRIPES AND THEIR RELATION WITH SUPERCONDUCTIVITY IN THE DOPED HUBBARD MODEL

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The dualism between superconductivity and charge/spin modulations (the so-called stripes) dominates the phase diagram of many strongly-correlated systems. A prominent example is given by the Hubbard model, where these phases compete and possibly coexist in a wide regime of electron dopings for both weak and strong couplings. Here, we investigate this antagonism within a variational approach that is based upon Jastrow-Slater wave functions, including backflow correlations, which can be treated within a quantum Monte Carlo procedure. We focus on clusters having a ladder geometry with M legs (with M ranging from 2 to 10) and a relatively large number of rungs, thus allowing us a detailed analysis in terms of the stripe length. We find that stripe order with periodicity l=8 in the charge and 2l=16 in the spin can be stabilized at doping d=1/8, in agreement with Ref. [1]. Here, there are no sizable superconducting correlations and the ground state has an insulating character. A similar situation, with l=6 appears at d=1/6. Instead, for smaller values of dopings, stripes can be still stabilized, but they are weakly metallic at d=1/12 and metallic with strong superconducting correlations at d=1/10, as well as for intermediate (incommensurate) dopings. Remarkably, we observe that spin modulation plays a major role in stripe formation, since it is crucial to obtain a stable striped state upon optimization. The relevance of our calculations for previous density-matrix renormalization group results and for the two-dimensional case is also discussed [2].

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#240 - CHEMICAL REACTIVITY AND INDUCED FERROMAGNETISM AT VSE2/FE INTERFACE

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Among 2D transition-metal dichalcogenides, monolayer VSe_2has been gaining major attention due to its unique combination of charge density wave and magnetic properties. Regarding the latter, its state is nowadays under debate, with contradictory results recently published. Here, we investigate the magnetic and chemical properties of VSe_2/Fe heterostructure. While x-ray magnetic circular dichroism spectra at V $L_{2,3}$edges of both bare bulk and monolayer/few layers VSe_2do not show any signature of ferromagnetic ordering, in the case of VSe_2/Fe bilayer a dichroic signal appears at room temperature at V L2,3 edges, with antiparallel alignment with respect to Fe. Combined measurements of XAS, ARPES and x-ray photoemission investigate the chemical reactivity at VSe2/Fe interface and its relation with interfacial magnetic coupling.

#241 - AMORPHIZATION PROCESSES IN PHASE CHANGE MATERIALS: EVOLUTION OF THE STRUCTURE AND ELECTRICAL PROPERTIES UPON DISORDERING

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Phase change materials are widely employed for many applications, thanks to the ability to rapidly switch between the amorphous and the crystalline phase. The crystallization has been widely investigated in literature, whilst there is a lack of information on the mechanisms governing the amorphization, mainly because it can be obtained only by driven conditions, largely far from equilibrium, usually implying melting and quenching.

With the aim to understand which are the accessible local atomic configurations towards amorphization, we have investigated the damaging process of crystalline GeSbTe alloys and of GeTe up to amorphization, by using ion irradiation. Light ions (Ar^+) have been employed to produce diluted cascades, which allows very low amount of disorder to be introduced and to follow then the structural evolution towards complete amorphization.

In situ reflectivity measurements and ex-situ resistance and Raman spectroscopy analysis have been employed to study the disordering process and its impact on the electrical properties and on the chemical bonds. Different compositions are compared: $Ge_2Sb_2Te_5$, $GeSb_2Te_4$ and GeTe. The effect of disordering is studied at low temperature (77K), at which the atomic mobility and disorder recovery is hindered, and at room temperature. Large differences are observed upon irradiation at low or room temperature, indicating that there is a large effect of dynamic annealing. Several phase transitions are observed before amorphization. The first change is the metal to insulator transition. In ternary GeSbTe alloys (with Ge < 30%) the disordering process is dominated by the presence of the stoichiometric vacancies. The van der Waals like gaps present in the stable hexagonal crystalline structure act as preferential sink for the diffusion of the displaced atoms, and are therefore effective in stabilizing the disordered material. The filling of the gaps tunes the electronic and structural properties, driving the metal-insulator transition and the successive conversion into the metastable rocksalt structure and then in the amorphous.

In the case of GeTe there are no structural vacancy layers. Nevertheless, the metal-insulator transition is observed anyway, at very low fluences and it seems to be induced by Te vacancy, characterized by an energy level into the gap. As the irradiation fluence increases, the displaced atoms form distorted octahedral bonds that, being energetically unfavourable, tend to disappear, going back to a more stable configuration. Such a process seems to be facilitated by the high atomic mobility that, according to crystal growth rate data available in literature, at room temperature is expected to be larger in GeTe than in GeSbTe alloys. As a consequence, GeTe exhibits unique marked self-healing properties and the irradiation fluence required for complete amorphization is one order of magnitude higher than that of GeSbTe alloys.

#242 - SYNTHESIS AND INVESTIGATION OF ZNO NANOWALLS FOR LOW CONCENTRATION GAS SENSING

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Zinc Oxide (ZnO) nanostructures, thanks to biocompatibility, non-toxicity, low cost, earth abundance, and chemical and thermal stability, have attracted a large industrial and academic interest for applications in gas sensing. Among the various typologies of ZnO nanostructures, nanowalls (ZnO

NWLs) have attracted increasing interest because of their huge surface-to-volume ratio and extremely thin wall thicknesses.

In this work we prepared NWLs by low cost by using chemical bath deposition (CBD) at the operating temperature of 70–95°C. In this way we were able to grow high-quality ZnO NWLs vertically on Al (covered) substrates, with an intertwined, honeycomb-like-pattern and c-axes parallel to the substrates, producing a huge surface-to-volume ratio and extremely thin wall thicknesses. These characteristics make them optimum candidates for detection of very low gas concentrations, for instance in environmental or medical fields.

In particular, we tested ZnO NWLs for detecting low concentration of NO2 and CO gases, by chemoresistive approach. Indeed, we grew ZnO nanowalls on the Pt interdigitated electrodes area of conductometric alumina platforms. The samples were deeply characterized by a structural and morphological point of view. Then, gas sensing properties of the films were studied by measuring the changes of electrical resistance upon exposure to low concentrations of carbon monoxide (CO) and nitrogen dioxide (NO2) in air. The sensor response to CO or NO2 evidenced a strong dependence on the operating temperature, providing a means to tailor the sensitivity and selectivity toward these selected target gases.

Given the excellent properties of ZnO NWLs for gas sensing at high temperatures, a detailed study of the electrical and optical properties was performed in order to find the way towards room temperature gas sensing. In particular, the opto-electrical properties were analyzed as a function of the growth time and post-growth annealing temperature to pursue the realization, in the future, of a UV-activated room temperature gas sensor. This strategy can be very promising because it doesn’t require alteration of the nanostructures by means of doping or surface functionalization that can compromise the versatility of the sensor.

#243 - STRUCTURE-BASED MODELING OF PH SENSING IN ZINC-BASED NANOWALLS

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The pH sensitivity reported in literature for different ZnO nanostructures (nanowalls, nanotubes, nanorods) spreads from sub- to super-Nernstian, with the microscopic mechanism behind the H^+ detection often unrevealed. Zinc based nanostructures are very promising material for pH sensing since they allow the realization of low-cost, sustainable, and high sensitivity electrodes. In this work we investigated the response towards pH sensing of two zinc based nanowalls (NWLs) which were synthesized by hydrothermal process. The NWLs consist of layered hydroxide zinc nitrate $Zn_5(OH)_8(NO_3)_2 \cdot 2H_2O$ (as grown) and zinc oxide ZnO (annealed) phases, respectively.

Scanning electron microscopy, micro Raman spectroscopy, X-ray photoelectron spectroscopy were used to characterize the morphology and structure of NWLs. Electrochemical chronopotentiometric analysis in standard buffer solutions was used to study the response towards pH in the range of 4-9.

The two zinc based NWLs have the same morphology (interconnected sheets 10-20 nm thin, 1.4-1.7 mm wide), but different behavior as pH sensitive electrodes. As grown NWLs show a super-Nernstian response (+83.7 mV/decade), whereas annealed NWLs show a sub-Nernstian response (+27.1 mV/decade). The data evidenced that the response towards pH sensing of the investigated systems is not related to the morphology of nanostructures. We satisfactorily modeled the experimental results by considering the crystallographic structures and assuming that layered hydroxide zinc nitrate NWLs is sensitive to only H^+ (with two simultaneous and independent mechanisms), while zinc oxide NWLs is simultaneously and independently sensitive to both H^+ and OH^-. These data and the proposed modeling are useful to further develop the pH sensitivity of electrodes based on ZnO nanostructures.

#244 - NI(OH)2@NI CORE-SHELL NANOCHAINS AS LOW-COST HIGH-RATE PERFORMANCE ELECTRODE FOR ENERGY STORAGE APPLICATIONS

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Energy storage performances of Ni-based electrodes rely mainly on the peculiar nanomaterial design. In this work, a novel and low-cost approach to fabricate a promising core-shell battery- like electrode is presented [1]. Ni(OH)$_2$@Ni core-shell nanochains were obtained by an electrochemical oxidation of a 3D nanoporous Ni film grown by chemical bath deposition and thermal annealing. This innovative nanostructure demonstrated remarkable charge storage ability in terms of capacity (237 mAh g^{-1} at 1 A g^{-1}) and rate capability (76% at 16 A g^{-1}, 32% at 64 A g^{-1}). The relationships between electrochemical properties and core-shell architecture were investigated and modelled. The high-conductivity Ni core provides low electrode resistance and excellent electron transport from Ni(OH)$_2$shell to the current collector, resulting in improved capacity and rate capability. The reported preparation method and unique electrochemical behaviour of Ni(OH)$_2$@Ni core-shell nanochains show potential in many field, including hybrid supercapacitors, batteries, electrochemical (bio)sensing, gas sensing and photocatalysis.

[1] M. Urso et al. Scientific reports 9 (1), 7736 (2019).

#245 - AB INITIO STUDY OF GRAPHENE INTERACTION WITH ALN

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In recent years the need to find a cheaper substrate than SiC on which Graphene can be grown lead the researchers to find a better alternative. In this context, project GraNiTe represents a combined effort between CNR- IMM, ST Microelectronics, CNRS-CRHEA and TopGaN to create devices for high frequency electronics combining Graphene and group III nitrades. The key advantage of using non-conducting substrates for graphene growth lies in the absence of a transferring step, which allows for the preservation of the quality of the material and reduces the overall cost of production. Group III nitride semiconductors have been successfully implemented in the felds of high-mobility electronics. The growth of graphene on these substrates could further enhance or even expand their features, allowing for high frequency modulation of the electrical current in vertical heterostructure designs. The substrate that we analyzed was AlN (Wurtzite). We used the code SIESTA to simulate a AlN-Graphene hetercostructure focusing on the study of four different surface reconstructions of the AlN, the two ideal surfaces(Al and N) and an Al-poor Al surface and Al-rich N surface. We found that there is a very weak interaction between the perfect Al face and graphene. A further analysis of the band structure shows that the graphene is n-doped and source of this doping has to be researched in the fermi level pinning of the surface. The structural analysis of the system with Al-poor face shows a stronger in- teraction, but still very low. This stronger interaction is well shown in the band structure. The system is still n-doped and the absolute level of doping is higher than the first case. We then analyzed the perfect N-face, the distance between the AlN and graphene is lower than perfect Al face. The unfolded band structure show us that the bands are not so perturbed, but the peculiar thing of this face is the inversion of the doping, the graphene is p-doped. The absolute level of doping is lower than the ideal Al face but still very high. We then analyzed the interaction with the Al-rich N face. In this case the distance between the AlN and graphene is higher than the perfect N-face. The unfolded band structure show us that the AlN bands are more perturbed than the Graphene ones, on this reconstruction the inversion of the doping is not present, we can conclude that the graphene is n-doped. The absolute level of doping is similar to the ideal Al face. The DFT results obtained for the graphene/AlN interface show peculiarities that could be interesting for the practical implementations of this system in high mobility, high power and high frequency microelectronics.

#246 - ORBITAL SELECTIVE CORRELATIONS AND THE PHASE DIAGRAM OF IRON-BASED SUPERCONDUCTORS

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Almost everyone believes that electron-electron correlations are the key to understand superconductivity in high-temperature superconducting cuprates. On the other hand, the strength and the role of electron-electron correlations in iron-based superconductors remain debated. We argue that solution of the debate lies in the orbital-selective character of the correlations [1], with some orbitals being significantly more correlated than others. This reconciles conflicting evidences and accounts for the dependence of the effective mass on doping and on the specific material considering the cases of electron- and hole-doped BaFe2As2 [2]. The orbital-selective Mott scenario also establishes a novel link between the iron-based superconductors and the cuprates, which suggests that the role of electron-electron correlations may be also the source of superconductivity. We finally discuss how such orbital-selective correlations influence the tendency towards a nematic ordering in FeSe and in other compounds [3] and the role of the same correlations in determining the properties and the symmetry of the superconducting state [4].

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#247 - HIBISCUS: HIGH PERFORMANCE-LOW COST IRON BASED COATED CONDUCTORS FOR HIGH FIELD MAGNETS

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High superconducting transition temperature, upper critical field, and critical current density are the three major requirements for high magnetic field applications of superconductivity.
Iron-based superconductors (IBS) discovered in 2008, could be a breakthrough of the intrinsic limits of low-Tc Nb_3Sn(20 T at 4.2 K) and of the extreme material complexity of copper oxide high-Tc superconductors (HTS), which leads to articulated and expensive processes for wire/tapes fabrication. The superconducting properties of IBS largely exceed those of Nb3Sn and theirintrinsic properties and preparation procedures appear less critical than those of HTSs.
The project HIBiSCUS aims at developing highly optimized IBS coated conductors (CCs), focusing on the trade-off between cost effectiveness and performances and taking advantage from an accurate material characterization.
We will develop new fabrication processes for IBS-CCs, relying on the advanced technologies developed in the last decades for HTS-CCs, but focusing on the possibility of simplifying the processes to drastically reduce fabrication costs and times. The optimization of IBS-CCs and their suitability for specific applications will be addressed by the combined use of complementary techniques including microstructure and superconducting properties on the local and macroscopic scale.

#248 - ULTRATHIN MOLYBDENUM DISULPHIDE AS A GATE-TUNABLE MULTI-VALLEY SUPERCONDUCTOR

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Gate-induced superconductivity (SC) at the surface of semiconducting transition metal dichalcogenides (TMDs) has attracted a lot of attention in recent years, thanks to the sizeable transition temperature, robustness against in-plane magnetic fields beyond the Pauli limit, and hints to a non-conventional nature of the pairing. A key information necessary to unveil its microscopic origin is the geometry of the Fermi surface hosting the Cooper pairs as a function of field-effect doping, which is dictated by the filling of the inequivalent valleys at the K/K’ and Q/Q’ points of the Brillouin zone. While it is often assumed that Cooper pairs reside only in the two electron pockets at K/K′, experimental and theoretical results suggest that a multi-valley Fermi surface (FS) is instead associated with the SC state, involving the six electron pockets at Q/Q′. Here, I will present a work combining low-temperature electric transport and Raman spectroscopy measurements in ion-gated MoS_2 thin flakes with ab-initio DFT calculations of the bandstructure to show that a fully multi-valley FS is associated with the onset of the SC state, and that a sizeable SC transition temperature does not appear until the Fermi level crosses both spin-orbit split sub-bands in the Q/Q’ valleys.This combined approach can be employed to map the dependence of the Fermi surface of gated MoS_2 on field-effect doping and demonstrates that the SC state is associated with the FS connectivity and promoted by multiple Lifshitz transitions due to the simultaneous population of multiple electron pockets. I will also discuss some possible implications that this peculiar FS geometry may have on the structure of the SC gap probed by tunnelling spectroscopy measurements.

#249 - FEASIBLE MODEL FOR LIGHT-INDUCED INTERBAND PAIRING

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Recent theoretical works [1,2] have highlighted the existence of a purely electronic mechanism for the appearance of non-equilibrium superconductivity in a resonantly driven semiconductor with repulsive interband interactions. The original proposals relied anyway on the existence of a specific fermionic dissipation mechanism and the careful simultaneous tailoring of the electronic dispersion relation and the electron-electron interaction.

In this work we show that this mechanism is actually more general and does not need any special tuning of the parameters. When considering a pair of bands with the same sign of concavity, we indeed demonstrate that interband pairing emerges under the natural assumptions of the presence of phononic baths and radiative recombination. In light of these findings, we show how the appearance of superconductivity can be understood in terms of standard equilibrium interband BCS theory. Finally, we conclude by presenting a phase diagram for the steady state of the model.

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#250 - NON-LINEAR I-V CHARACTERISTICS IN TWO-DIMENSIONAL SUPERCONDUCTORS: BEREZINSKII-KOSTERLITZ-THOULESS PHYSICS VS INHOMOGENEITY

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The progresses made in the last decades in material science make nowadays available a wide class of systems whose thickness ranges from few nanomenters up to the atomic-layer limit. In some interesting cases, the ground state can be tuned from the metallic to the superconducting (SC) one. In 2D SC materials the transition is expected to be described by the Berezinsky-Kosterlitz-Thouless (BKT) theory, where the relevant excitations are topological vortex-like configuration. One of the hallmarks of BKT transition in 2D superconductors is the universal jump of the superfluid density, that can be indirectly probed via the non-linear exponent of the current-voltage *I-V* characteristics. In this scenario, the non-linearity of current-voltage *I-V* characteristics is ruled by the unbinding of vortex-antivortex pairs induced by a large enough current and the exponent of the current *I* is expected to jump from 3 to 1 (ohmic behaviour) as the temperature increases above the critical temperature. However, the experimental observation of the BKT transition in real systems is far from being straightforward. We compared two paradigmatic cases, namely NbN thin films and STO-based interfaces. In the former case, although the superfluid-density jump is smeared by disorder it is still observable, either via direct measurements of the inverse penetration depth or via the measurement of the exponent of the non-linear *I-V* characteristics near the critical temperature. On the other hand, in STO-based interfaces direct measurements of the superfluid-density is rather challenging, while the analysis of the *I-V* characteristics does not seem to be justified in order to infer the occurrence or not of a BKT-like transition. We argue that in the case of inhomogeneous superconductors, where there has been increasing evidence that the SC background organizes in islands of larger size, the non-linearity arises from the pair-breaking effect in the weaker SC regions due to a finite applied current *I*, non-linearly increasing the global resistivity. In these systems, the broadening of the resistive transition itself has been ascribed to a percolation mechanism via a network of SC puddles. Likewise, with a simple random resistor network (RRN) model in effective medium (EM) approximation, we can reproduce the *I-V* non-linearity in qualitative agreement with experiments.

#251 - EVIDENCE OF THE ISOELECTRONIC CHARACTER OF F DOPING IN SMFEASO(1−X)F(X).

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The $SmFeAsO_{1-x}F_x$ superconducting alloy has attracted much attention because of its high transition temperature ($\mathbf{T}_C = 58$ K) at optimal doping [1]. Recent experiments [2] show that the Shubnikov de-Haas oscillations in the $SmFeAsO_{1-x}F_x$ do not change with F concentration. This behavior is somewhat surprising because it contradicts the common believe that F should behave as a donating impurity. In a semimetal, as the SmFeAsO, electron doping should widen the size of the Fermi surface for the electrons and shrink those related to the holes. Instead, experimental evidence suggests that the size of the Fermi surfaces is independent of F concentration. To shed light on this anomalous behavior, we study the electronic structure of the $SmFeAsO_{1-x}F_x$ alloy by means of first-principle calculations [3]. We find that, contrary to common believe, F-doping does not change the charge balance between electrons and holes free-carriers in $SmFeAsO_{1-x}F_x$. Indeed, within a narrow energy range across the Fermi energy, the effect of F-doping on the band structure dispersion is tiny in both the paramagnetic and stripe antiferromagnetic phase of $SmFeAsO_{1-x}F_x$. Using the concept of Baders charge, we discuss the charge balance between the conducting FeAs-layer and the $SmFeAsO_{1-x}F_x$ charge reservoir layer as a function of F concentration. The results of our calculations show that the charge state of the FeAs-layer is not influenced by the compositional change. Such a surprising behavior can be explained looking at the evolution of the band structure as a function of F concentration. We discover that the additional charge carried by fluorine, with respect to the oxygen, is compensated by a change in the oxidation state of the Sm ion from 3+ to 2+. A comparison with the $SmFe_{1-x}Co_xAsO$ system shows that such a charge compensation by the Sm ion is not shared by donors substituting at the Fe site.

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#252 - ITICAL FIELDS ANISOTROPY IN IRON-CHALCOGENIDE FE(SE, TE) THIN FILMS

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The anisotropy of superconducting and pinning properties is one of the key parameters, which determines whether or not a material is suitable for high field applications. Iron-chalcogenides are known to be weak anisotropic superconductors. Among them, Fe(Se,Te) thin films are characterized by very low and robust values of the anisotropy factors $g_J$and g_H. The origin of this behaviour is still a puzzling question whose answer requires deeper analysis on fundamental superconducting properties. In this work, we report about the angular dependence of the critical fields evaluated with different criteria. Different behaviours have been observed, which are anyway in between the behaviours of a fully 2D and an anisotropic 3D material. In order to compare our results with those on a well-known 3D HTSC, we have carried out the same analysis on YBCO thin films. Moreover, we make a comparison also with the case of 2D ultra-thin superconducting films.

#253 - TIME-REVERSAL SYMMETRY BREAKING IN RE-BASED SUPERCONDUCTORS

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As possible systems to harbor unconventional pairing symmetries, noncentrosymmetric superconductors (NCSCs) are under intense study. Here, relaxed space-symmetry requirements lead to anti-symmetric spin-orbit coupling (SOC), possibly inducing a mixture of spin-singlet and spin-triplet pairing. In addition, some NCSCs are known to break also the time-reversal symmetry (TRS). Since, in principle, time-reversal and space-inversion symmetries may occur independently, their concomitant breaking among numerous Re-based NCSC compounds remains puzzling.

To trace the origin of time-reversal symmetry breaking in Re-based superconductors, we performed an extensive study of numerous cases [1, 2]. Among these, the $Re_{1-x}Mo_x$ alloys [3, 4], which are all superconductors, yet with either centro- or non-centrosymmetric structure, represent one of the most suitable systems for studying the interplay of space-inversion, gauge-, and time-reversal symmetries. By performing comparative muon-spin relaxation/ rotation (μSR) measurements, we address the key question of TRS breaking in ReT systems. The observation of a gradual increase of ZF-μSR relaxation rate below T_c, yet its independence of crystal-structure symmetry, suggests the rhenium presence to be the key factor for the appearance and the extent of TRS breaking in ReT superconductors.

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#254 - HOW TO MIMIC NATURAL ORGANELLES BY ENGINEERING BIO-SYNTHETIC NANOCOMPARMENTS WITH IN VIVO FUNCTIONALITY

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New concepts that combine active compounds with stable, safe carriers or membranes resulting in functional systems are on focus in a variety of domains, such as medicine, catalysis, environmental science, food science and technology. In particular, suitable amphiphilic block copolymers are ideal candidates for generation of 3D supramolecular assemblies, such as compartments, micelles, nanotubes or planar membranes. Such synthetic flexible membranes have a superior stability, and robustness compared to the lipid based membranes, and can be obtained with a variety of physical and chemical properties. By combining such polymeric nanocompartments with suitable biological entities, e.g., by enzyme encapsulation inside the cavity, membrane proteins insertion in their synthetic membranes or biomolecules attachment at their surface, it is possible to provide welldefined functions, such as molecular recognition, cooperation, and catalytic activity.1

Here, we present distinct spaces for desired reactions at the nanometer scale based on protein-polymer assemblies as compartments with triggered activity that play the role of artificial organelles when internalized in cells.2

Biopores/channel proteins inserted into the polymer membrane selectively control the exchange of substrates and products, resulting in development of stimuli-responsive compartments, which preserve their architecture, while allowing specific in situ reactions. Generation of nanocompartment clusters represents a step further in more complex architectures mimicking intracellular artificial organelles.3 This general strategy based on combination of synthetic assemblies and biomolecules supports the development of artificial organelles, proved to be functional in vitro and in vivo, in Zebra fish.2

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#255 - PULSED X-RAY SOURCES FOR TIME-RESOLVED STRUCTURAL STUDIES ON PHOTOSENSITIVE PROTEINS

Giorgio Schiro' (I) - CNRS - Institut de Biologie Structurale

Biological macromolecules are characterized by specific structural and dynamic features that are at the basis of their biological activity. Understanding macromolecular activity thus requires studying structural changes over time and on various time-scales down to the femtochemistry regime. Electron accelerators for X-ray production (X-ray free electron lasers - XFEL - and synchrotrons) are able to deliver short (~100 ps at syncrothrons and ~10 fs at XFELs) and bright X-ray pulses. If synchronized with optical lasers to trigger a photoreaction, X-rays can provide structural snapshots after the photoreaction with high time and space resolution. Time-resolved X-ray scattering and diffraction permit tracking macromolecular conformational changes along a photoinduced reaction pathway, and their characterization at the atomic level of resolution [1]. I will show results from our recent studies of light-induced protein structural dynamics in model systems [2] and in photoactive proteins on the femtosecond to millisecond time scale [3-5].

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#256 - THERMAL IMAGING BY SUB-DIFFRACTION LOCALIZATION OF PHOTOACTIVATED ABORBERS

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Conventional thermal imaging provides temperature spatial maps based on the intensity of infrared radiation emitted by the sample and detected by a microbolometer-based thermal camera under the assumption of grey body radiance. Active thermal imaging measures the temperature response of the sample following a laser induced heating, thereby giving a thermal contrast that can be employed to reconstruct the image. However, the typically low numerical aperture of collecting Germanium lenses sets a diffraction-limited spatial resolution of ∼0.1-0.5 mm that can be worsened to ∼1 mm by the thermal waves diffusion in the sample, preventing high sensitivity (∼0.1°C) temperature mapping with tens-of-microns resolution across extended (mm-/cm- sized) fields of view.

By employing a time modulated laser light scanning of sparse heat absorbers in the sample we introduce and validate here a photo-thermal super-resolution image acquisition approach. Heat centers localization occurs by the non-linear surface fit of the isolated temperature peaks in the time stacks acquired by the thermal camera, and a final super-resolved image is obtained that contains both the morphological information of the absorbing sample through the peak coordinates and the temperature variations gained from the best-fit amplitudes.

Proof-of-principle experiments on synthetic ink samples demonstrate photo-activated super-resolution thermal imaging: by comparison of our results with conventional transmitted-light images of the same samples a 60-μm attainable resolution on the adopted setup configuration is shown, increasing up to 20 times the effective (1200±180)-μm resolution of our thermal camera in conventional operation.We also applied the method to detect the distribution of photothermal nanoparticles in tissues by imaging an explanted murine skin biopsy treated with Prussian blue 30-nm nanocubes. This is a very interesting tool to analyze the distribution of nanoparticles either in treated pathological tissues, or in organ biopsies to uncover their biodistribution in vivo experiments. We envision potential applications and future impact of photo-activated super-resolved thermal imaging in both the biotechnological and nano-medical fields.

#257 - EFFECT OF CHOLESTEROL ON THE PROTEOLYTIC PROCESSING OF APP

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Several findings point at high cholesterol levels as a risk factor for the development of Alzheimer's disease. An intriguing hypothesis suggests that high cholesterol content in the plasma membrane can promote the translocation of the amyloid precursor protein (APP) in proximity of the β-secretase (BACE1) and the gamma-secretase complex at the level of membrane-rafts, increasing therefore the production of toxic Aβ peptide. By contrast, the a-secretase (ADAM10), responsible for the nonamyloidogenic pathway, seems to stably localize in the non-raft regions, and its activity should not be influenced by cholesterol levels.

Here we have elucidated the effect of cholesterol on the proteolytic processing of APP in living cells using a prototypal fluorescence bioassay coupled with flow cytometry. Our findings clearly indicate a strong correlation between cholesterol concentration and APP cleavage degree. Similar results were obtained for cells overexpressing a mutant APP variant that cannot be processed by ADAM10, highlighting the significant role of cholesterol on the first event involving the cleavage of APP by BACE1.

In addition, we have been investigating, for the first time, the influence of cholesterol on the dynamics of APP and secretases at the plasma membrane level with single molecule tracking experiments. Preliminary data suggest that no correlation exists between the lateral diffusion of APP, BACE1 and ADAM10, and the cholesterol content, assuming that cholesterol affects the processing of APP with mechanisms different from those postulating the involvement of membrane-rafts. However, other experiments are required to confirm this result.

#258 - INVESTIGATION OF PROTEIN AGGREGATION IN HEALTH AND DISEASE BY AFM-BASED METHODS

Francesco Simone Ruggeri - University of Cambridge

Today, more than 40 million people worldwide are affected by dementia and neurodegenerative disorders. Onset of these diseases is associated at the molecular level with the misfolding and aggregation of proteins into insoluble fibrillar protein aggregates termed amyloids, forming intracellular inclusions or extracellular plaques in the brain of patients. The molecular origin and mechanistic link between amyloid formation and neurodegeneration aetiology remain unclear and no therapies, able to cure or delay the onset of these pathologies, are available. Despite its fundamental role in biological function and malfunction, the mechanism of protein self-assembly and its link with cellular toxicity and neurodegeneration remains challenging to elucidate, mainly because unraveling amyloid species biophysical properties at the nanoscale still represents a formidable experimental challenge.

Here, we first show that the limitations of manual samples deposition for AFM single molecule imaging can be overcome with a single-step microfluidic spray deposition platform. This method transfers biological solutions to substrates as microdroplets with sub-picoliter volume, drying in milliseconds, preserving the molecular architecture and heterogeneity of the sample under investigation. Furthermore, exploiting high-resolution AFM and force spectroscopy, we demonstrate the identification and characterisation of the smallest elementary unit in the hierarchical assembly of amyloid fibrils, which we termed single-strand protofilaments. We demonstrate that these new species possess sub-nanometer diameter and form from the direct interaction and assembly of unfolded monomeric polypeptide chains. Finally, we prove that the combination of AFM with infrared spectroscopy (AFM-IR) can successfully characterise the chemical properties of individual amyloid aggregates at the nanoscale both in air and native liquid environment.

Unraveling the biophysical properties of protein aggregates at the single species scale is fundamental in order to develop a model of their toxicity as well as new pharmacological approaches to tackle neurodegeneration.

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#259 - LIBRATIONAL CHAIN DYNAMICS IN UNSATURATED LIPID BILAYERS AT CRYOGENIC TEMPERATURE

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Electron Spin Resonance (EPR) experiments at cryogenic temperature allow to unravel dynamic properties of biosystems that would be otherwise hidden at higher physiological temperatures. An interesting motion that manifests itself in the echo-detected EPR spectra of spin-labeled samples in the frozen state is the librational motion. It consists of high-frequency segmental oscillations of small angular amplitude. The librational dynamics of chain-labeled lipids incorporated in lamellar phases composed of saturated and unsaturated lipids, namely DPPC, POPC and DOPC bilayers, is studied by combining two-pulse echo detected EPR spectra and continuous wave EPR data in the temperature range 77-270 K. The temperature dependences of the mean-square angular amplitude of libration and the rotational correlation time of motion are investigated for positions of labeling at the first segments and at the terminal methyl end of the lipid chain. Whereas the rotational correlation time lies in the sub- to nanosecond timescale in any lipid bilayer, the mean-square angular amplitude at the chain termini is larger in unsaturated than in saturated bilayers and larger in DOPC than in POPC bilayers. Interestingly, the results also show that, similar to other hydrated biosystems including proteins and membranes of various nature and composition, the lipid bilayers cross low-energy barriers ($E_a \approx$ 15-20 kJ/mol) at the dynamical transition occurring at T_d around 200 K and associated with the onset of stochastic motions. The present results obtained at cryogenic temperature highlight molecular properties of lipid bilayers that are also relevant in a physiological temperature range where they impact on the structure-dynamics-function relationship in membrane.

#260 - STAPHYLOCOCCUS AUREUS ISDB AND HUMAN HEMOGLOBIN: A BIOPHYSICAL DESCRIPTION OF A PROTEIN-PROTEIN INTERACTION

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*Staphylococcus aureus*exploits different mechanisms for iron supply, but the preferred one is acquisition of organic iron through the expression of hemoglobin (Hb) receptors. One of these, IsdB, is a recognized virulence factor and its interaction with Hb represents a target for the design of antibacterial molecules. However, many structural and mechanistic details of complex formation are still lacking. By combining absorption spectroscopy and surface plasmon resonance to small (SAXS) and wide (WAXS) angle X ray scattering and computational methods, we obtained i) the exact complex stoichiometry, ii) the microscopic kinetic rates describing of complex formation and heme extraction and iii) the structural/dynamic description of the effect played by IsdB on Hb.

#261 - EXPLORATION-EXPLOITATION TRADEOFFS DICTATE THE OPTIMAL DISTRIBUTIONS OF PHENOTYPES FOR POPULATIONS SUBJECT TO FITNESS FLUCTUATIONS

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We study a minimal model for the growth of a phenotypically heterogeneous population of cells subject to a fluctuating environment in which they can replicate (by exploiting available resources) and modify their phenotype within a given landscape (thereby exploring novel configurations). The model displays an exploration-exploitation trade-off whose specifics depend on the statistics of the environment. Most notably, the phenotypic distribution corresponding to maximum population fitness (i.e. growth rate) requires a non-zero exploration rate when the magnitude of environmental fluctuations changes randomly over time, while a purely exploitative strategy turns out to be optimal in two-state environments, independently of the statistics of switching times. We obtain analytical insight into the limiting cases of very fast and very slow exploration rates by directly linking population growth to the features of the environment.

#262 - PLASMONS IN REALISTIC GRAPHENE/HEXAGONAL BORON NITRIDE MOIRÉ PATTERNS.

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van der Waals heterostructures employing graphene and hexagonal boron nitride (hBN) crystals have emerged as a promising platform for plasmonics thanks to the tunability of their collective modes with carrier density and record values for plasmonics figures of merit. In this work [1] we investigate theoretically the role of moiré-pattern superlattices [2] in nearly aligned graphene on hBN by using a continuum-model Hamiltonian derived from ab initio calculations [3]. We calculate the system's energy-loss function for a range of chemical potential values that are accessible in gated devices. Our calculations reveal that the electron-hole asymmetry of the moiré bands leads to a remarkable asymmetry of the plasmon dispersion between positive and negative chemical potentials. We point out that the asymmetry of the plasmon dispersion must be taken into account when designing plasmonic devices based on gate-tunable graphene/hBN heterostructures. Below the Dirac point, the spectral reconstruction induced by the moiré pattern results in a band gap. Across the gap we find and instance of the plasmon morphing phenomenon [4] where the plasmon mode is supported by collective oscillations of either electrons or holes on different sides of the energy gap.

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#263 - ULTRAFAST NONLINEAR DYNAMICS OF PLASMONIC MATERIALS

Andrea Marini - University of L'Aquila

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We investigate the ultrafast nonlinear response of silver upon excitation by infrared electromagnetic radiation pulses with a duration of a few femtoseconds. By adopting the Landau weak coupling approach to account for electron–electron and electron–phonon collisions, we solve the Boltzmann equation through the method of moments obtaining a novel set of hydrodynamical equations describing the ultrafast nonlinear dynamics of electrons in silver. While the novel hydrodynamical model that was obtained reduces to the Drude model for small intensities of the driving field, it predicts that absorption saturates for large but experimentally attainable peak intensities of the order of GW/cm^2. Our results are important for absorption mitigation in plasmonic devices, with potential impact for low-loss plasmonic waveguides and interconnects.

#264 - LASER SYNTHESIS OF SERS-BASED SENSORS FOR THERAPEUTIC DRUG MONITORING

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Therapeutic Drug Monitoring (TDM) is a clinical practice to assess the drug concentration in a biological fluid, usually blood plasma. TDM is critically important for Narrow Therapeutic Index (NTI) drugs, including Anti-Epileptic Drugs (AEDs), where small differences separate therapeutic from toxic doses. Blood concentration of AEDs is measured with the time consuming and costly Immunoassay tests, or High-Performance Liquid Chromatography+Mass Spectrometry (HPLC-MS).

Light scattering with *ad hoc*engineered plasmonic substrates made of noble metal (Au) nanoparticles (NPs) grown by pulsed laser ablation is a fast and comparatively inexpensive TDM approach for AEDs. Ablating in a transparent liquid a colloidal solution of Au NPs is obtained, while in a dense, inert, massive gas (Ar) NPs form in the expanding plasma plume and are deposited on an inert support (100-Si). Ambient gas pressure and laser pulse number in gas-phase synthesis and pulse duration and laser energy density in liquid-phase ablation affect the size, size distribution, shape and optical properties of the NPs and the NP arrays that self-assemble on the support, making possible to adjust the wavelength of the Surface Plasmon Resonance (SPR) peak. Thus, Surface Enhanced Raman Scattering (SERS) on samples of different origin, with various AEDs at concentrations of clinical interest become feasible. Our results on the SERS response of the AEDs Lamotrigine and Perampanel of relevant clinical interest are discussed.

#265 - NONLINEAR RESPONSE OF GRAPHENE: IMPURITY IMPACT

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Anharmonic oscillation of charged carrier in response to an intense external field such as laser field is the origin of the nonlinear property of the medium. Because of the nonlinearity, the superposition principle will be violated and new phenomena emerge such as higher harmonic generation and rectification of an ac-drive. There are a lot of technological applications of strong nonlinear materials in microscopy, therapy, solar energy harvesting, photodetectors, saturable absorbers in ultrafast lasers, frequency conversion and etc.

Recently, the strong nonlinear response of two-dimensional materials such as graphene is confirmed experimentally [1-4]. The third harmonic optical conductivity of graphene with massless Dirac quasiparticle contains three logarithmic singularities corresponding to single, two and three-photon transitions, respectively [5-7]. Because the cumbersome nature of the nonlinear response functions to evaluate, most of the theoretical studies of this subject are limited to clean and non-interacting systems. However, disorder and many-body scatterings are inevitable in realistic systems. Considering electron-electron interaction allows incorporating the plasmonic effect on nonlinear susceptibilities. Plasmon emergence could significantly enhance the local field strength leading to a considerably large nonlinear effect [8,9].

In this project, we develop a systematic theoretical framework for the third order response function in order to go beyond non-interacting and clean limit and incorporate impurity impact within a conserving approximation which takes both self-energy and vertex corrections into account. Our result manifests a counter-intuitive enhancement of third harmonic generation due to impurity scattering. Particularly, the finite lifetime of Dirac quasiparticles plays a crucial role in the nonlinear response of graphene at low-frequency.

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#266 - MODELING OPTICAL FORCES ACTING ON A RESONANT GAIN-ENRICHED SILVER NANOSHELL IN OPTICAL TWEEZERS CONFIGURATION

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Optical tweezers are a crucial tool for the manipulation and study of micro- and nanoscopic particles of different nature without mechanical contact. Among the various applications, the study of optical forces in optically trapped gain-enriched plasmonic nanostructures appears to be of particular interest. In fact, a plethora of remarkable phenomena occurs in these systems due to the resonant interplay between plasmonic structures and gain media (*e.g.* dye molecules or quantum dots). In particular, the coupling with a gain medium located in the core of a metallic nanoshell, when excited by means of an external pump, produces intense changes of the electromagnetic fields around the structure. Therefore, this phenomenon affects profoundly the optical forces acting on the nanostructure itself, thus making possible to produce new features which can be useful over a variety of applications.

Here, we present a theoretical study of the optical forces acting on a gain-enriched silver nanoshell in the quasi-static limit. Specifically, we have analyzed the optical trapping of this nanostructure in a counterpropagating Gaussian beam optical trap. About that, we have studied the trend of trap stiffnesses as a function of wavelength and for different gain levels (which can be achieved by fixing the molecular density of the gain medium and varying the power of the external pump).

The characterization we ran shows that optical trapping strongly depends not only on the wavelength (as expected) but also on the gain level. This suggests that the measure of the trap stiffnesses could be used as a signature of the coupling between plasmonic particles and gain media, thus representing a powerful tool to unravel the near field Physics in these systems.

#267 - ACOUSTIC PLASMONS AT THE CROSSOVER BETWEEN THE COLLISIONLESS AND HYDRODYNAMIC REGIMES IN TWO-DIMENSIONAL ELECTRON LIQUIDS

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Hydrodynamic flow in two-dimensional electron systems has so far been probed only by dc transport [1-2] and scanning gate microscopy measurements [3]. We discuss theoretically signatures of the hydrodynamic regime in near-field optical microscopy. We analyze the dispersion of acoustic plasmon modes [4-5] in two-dimensional electron liquids using a non-local conductivity that takes into account the effects of (momentum-conserving) electron-electron collisions, (momentum-relaxing) electron-phonon and electron-impurity collisions, and many-body interactions beyond the Random Phase Approximation. We derive [6] the dispersion and, most importantly, the damping of acoustic plasmon modes and their coupling to a near-field probe, identifying key experimental signatures of the crossover between collisionless and hydrodynamic regimes. Finally, we compare our theory with experimental data.

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#268 - CHIRAL METASURFACE OPTOMECHANICS AND ADVANCED DESIGN OF ANISOTROPIC METASURFACES

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The coupling between electromagnetic fields and mechanical motion has recently produced intriguing fundamental physics, such as the observation of mesoscopic optomechanical phenomena in objects operating in the quantum regime. It is also yielding innovative device applications, for instance in the manipulation of the optical response of photonic elements. Following this concept, we show how combining a chiral metasurface with a GaAs suspended micromembrane can open new scenarios where the mechanical motion affects the polarization state of a light beam, and vice-versa. We will present optical characterization of the fabricated samples, assisted by theory and numerical modeling. This work represents a first example of “Polarization Optomechanics”, which could give access to new form of polarization nonlinearities and control, possibly down to the single photon-single phonon quantum level. It could also lead to wide applications in fast polarimetric devices, polarization modulators and dynamically tunable chiral state generators and detectors.

Band structures are a typical fingerprint of periodic optical structures, and are usually observed in spectroscopic quantities such as transmission, reflection and absorption. We will show that the metasurfaces employed for the optomechanical experiments also show a rich photonic band structure, where intrinsic and extrinsic chirality effects are clearly recognized and connected to localized and delocalized resonances. Superchiral near-fields can be excited in correspondence to these resonances, and anomalous behaviors as a function of the incidence polarization occur. Moreover, we will introduce a singular value decomposition (SVD) approach to show that the above mentioned effects are connected to specific fingerprints of the SVD spectra. Finally, we will demonstrate that a metasurface based on a simple L-shaped hole array is a *minimal metasurface*, as it is always possible to conceive a unit cell geometry that implements arbitrary transmission matrices. These observations open new avenues for optical wave propagation.

#269 - LIGHT HARVESTING ANTENNA BASED ON SI NANOWIRES

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The recent rise of semiconductor nanowires opens new opportunities due to the unique one-dimensional structure with remarkable electrical and optical properties. Particularly, involving one of the most earth-abundant materials, silicon nanowires (Si NWs) represent one of the most promising resources to be employed in modern nanodevices although their fabrication is still challenging. We demonstrated the realization of a dense array of vertically aligned Si NWs with tunable aspect ratio by a low-cost, mask-less approach compatible with the current Si technology [1]. Si NWs with an efficient room temperature (RT) light emission would represent a great industrial advancement, opening the route to a wide range of unexpected photonic applications. We demonstrated the fabrication of light emitting Si NWs (10^{12} NWs/cm^2) by using a modified metal assisted chemical etching without any type of mask or lithography. NWs achieved by this technique exhibit a very bright RT PL and EL, tunable with NWs size in agreement with the occurrence of quantum confinement effect [2]. We demonstrated the possibility to realize a new class of luminescent antennae constituted by the coupling of Si NWs with different dyes (Ru_4, Ru_3Os). These hybrid light-harvesting antenna are very promising for different applications in the bio-imaging, sensors, photonics and energy fields. When a dye is introduced in these NWs a strong NW-dye interaction sets in and the energy is preferentially transferred from the NW to the dye. The NW-related luminescence is partially quenched and the dye-related luminescence appears. Moreover, by increasing the dye concentration the NWs emission decreases while the dye emission increases. This hybrid antenna has a potential application for different fields, with a strong standard silicon technology compatibility.

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#270 - QUANTUM DYNAMICS OF STRONGLY-CORRELATED ATOMS IN LIGHT POTENTIALS

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I will report on recent theoretical work on systems composed by ultracold atoms strongly coupled to the field of an optical resonator. The quantum phases and dynamics result from the interplay between quantum fluctuations, van-der-Waals collisions, and the effective long-range forces mediated by the cavity. I will focus in particular on dynamical phase transitions and discuss thermalization in these systems.

#271 - DISCRETE TIME CRYSTAL IN A FINITE CHAIN OF RYDBERG ATOMS WITHOUT DISORDER

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We study the collective dynamics of a clean Floquet system of cold atoms, numerically simulating two distinct realistic set-ups based on a regular chain of interacting Rydberg atoms driven by laser fields. In both cases, the population evolution and its Fourier spectrum show clear signatures of a discrete time crystal (DTC), exhibiting the appearance of a robust subharmonic oscillation which persists on a time scale increasing with the chain size, within a certain range of control parameters. We also characterize how the DTC stability is limited by dissipative processes which are typically present in the system.

#272 - GAUGE AMBIGUITIES AND THEIR RESOLUTION IN CAVITY QED

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In quantum electrodynamics (QED), the choice of gauge influences the form of light–matter interactions. However, gauge invariance implies that all physical results should be independent of this formal choice.

Recently, it has been claimed that the quantum Rabi model, describing the dipolar coupling between a two-level atom and a quantized electromagnetic field, violates this principle.

This failure is attributed to the finite-level truncation of the matter system. Very recently, we identified the origin of these gauge ambiguities and showed that a careful application of the gauge principle is able to restore gauge invariance even for extreme light-matter interaction regimes [1]. The resulting quantum Rabi Hamiltonian in the Coulomb gauge differs significantly from the standard model and provides the same physical results obtained by using the dipole gauge. It contains field operators to all orders that cannot be neglected when the coupling strength is high.

These results shed light on gauge invariance in the nonperturbative and extreme interaction regimes [2], which are now experimentally accessible, and solve all the long-lasting controversies arising from gauge ambiguities in the quantum Rabi and Dicke models.

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#273 - CAVITY QED OF STRONGLY CORRELATED ELECTRON SYSTEMS: A NO-GO THEOREM FOR PHOTON CONDENSATION

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Despite decades of work, it is still unclear whether an equilibrium superradiant quantum phase transition (which will be referred to as "photon condensation”) can occur or not in quantum many-body models of condensed matter relevance. Firstly, we show that gauge invariance forbids photon condensation when a non-relativistic quantum many-body system is coupled to a cavity field.
We then present a microscopic theory of the cavity quantum electrodynamics of an extended Falicov-Kimball model, showing that, in agreement with the general theorem, its insulating ferroelectric and exciton condensate phases are not altered by the cavity and
do not support photon condensation.

#274 - GROUND STATE OF WEAKLY-INTERACTING BOSONS: A VARIATIONAL STUDY

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The properties of a macroscopic assembly of weakly-interacting bosons at zero temperature are well described by Gross-Pitaevskii mean-field theory. We apply this formalism to a system of penetrable bosons, providing a model for ultracold gases of atoms dressed with Rydberg states. We develop a thermodynamic treatment of the different phases of the system, using an accurate variational formulation of the condensate wave function that is amenable to exact manipulations. While quantum fluctuations keep the system fluid at low density, upon compression it eventually forms a cluster crystal, i.e., particles gather together in clusters centered at the sites of a lattice. Depending on the crystalline structure, the transition from fluid to cluster crystal is first-order or continuous, a lower coordination entailing a milder transition [1,2]. The analysis is then repeated for bosons embedded in a spherical surface, like in forthcoming experiments on atoms trapped in a thin spherical shell. For radii up to a few interaction ranges we examine the stability of a number of crystal-like arrangements having the symmetry of a regular or semi-regular polyhedron. As the radius increases, we observe a sequence of transitions between different cluster phases, which, within our mean-field description, are all supersolid [3].

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#275 - OBSERVATION OF QUANTUM DROPLETS IN A HETERONUCLEAR BOSE-BOSE MIXTURE

Chiara D'Errico - CNR-INO

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We report on the formation of heteronuclear quantum droplets in an attractive Bose-Bose mixture of 41K and 87Rb. We observe long-lived localized states, both in free space and in an optical waveguide.

In the latter case the dynamics under the effect of a species-dependent force confirms their bound nature. By tuning the interactions from the weakly to the strongly attractive regime, we study the transition from freely expanding clouds to the self-bound states, in both geometries. We compare the experimental results with numerical predictions and we found a good agreement in the full range of explored interactions.

We report on the formation of heteronuclear quantum droplets in an attractive Bose-Bose mixture of ^{41}K and ^{87}Rb. We observe long-lived localized states, both in free space and in an optical waveguide. In the latter case the dynamics under the effect of a species-dependent force confirms their bound nature. By tuning the interactions from the weakly to the strongly attractive regime, we study the transition from freely expanding clouds to the self-bound states, in both geometries. We compare the experimental results with numerical predictions and we

found a good agreement in the full range of explored interactions

#276 - BLACK HOLE SUPERRADIANCE AND VORTICES IN BOSE-EINSTEIN CONDENSATES

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Other Authors: Iacopo Carusotto (INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento)

Superradiance is a radiation enhancement phenomenon in which radiation scattering on a rotating black hole is reflected in an amplified way. Through the ideas of analogue gravity, in which sound in a moving fluid is described as a field propagating in a curved spacetime, this phenomenon can be investigated in Bose-Einstein condensates (BECs). Besides giving insight on the gravitational effect, this study provides new perspectives on the physics of condensates. In this spirit we investigate different configurations in which these amplification phenomena occur and show that the instability of multiply quantized vortices in BECs is linked to these superradiance effects. In doing so we clarify the nature and the characteristics of these instabilities and correct some misconceptions present in the literature on trapped BECs.

#277 - CHARGE DENSITY WAVES AND TEMPERATURE-DEPENDENT PHONONS IN BULK AND MONOLAYER OF DICHALCOGENIDES.

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Anharmonic effects can generally be treated within perturbation theory. Such an approach breaks down when the harmonic solution is dynamically unstable or when the anharmonic corrections of the phonon energies are larger than the harmonic frequencies themselves. This situation occurs near lattice-related second-order phase-transitions such as charge-density-wave (CDW). Interestingly, even in these cases, phonons can be observed and measured. In order to treat such cases, we developed a stochastic implementation of the self-consistent harmonic approximation valid to treat anharmonicity in the nonperturbative regime and to obtain, from first-principles, the structural, thermodynamic and vibrational properties of strongly anharmonic systems. I will present an application to the study of CWD transitions in NbS2, NbSe2 and in TiSe2 (in the bulk and monolayer phases), where we are able to reproduce the experimental behavior. Our results identify in the vibrational entropy (and not in the electronic one) the driving force for the CWD melting.

#278 - STRAIN RELAXATION MECHANISM OF FREESTANDING, EPITAXIAL LAO/STO MICRO-HETEROSTRUCTURES INVESTIGATED BY TRANSMISSION ELECTRON MICROSCOPY

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Since more than a decade, the $LaAlO_3/SrTiO_3$ (LAO/STO) system has gained the attention of researchers world wide, as an intriguing example of the fascinating properties stemming at the interface between complex oxides compounds. Despite there is a general experimental agreement on the minimum critical thickness below which the samples are insulating (4 u.c.), the value of the maximum thickness for conducting LAO/STO samples changes noticeably from sample to sample. The disappearance of the interface conductivity is generally ascribed to defects induced by the gradual relaxation of the tensile strain related to the relatively large lattice mismatch between LAO and STO (∼3% at room temperature). The maximum thickness reported in literature for conducting LAO films is around 30 u.c, but there are seldom reports on such topic.

Interestingly, we are able to obtain a stable layer-by-layer growth even for extremely thick films, as confirmed by RHEED intensity oscillations. This layer by layer growth pushed up to a noticeable thickness (200 u.c.) leads to the film cracking resulting in LAO/STO flakes, as the topmost layer of the STO substrate is cut away from the rest of the STO substrate, because of the strong bonding at the interface with the grown thick film. These defect free flakes, shows transport properties similar to the standard LAO/STO samples. In this talk, we focus on TEM characterization of these micro-membranes aimed to investigate its strain relaxation mechanism.

#279 - SINGLE SPIN-POLARISED FERMI SURFACE IN SRTIO3 FILMS

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Transition metal oxides are expected to play an important role in next generation electronics and devices [1], mainly due to the interplay of lattice, charge, orbit, and spin degrees of freedom in combination with correlation effects [2]. In particular, a prominent sub-class are the titanates with a perovskite structure ($ATiO_3$), which despite being band insulators in bulk form, at interfaces to other materials or vacuum, a high mobility two-dimensional electron gas (2DEG). The 2DEG on $SrTiO_3$ (STO) [3, 4, 5] has been extensively studied, and one of its promising aspects of the 2DEG at the $SrTiO_3$(001) surface is the large Rashba-like splitting of the 2EG, marked by a helical spin texture and energy gap around the surface Brillouin zone (SBZ) centre [6].
I will present our (Spin and) Angle Resolved Photoemission (S)ARPES on $SrTiO_3$ films grown by Pulsed Laser Deposition (PLD) on Nb-doped STO substrates. The films were grown with different thicknesses and on substrates with different amounts of Nb doping. Our main finding is that for films from 3 to at least 20 unit cells on 0.5 Nb wt.% substrates the band filling is such that the Fermi level is exactly in the Zeeman gap at the SBZ centre, thus resulting in a single spin-polarised 2D Fermi surface. Further, we show that it is possible to change the position of the Fermi level by varying the amount of Nb dopants in the substrate. The similarities of the 2DEGs found in films with different thicknesses indicate that the difference between single crystals and the films is not due to finite size effects, but due to a distinct dielectric response of the system. This in turn is expected to change the properties of the polaronic excitations and thus the band characteristics.

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#280 - ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF FEW-LAYER CR2GE2TE6: THE KEY ROLE OF NONLOCAL ELECTRON-ELECTRON INTERACTION EFFECTS

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Atomically-thin magnetic crystals have been recently isolated experimentally, greatly expanding the family of two-dimensional materials. In this work we present an extensive comparative analysis of the electronic and magnetic properties of $Cr_2Ge_2Te_6$, based on density functional theory (DFT). We first show that the often-used DFT + U approaches fail in predicting the ground-state properties of this material in both its monolayer and bilayer forms, and even more spectacularly in its bulk form. In the latter case, the fundamental gap decreases by increasing the Hubbard-U parameter, eventually leading to a metallic ground state for physically relevant values of U , in stark contrast with experimental data. On the contrary, the use of hybrid functionals, which naturally take into account nonlocal exchange interactions between all orbitals, yields good account of the electronic gap
as measured by ARPES. We then calculate all the relevant exchange couplings (and the magneto-crystalline anisotropy energy) for monolayer, bilayer, and bulk $Cr_2Ge_2Te_6$ with a hybrid functional,

with super-cells containing up to 270 atoms, commenting on existing calculations with much smaller super-cell sizes. In the case of bilayer $Cr_2Ge_2Te_6$, we show that two distinct intra-layer second-neighbor exchange couplings emerge, a result which, to the best of our knowledge, has not been noticed in the literature. We also show the effects of the electrochemical doping on the electronic and magnetic properties of few-layer $Cr_2Ge_2Te_6$.

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#281 - DISORDER-INDUCED POLARONS IN STRONGLY DISORDERED METALS

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The nature of the disorder-driven metal-insulator transition is fundamentally changed with respect to the noninteracting Anderson scenario when the interaction of electron with lattice is taken into account.

For strong disorder, even a modest electron-phonon interaction is found to dramatically renormalize the random potential, opening a mobility gap at the Fermi energy. [1]

In the strongly disordered metallic phase the change of sign of the temperature coefficient of resistivity is a signature of the onset of a disorder-induced polaronic phase.

This phenomenon though physically distinct to Anderson localization, still realizes early seminal ideas of Anderson himself, concerning the interplay of disorder and lattice deformations. [2]

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#282 - FREE-STANDING MAGNETIC MEMBRANES FOR SPIN POLARIMETRY

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This work deals with the fabrication of free-standing magnetic membranes for spin polarimetry of an electron beam, either generated by an electron gun or by photoemission experiments. The working principle of membranes is to selectively transmit electrons with spin parallel or anti-parallel with respect to a quantization axis defined by the direction of the magnetization of the ferromagnetic layer [1]. A proper fabrication process is needed to obtain the free-standing membranes, that must be thin, mechanically robust and self-sustaining, and yielding efficient transmission (>0.05) and asymmetry (~0.5) [1].

Different solutions have been considered, from free-standing oxide membranes to single graphene layers where to deposit the spin filtering heterostructure. The material stack is composed by a layer which increases the mechanical resistance of the membranes, a layer which acts as a capping, the active magnetic layer and a final gold layer to prevent the film from oxidation. According to the magnetization direction desired (in-plane or out-of-plane), different materials would be chosen, e.g. Co or CoFeB for the in-plane configuration and heterostructures as Co/Pt or CoFeB/Ta for the out-of-plane one. The whole structure cannot exceed the thickness of ten nanometers in order to guarantee a reasonable transmission of the device.

Here we present the first magnetic characterizations of out-of-plane stacks with micrometric honeycomb geometry, based on Ta/CoFeB/Ta heterostructures grown by magnetron sputtering. The out-of-plane behavior is realized by a proper choice of CoFeB thickness and annealing temperature, and characterized by Vibrating Sample Magnetometer, Faraday Effect and micro-Kerr effect, which allows to locally probe (at the micrometric scale) the magnetic properties of the devices:the ferromagnetic remanence and coercive field, and the presence of magnetic domain structure.

The next step of the work will be the characterization of the membrane spin filtering properties through a of a spin-polarized beam of low energy electrons, in order to determine the transmitted beam polarization [2] and the final figure-of-merit of the device.

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#283 - DIRECT X-RAY DETECTION BY STABLE AND RADIATION HARD MIXED LEAD-HALIDE PEROVSKITE THIN FILMS

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The demand for large area high-energy radiation detection systems combining high sensitivity and low-cost fabrication, has pushed the research in the last ten years to develop and design both novel materials and device geometries. Despite organic semiconductors have attracted a great attention, their low atomic number strongly limits the high-energy radiation absorption. Hybrid organic-inorganic perovskites have been recently proposed as alternative materials for X- and γ-photon direct detection, thanks to their high Z atoms, combined with high charge mobility. In this work we report on thin film X-ray detectors made of solution processed Cesium-containing triple cation perovskite, namely $Cs_{0.05}(MA_{0.17}FA_{0.78})Pb(I_{0.8}Br_{0.2})_3$ (CsFAMA), where cesium (Cs) has added to mixed organic cations (methylammonium (MA) and formamidinium $CH_3(NH_2)2$ (FA)) and mixed halides (I and Br). We demonstrate how X-ray detectors based on solution processed CsFAMA film possess a high sensitivity, with values up to 80 µC mGy^{-1} cm^{-3} in short-circuit conditions, and up to 380 µC Gy^{-1} cm^{-2} when operated under small (i.e. 4V) bias conditions: two orders of magnitude higher than previous reported perovskite thin films and comparable to state-of-the-art perovskite single-crystal at 50V operating bias. It is noteworthy that using low-voltage or zero-bias operation reduces the material degradation, the system power consumption allowing non-invasive, safe and wearable applications of these devices.

We tested perovskites thin films with enhanced stability in air. Remarkably, the electrical performance of the final detectors is still working after 50 days of storage in air, with degradation of X-ray sensitivity limited to 15%. Radiation hardness test assessed that the detectors are still properly working after receiving a total dose of 10 Gy in few minutes. Indeed, the combination of thin films and long carrier diffusion length allows in perovskites the efficient collection of photogenerated charges, even in presence of defects or radiation-induced traps, resulting in a higher radiation tolerance than thicker films and single crystals.

In conclusion, we reckon that thin film perovskite devices: i) surpass the state-of-the-art performance of inorganic large area detectors (a-Se and poly-CZT); ii) overcome the scalability limitation of thick layers and single crystals; iii) allow to envisage battery-operated wearable detectors thanks to their low voltage operation.

#284 - ORGANIC PHOTOTRANSISTORS FOR INDIRECT PARTICLES DETECTORS

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Photodetectors based on organic materials have gained considerable attention because of their unique and attractive features, in particular the low-temperature process fabrication that allows the of flexible plastic substrates, making possible new photodetector structures and applications. Large area, low fabrication costs, lightweight and possible biocompatibility are other features that make organic photosensors very interesting for applications such as imaging, radiation detectors and biomedical sensing. Furthermore, the wide number of organic materials with different absorption spectra makes possible to develop photosensors with large spectral sensitivity or tuned to specific wavelengths. The phototransistors (OPTs) are particularly promising since they combine light detection, typical of the photodiodes (OPD), with the intrinsic signal amplification that increases the device sensitivity. In addition, the OPTs can share most of the fabrication steps with the circuitry devices surround them, leading to an easy and inexpensive integration of optical and electrical circuits on the same substrate. In this work we will show the development of a phototransistors based on organic semiconductor

(DNTT) on flexible polyethylene Naphthalate (PEN substrate), aiming to develop an indirect detector based on OPTs coupled with plastic or inorganic scintillators.
Bottom gate/bottom contact device structure was used to simplify the device coupling with scintillator film while multi-finger structure was used to increase the device area. High quality silicon dioxide gate dielectric was deposited by ECR-PECVD at low temperature (150 °C), compatible with the plastic substrate. Thin (30nm) semiconductor layer of DNTT was thermally evaporated on top of gate dielectric and S/D contact after SAM treatment of the metal surface to reduce contact resistance. Cytop passivation layer was spin-coated on top of the semiconductor film to reduce the device degradation induced by the environment without introducing attenuation of the light from the scintillator. Thanks to the high quality of the semiconductor and of the dielectric/semiconductor interface, the devices show good electrical characteristic, with field effect mobility in excess of 0.1 cm^2/Vs, low threshold voltage (about -1÷-2 V) and very steep subthreshold voltage (less than 1V/dec). The devices show sufficient reliability, with low hysteresis, also in air, and low electrical characteristics variation under substrate bending. The OPTs were characterized by electrical and optical measurement in order to evaluate the figures of merit parameters of the photodetectors, such as the photo-switching speed, the responsivity, and the photocurrent on/off ratio (also indicated as photosensitivity). The results show that these devices are promising as UV (λ< 450 nm) detectors.
This work is supported by INFN-CNS5 project "FIRE".

#285 - FLEXIBLE ELECTROCHROMIC-OLED INTEGRATED DEVICES FOR HIGH TRANSPARENT SMART GLASSES AND DISPLAYS

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In the last decade industrial research focused its attention on advanced “smart” glasses based on electrochromic (EC) devices. EC windows can improve energy efficiency in buildings with a reduction of the expense for heating and cooling by modulating the light transmittance and dynamic shading control, with further benefits in terms of thermal gain and visual comfort. In this context, the development of innovative devices which integrate EC devices with an organic light emitting diodes (OLEDs), is of growing interest thanks to the possibility to generate light and modulate the total transmittance in a very efficient way. However, the development of an effective EC-OLED device on flexible substrates represents an emerging challenge for the realization of novel multifunctional devices on any kind of surface and geometric configuration.
We present for the first time a flexible EC-OLED device fabricated on plastic substrate, by the integration of an OLED unit with a solid-state EC cell in one monolithic system. The integration of the EC cell, based on WO_3 layer and high performing solid polymer electrolyte, with OLED was achieved by the adoption of a common ITO electrode: the top electrode of EC device acts as anode for the OLED, which in turn is fabricated on its top by thermal evaporation.This multifunctional device is capable to tune its transmittance properties in the visible and near-IR optical region and to produce light by electroluminescence, simultaneously or independently. This outcome represents a further step towards the developments of next-generation multifunctional EC devices and, importantly, it can open the way for new flexible “smart” windows systems such as the retail display windows or display EC glasses for augmented reality.

#286 - GROWTH, STABILITY AND METALATION OF 5,10,15-TRIPHENYLCORROLE (TPC) ON CU(111) AND CU(110) SURFACES

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Metallo-porphyrin are a very important class of organic molecules for their possible use in novel devices based on the interaction of an active nanoscale site with the surrounding medium. Moreover, they can be exploited as templates for the ordered organization of i) “isolated” metallic atoms, which correspond the metallic ions at the center of the macrocycles and/or ii) of active sites that can bind, via molecular recognition, guest species on surfaces. The fine control on the self-assembling and, possibly, on the metalation of the molecules represent a key issues in the development of these organic-substrate interfaces with the aim of tailoring suitable properties for organic-based devices. Therefore it is fundamental to understand how porphyrins (metalated or not) interact with the substrates and in which way the self-assembled organic monolayer can becontrolled and modified. Here we report on the study of 5,10,15-triphenylcorrole (TPC), which presents a inner macrocycle with 3 pyrrolic units and 1 iminic one, at variance with the more studied 5,10,15,20-Tetraphenyl-21H,23H-porphyrin (H2TPP) where the pyrrolic and iminic units are 2 each. This is the first time to our knowledge that TPC is deposited in Ultra High Vacuum (UHV). We studied its growth and stability as a function of the temperature by growing thin films (max 20 Å) onto the clean and the oxidized Cu(111) and Cu(110) surfaces by means of X-ray Photoemission (XPS) and Near Edge X-ray Absorption Spectroscopy (NEXAFS). For the metal free porphyrins H2TPP the metalation temperature is lowered in the case of oxidized substrates of about 200K [1],[2], and thus fast XPS spectra measurements of the N 1s core level: the spectra have been recorded during annealing in order to find the temperature at which the metalation sets up for the different surfaces. We can confirm the role of the oxygen in the metalation process, finding a lowering of the metalation temperature, with respect to the clean surface, of about 90K and 70K for the Cu(111) and the Cu(110) surfaces, respectively. Moreover, by monitoring the relative peak height of the N 1s XPS spectrum of the TPC: on the non oxidized Cu(111) and Cu(110) surfaces we observe a 1:1 peak ratio between the pyrrolic and the iminic components, instead of the stoichiometric 3:1, evidencing a surface-induced loss of one of the 3 H atoms of the pyrrolic group even at temperatures of 200K. For both clean and oxidized Cu(111) and Cu(110) surfaces, NEXAFS measurements have been performed, showing that pristine molecules display a strong dichroism, indicating a macrocycle lying parallel to the surface; while metalated molecules show a reduced dichroism, indicating a strong interaction with the substrate that bends the macrocycle towards the surface.

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#287 - CHEMICAL VAPOUR DEPOSITION OF CONJUGATED PORPHYRIN TAPES ON SENSITIVE SUBSTRATE: SYNTHESIS, DEPOSITION AND OPTOELECTRONIC PROPERTIES.

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Directly fused porphyrin tapes own outstanding physical properties such as two photons and NIR absorption, small band gaps, improved photocatalytic activity and low attenuation factor. In spite of their outstanding properties, the application of directly fused porphyrins is been limited by their extremely low solubility that hinder the production of thin films required for advanced applications.

In this work, we present a single step and upscalable Chemical Vapour Deposition (CVD) approach towards the direct synthesis, deposition and doping of conductive directly fused porphyrin thin films. The CVD approach do not require any solubilizing pendant groups allowing more compact arrangements that drastically improve the electrical properties of the films. The effect of the central metal ion and substituents are evaluated. The developed CVD route is substrate independent and allow the patterning on sensitive substrates, such as paper and plastic, thus representing a direct route for the integration of directly fused porphyrin coatings into organic optoelectronic devices.

#288 - RESONANT SOFT X-RAY REFLECTIVITY OF ANISOTROPIC ORGANIC FILMS FOR MOLECULAR ELECTRONICS

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Reflectivity is typically carried out in the hard X-ray range, where electron density contrast between different materials is exploited. In the soft X-rays, elastic scattering (reflectivity) at resonance provides additional advantages in terms of atomic and depth-resolved investigation of the chemical, structural and magnetic properties of a variety of systems, including polymeric and organic materials, liquid interfaces, spintronic systems and inorganic layered materials. Element selectivity together with high contrast between different structures is obtained. The technique is non-destructive. The sampling depth is not limited to the near-surface region, as for electron yield spectroscopies, but deep buried interfaces can be accessed as well (several tenths of nm).

The recent advances in the application of resonant soft X-ray elastic scattering will be presented. In particular, we developed a protocol to get simultaneous quantitative information on the structure, interface morphology, chemical properties and optical anisotropies of layered materials with sub-nm depth resolution. The method is based on the quantitative prediction of the spectral line-shape across specific elemental edges through: 1) the simulation from the first principles of the dielectric tensor of each material in a given layered system; 2) the simulation of the propagation of the electromagnetic field in the stack of layers and the computation of the (anisotropic) optical properties (reflectivity, transmission); 3) the comparison and fitting of the simulation to the experiment.

The method has been successfully applied to study anisotropic thin and ultrathin organic films on metals and insulators and to get quantitative information on chemical composition, layer-resolved molecular orientation, optical anisotropies and overall thickness of the films, simultaneously. In particular, the following prototypical cases will be discussed: 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA) on Au(111), pentacene on SiO_2, tetracene single crystal.

The method transfers to the soft-X range the knowledge gained in the years in the field of visible and infrared spectroscopy of thin anisotropic films and offers a tool of quantitative investigation in those cases where electron spectroscopy cannot be applied due of the presence of nonconductive materials, poor vacuum or materials buried at distances from surfaces higher than the electron free collision path.

#289 - ORDERED ADSORPTION AND DEMETALLATION OF ZINC-PHTHALOCYANINE ON ALUMINUM (100)

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In recent years, thin films of organic molecules have attracted increasing interest. Among them, thin films of metal-phthalocyanines (MPcs) deposited on solid state substrates are of importance. MPcs can absorb light in the visible range and this makes MPc heterostructures particularly useful for optoelectronic applications, like solar energy conversion or organic-light-emitting diodes (OLEDs) production. In all areas of utilization, the electronic and structural properties of those complex structures play a crucial role. They depend, not only on the intrinsic properties of the constituents, but also on the molecule-molecule and molecule-solid interaction.

In this work zinc-phtalocyanine (ZnPc) molecules were thermally deposited on Al(100) surface. The chemical and electronic properties and the ordering of the molecular films were investigated by combining photoemission spectroscopy (PS) and low energy electron diffraction (LEED).

As for CuPc/Al(100) [1], at low coverage (1 ML), a sizable charge transfer from the substrate to the molecules is observed, this indicating a strong interaction at the organic-inorganic interface. However, this does not prevent diffusion of the molecules and ordering on the substrate. LEED patterns clearly show a (5x5) reconstruction, characteristic of flat-lying molecules forming a long-range-ordered structure with square unit cell. The degree of ordering (i.e. the average domain size) is increased when the substrate is held above 100°C during the deposition. As a consequence of the thermal treatment the zinc atom (held in the ZnPc central cavity) is removed and diffuses into the aluminum substrate. This chemical modification does not affect π-conjugation leaving the molecular structure intact.

#290 - USE OF CVD-GRAPHENE AS ELECTRODE IN N-TYPE OFETS: TOWARDS THE SUB-MICROMETER SCALE

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Despite considerable advances in understanding the fundamental mechanisms, several bottlenecks still restrict the miniaturization of Organic Field Effect Transistors (OFETs) towards the nanometric scale where charge transport is often dominated by non-linear Space Charge Limited Current (SCLC) and high off-state currents.

In this scenario, careful choice of materials or chemical treatment of contact electrodes, and generally, of the overall device architecture are needed in order to optimize the OFET response at nanometric scales. At this regard, graphene has been recently considered as a novel electrode material in organic field-effect devices, taking advantages from their work function tunability, permeability to the transversal electric field and overall chemical stability. In this contribution, we report on the use of CVD-graphene as electrode material in both nanometric and micrometric channel n-type OFETs based on thermally evaporated thin films of perylene diimide derivatives (PDIF-CN2 and PDI8-CN2). We firstly explored the electrical response of nano devices by a thorough comparison with short channel transistors made with reference gold electrodes. Electrical characteristics of the graphene-based devices suggests that short-channel effects are effectively suppressed and an enhanced response for high longitudinal biases is demonstrated for channel lengths (L) down to 140 nm. Further advances have been reached by the use of a proper device architecture with patterned local gate tracks and an ultra-thin films (8nm) of Hafnium Dioxide as gate dielectric for which excellent transistor operation is ensured with supply biases of few volts. Overlap capacitances and the overall AC response of CVD-graphene electrodes have been investigated as well, with the indirect evaluation of the maximum operational frequencies as final goal. In this case, values of the order of 10^5 Hz has been obtained for L=200nm. Lastly, we focused on the organic/graphene interfaces investigated by Scanning Kelvin Probe Force Microscopy, in micrometric graphene-based and hybrid gold/graphene architectures (L=10 µm). By comparing data again with reference gold-based layouts, we observed neat differences in terms of surface voltage profiles. Contact resistances affect solely the source electrode, in contrast with gold architectures where voltage drops are equally distributed at the injection (source) and extraction (drain) interfaces, and an enhanced response of contact effects as function of the gate voltage and of the temperature is observed. Results have been rationalized taking into account the morphological peculiarities of the graphene/organic interface given by the negligible thickness of the graphene and its permeability to the transversal electric field.

#291 - X-RAY SYNCHROTRON STUDY OF A BLATTER-TYPE STABLE ORGANIC RADICAL AT THE METAL-MOLECULE INTERFACE

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Stable organic radicals have potential applications for building organic spintronic devices. To fulfill this potential, the interface between organic radicals and metal electrodes must be well characterized. Employing a combination of synchrotron based techniques, X-ray photoemission (XPS), X-ray absorption (NEXAFS) and resonant photoemission (RESPES), we have probed the electronic interaction between gold metal substrate Au(111) and a custom synthesized benchtop stable radical – a Blatter radical with two gold-binding thiomethyl groups – under ultrahigh vacuum. We find that despite its open-shell character and having a half-filled orbital close to the Fermi level, the radical remains stable on the gold substrate. Nitrogen K-edge NEXAFS measurements show a preferentially flat adsorption geometry, with the singly unoccupied molecular orbital (SUMO) intact even in the case of a monolayer deposition, where the metal-molecule coupling is essential. Furthermore, XPS N1s core-level measurements confirm these results, showing three chemically inequivalent nitrogen peaks as expected for the intact radical. Our DFT computations of N1s core-electron binding energies and half core-hole NEXAFS calculations on isolated molecules additionally corroborate the experimental results. Interestingly, complementary solution-based single-molecule conductance measurements, performed by our collaborators, show that the radical character is lost through oxidation with charge transfer occuring from the molecule to the metal. These experiments therefore show the importance of metal-molecule coupling to the stability of radical states that can be very sensitive to the environment around the molecule itself.

#292 - TOWARDS ROOM TEMPERATURE SUPERCONDUCTIVITY

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The old dream of room - temperature superconductivity is nowdays nearly achieved thanks to the recent synthesis of hydrogen-rich materials at megabar pressure, SH_3 and LaH_10. In this talk we will present the state-of-the-art of this fashinating research field, the fundamental hystorical steps and the most important experimental and theoretical advances which led to these astonish discoveries: in particular, the modern theoretical and computational techniques allowing the "in-silico" synthesis of new superconductors thanks to their predicting power.

Furthermore, we will evidence general trends in the electronic structure and chemical bonding of superconducting hydrides under pressure, trying to give empirical and simple rules to guess new supercondutors. Finally, in the last part we will discuss strategies and future directions for high-temperature superconductivity.

#293 - SCREENING OF PAIR FLUCTUATIONS IN SUPERCONDUCTORS WITH COUPLED SHALLOW AND DEEP BANDS: A ROUTE TO HIGHER TEMPERATURE SUPERCONDUCTIVITY

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A combination of strong Cooper pairing and weak superconducting fluctuations is crucial to achieve and stabilize high-T c superconductivity. We demonstrate that a coexistence of a shallow carrier band with strong pairing and a deep band with weak pairing, together with the Josephson-like pair transfer between the bands to couple the two condensates, realizes an optimal multicomponent superconductivity regime: it preserves strong pairing to generate large gaps and a very high critical temperature but screens the detrimental superconducting fluctuations, thereby suppressing the pseudogap state. Surprisingly, we find that the screening is very efficient even when the inter-band coupling is very small. Thus, a multi-band superconductor with a coherent mixture of condensates in the BCS regime (deep band) and in the BCS-BEC crossover regime (shallow band) offers a promising route to higher critical temperatures [1,2].

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#294 - VORTEX PHYSICS IN 2D SUPERCONDUCTORS

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The study of quasi-two-dimensional (2D) superconductors can hardly avoid taking into account the presence of vortices. Many real systems, of both conventional and unconventional superconductors, undergo the superconductor-insulator transition via the Berezinskii-Kosterlitz-Thouless (BKT) transition, at which the phase coherence of the condensate is destroyed by means of free-vortices proliferation. When a finite flux of magnetic field is applied to the films, the role of vortices becomes even more crucial for the understanding of the superconducting (SC) transition. Indeed, in this case, the transition is no longer driven by the vortex-antivortex unbinding, but rather by the melting of the 2D Abrikosov lattice of vortices. Such melting, as predicted by the BKT theory, afterward refined by Halperin, Nelson and Young (BKTHNY), can occur in two steps via an intermediate state called hexatic phase. In real systems, the observation of the two-step BKTHNY melting could be hindered by the presence of additional ingredients, such as random pinning, and also competing phases. In [1], we have shown that the 2-dimensional vortex lattice in a-MoGe thin film follows the BKTHNY sequence of melting as the magnetic field is increased. Identifying the signatures of various transitions on the bulk transport properties of the superconductor, we construct a vortex phase diagram for a 2D superconductor. From a theoretical standpoint, the classical XY model with a transverse magnetic field is a very promising candidate to capture the physics experimentally observed and to explore stronger disorder regimes. It constitutes hence a perfect playground for the investigation of the long-standing issue of the emergent glassy-state of the vortex lattice in the presence of disorder.

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#295 - NANOSCALE EFFECT ON VOLTAGE SWITCHING FOR SUPERCONDUCTING PHOTON DETECTION

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In the quest of superconducting nanostructures for photon detectors, ultra-thin films made of appropriate superconducting materials can provide a suitable geometry by reducing the thickness just down few nanometers. We study the voltage switching behavior in NbN and NbTiN ultra-thin films patterned in microbridges by standard UV lithography. Measurements of critical currents as well as switching currents are performed in a magnetic field applied parallel and perpendicular to the sample surface. Regardless of the superconducting material, the nanoscale effect of the thickness in the superconducting microbridges lead to the conclusion that by lowering the thickness of wide microbridges to few nanometers and with a sufficiently low in-plane applied magnetic field, the bridge achieves a direct voltage switching from the superconducting to the normal state as it happens in nanowires. Thus, a comparable performance can be foreseen, becoming relevant for photon detection applications involving nanostructures.

#296 - TUNING OF MAGNETIC ACTIVITY IN SPIN-FILTER JOSEPHSON JUNCTIONS TOWARDS SPIN-TRIPLET TRANSPORT

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Ferromagnetic Josephson junctions present a rich emerging physics due to the coupling between ferromagnetism and superconductivity. The interplay between the two competing phases causes an oscillation of the superconducting order parameter within the ferromagnetic barrier, which is responsible for the appearance of a \pi ground state, and of triplet correlations in the Josephson junction. Because of such properties, SFS junctions are sought to have applications in the emerging field of superconducting spintronics and in quantum and digital superconducting computation as phase shifters or as auxiliary circuit elements for error correction, readout and memory elements. Currently, their use is limited by their metallic, highly dissipative nature. In this work we will review the properties of a specific category of SFS, namely low dissipation spin filter junctions. In particular, we will present a low temperature characterization of such devices down to 0.3K. We measured several junction parameters as a function of thickness, focusing our attention on critical current versus temperature dependencies at different thicknesses. We developed a model to describe the anomalous behaviour and the incomplete transition found in experimental data using short-range triplet correlations. These results offer new perspectives for the study of the role of short-range triplet correlations in the transport properties of low dissipation ferromagnetic junctions.

#297 - PHOTOASSISTED TRANSPORT IN SUPERCONDUCTING POINT CONTACTS

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We investigate the transport properties of a superconducting quantum point contact in the presence of an arbitrary periodic drive. In particular, we calculate the dc current and noise in the tunnel limit, obtaining general expressions in terms of photoassisted probabilities. Interesting features can be observed when the frequency is comparable to the gap. Here, we show that quantized Lorentzian pulses minimize the excess noise, further strengthening the hierarchy among different periodic drives observed in the electron quantum optics domain. In this regime, the excess noise is directly connected to the overlap between electron and hole energy distributions driven out of equilibrium by the applied voltage. In the adiabatic limit, where the frequency of the drive is very small compared to the superconducting gap, we recover the conventional Shapiro-spikes physics in the supercurrent.

#298 - THERMAL NOISE EFFECTS IN A Φ0 JOSEPHSON JUNCTION

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Recently, much interest has been addressed to the theoretical study of superconductor-ferromagnet-superconductor Josephson junctions with a Rashba-like spin-orbit coupling (SOC). Such a junction may have a finite phase shift,φ_0, in the current-phase relation and is referred as φ_0-junction, and allows for a magnetization switching of the ferromagnet by an electric current. Even if it was earlier suggested by Buzdin [1] more than ten years ago, only recently the anomalous phase shift was observed experimentally in hybrid JJs fabricated with the topological insulator Bi_2Se_3 [2].
Although the features of a φ_0 junction has recently attracted a lot of attentions [3,4], the fundamental issue of unavoidable thermal fluctuations effects on magnetization dynamics has not been addressed concretely yet. Specifically, the pursuit of specific conditions giving a current-induced magnetization reversal [4] must necessarily involve the environmental thermal noise in which the device is embedded.
In our work, we discussed the bistable behavior of the magnetization of a current-biased φ_0 junction, with the aim to eventually conceive a superconducting memory based on the current-induced

magnetization reversal. We studied the robustness of the device against unavoidable thermal fluctuations, and we observed that a sufficiently intense noise contribution can even prevent the magnetization reversal phenomenon. Our finding can therefore be used for carefully setting the temperature of the system, in order to assure the magnetization reversal induced by a current pulse, regardless of thermal noise disturbances.

Moreover, in the case a ferromagnetic layer with a Rashba-Dresselhaus type SOC, we discuss the feasibility of a perfect decouple between phase and magnetization dynamics, in order to eventually protect the state of the system from any external input. In this case, we take advantages of the possibility of tuning, by using a gate voltage, the Rashba SOC, so that when it matches the Dresselhaus contribution the anomalous phase shift φ_0 vanishes.

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#299 - NONCLASSICAL LIGHT SOURCES FOR SILICON PHOTONICS

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Silicon and silicon-based materials are rapidly becoming the platforms of choice for on-chip integration of high performing photonic devices, now extending their functionalities to quantum applications. We review recent progress in this growing field, focusing on nonclassical light sources based on four-wave mixing in resonant nanostructures. We discuss the use of state-of-the-art integrated devices like microring resonators and photonic crystal cavities for the ultra-efficient generation of entangled photon pairs and heralded single photons, and we highlight the challenges that need to be overcome to make silicon quantum photonics a reliable and widespread technology.

#300 - SILICON NANOWIRES FOR PHOTONICS, PHOTOVOLTAICS AND SENSING

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The quantum confinement of Si in 1D nanostructures such as nanowires (NWs) is a striking strategy to improve its radiative efficiency with great perspectives for integrated photonics. NWs synthesis was optimised with a low-cost and Si compatible approach based on the chemical etching of Si wafers by using thin Au layers. The method allows the realization of Si nanowires with controlled structural features in term of length, quantum confined Si NWs diameter (5-7 nm), high density (1012 NWs/cm2) and with the same doping of the starting wafer.NWs obtained by this approach shows promising physical properties arising from their quantum confinement, such as room temperature light emission at wavelengths tunable with their size. Indeed, light emitting devices based on Si NWs with efficient room temperature electroluminescence at low voltage were also reported, opening the route towards low-cost, Si-based photonics. Moreover, we fabricated low-cost multiwavelength light sources working at room temperature by combining Si NWs and carbon nanotubes (CNT). The NW/CNT hybrid systems exhibit a tunable emission both in the visible range, due to Si NWs, and in the IR range from CNTs for future perspective in the telecom sector [3]. Achieving light management in nanostructured materials is a recent challenge of great resonance among the scientific community, which is generally attained by expensive surface patterning requiring advanced technologies. In this paper, the realization of 2D random fractal arrays of silicon nanowires (NWs) synthesized with a low cost approach compatible with Si technology, without the use of any lithography or mask is also reported by engineering the synthesis process. Strong in-plane multiple scattering and efficient light trapping overall the visible range were observed due to the fractal structure, remarking the promising potential of Si NWs for both photovoltaic and photonic applications1. NW fractal arrays present unique optical properties, such as multiple scattering that determines a strong light trapping and the observation of remarkable coherent effects for Raman scattering. We report the first experimental observation of Raman coherent backscattering arising from the constructive interference of Raman light in the strongly diffusing NW arrays. Finally, we also demonstrate the performances of label-free optical biosensors based on the room temperature luminescence of Si NWs for the selective detection of proteins, biomolecules and pathogen genome without amplification with tailored ultrasensitivity in biofluid matrices over a unable and broad concentration range with perspectives for noninvasive analysis in saliva for the early diagnosis of major cardiovascular biomarkers3-4.

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#301 - SLOW-LIGHT MODULATORS WITH INTERLEAVED P-N JUNCTION IN SILICON WAVEGUIDES GRATINGS

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Integrated Mach-Zehnder modulators are key components in silicon photonic devices, which rely on a reverse-biased p-n junction to modulate the optical signal via a change of the waveguide refractive index [1]. Reducing their energy consumption is a crucial issue towards applications of silicon photonics to optical communication. In this presentation, we describe the design of slow light structures consisting of silicon grating waveguides, which have an increased group index close to the photonic band edge [2]. Also, we discuss how the design of p-n junctions that are interleaved along the waveguide direction and with the same periodicity of the grating structure, in order to optimize spatial matching between the optical field mode and the depletion region [2]. The combination of slow light and interleaved p-n junction improves the modulation efficiency and reduces the energy dissipation per bit of the modulator, while maintaining a wide bandwidth and modulation rate. This design may allow implementation of slow light concepts in actual silicon photonic devices.

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#302 - RESHAPING HYBRID PEROVSKITES EMISSION WITH FLEXIBLE POLYMER MICROCAVITIES

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Thanks to a high photoluminescence quantum yield, large charge carrier diffusion, and ease of processing from solution, hybrid perovskites are in the spotlight of flexible optoelectronic devices.[1-2]However, their deposition requires wide range solvents that are incompatible with many other flexible and solution-processable materials, including polymers.[3-4]In this work, we demonstrate that methylammonium lead iodide ($MAPbI_3$) films can be directly synthesized on all-polymer microcavities via simple addition of a perfluorinated layer which protects the polymer photonic structure from the perovskite processing solvents. The new processing provides microcavities with a quality factor Q = 155. This value is in agreement with modelling and is currently the largest value reported for fully solution processed perovskite microcavities.[5]The obtained microcavities shows strong spectral and angular redistribution of the perovskite photoluminescence spectrum, whose intensity results enhanced by a 3.5 fold with respect to the detuned reference. The capability to control and modify the emission spectrum of a solution processable perovskite via a simple spun-cast polymer structure is of great interest in advanced optoelectronic applications requiring high color purity or emission directionality.Furthermore, thanks to the ease of fabrication and scalability of solution-processed photonic crystals, this approach could enable industrial scale production of low-cost, large area, lightweight and flexible polymer-perovskite lighting devices, which may be tuned without resorting to compositional engineering.

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#303 - OPTICAL INVESTIGATIONS ON YB3+/ER3+ DOPED SZO PHOSPHOR FOR THE APPLICATION IN FORENSIC FINGERPRINT DETECTION & BIO-IMAGING

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Herein, the energy up conversion emission studies on solid state route prepared $SrZrO_3$:Yb^{3+}/Er^{3+} phosphor for the application in forensic fingermark detection & bio imaging has been done. The up conversion emission of $SrZrO_3$:Yb^{3+}/Er^{3+} phosphor has been recorded using 980 nm laser excitation with various temperature treatments. The upconversion (UC) emission intensity ratio of green to red bands is found too high to neglect the contribution from the red emission band, which is not observed normally in Yb^{3+}/Er^{3+} doped materials under the exposure of 980 nm wavelength excitation. An observed comparison between UV vs. NIR excited fingerprint images shows that fingerprint images exposed by NIR excitation have more clear edges than the UV excitation. Hence upconversion emission of in Yb^{3+}/Er^{3}doped SZO phosphor is preferred by the authors for the application in fingerprint detection which has a great importance in forensic data. The emission dynamics is studied with respect to its dependence on input power and external temperature including lifetime. Furthermore, the present phosphor could be useful for bio-imaging regime. The 808 nm wavelength excitation produces lesser heating in a biological medium compared to the 980 nm excitation and hence in this regardEr^{3+} can be a good option for transparency across 2nd biological window. UC/DC emission in “NIR biological windows” has less absorption in biological medium and hence can be imaged easily [1].

#304 - EXPERIMENTAL EVALUATION OF FREQUENCY NOISE IN INTERBAND CASCADE LASERS

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Among mid-infrared laser sources, Interband cascade lasers (ICLs) present the appealing features of compactness, low-power consumption and frequency tunability. They are different from any other class of semiconductor lasers due to their structure and internal carrier generation and transport processes. However, a complete evaluation of their potential has not been possible till now mainly because of a poor understanding of their internal physics. In this work the frequency noise characteristics and intrinsic linewidth of ICLs are unveiled for the first time. Understanding the noise features is especially important for demanding applications, like frequency metrology, and is a necessary step for a deeper knowledge of the physical behavior for this class of lasers. We experimentally evaluate the frequency noise power spectral density (FNPSD) of a commercial ICL emitting at. Our analysis is focused on the identification of the main frequency noise contributions in ICLs, showing similarities and differences with respect to standard diode lasers and to QCLs, and to measure intrinsic linewidths, at different power levels, down to the 10-kHz level.

#305 - LABEL-FREE LUMINESCENT BIOSENSORS BASED ON SILICON NANOWIRES

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The integration of silicon and light is still one of the most interesting challenges in research as well as in industry. Innovative Si based nanomaterials have arisen in order to address this point. Among them silicon nanowires (Si NWs) are becoming a building block for a wide application range, from energetics to photonics and even biosensing. Indeed, their robustness, easier integration with Si wafer and easier electrical addressing are just few advantages with respect to other nanostructures. However, common synthesis methods as Vapor-Liquid-Solid or Reactive Ion etching suffer of different limitations on the size, and in particular for the VLS, on doping and metal impurities. These several drawbacks afflict the Si NWs performances in each device type. By using a Metal-Assisted Chemical Etching (MACE) approach we realized quantum confined and room temperature (RT) luminescent Si NWs. This method is based on an anisotropic wet etching by a HF and H_2O_2 solution driven by a thin Au metal film. The Au catalyze the Si oxidation just underneath the metal. Si NWs are formed on the uncovered Si region with the same doping of the starting Si wafer. All the process is at RT and Au impurities are not present inside Si NWs. By changing metal type and thickness is possible to tune the average NWs diameter in the quantum confinement range [1]. Recently, the use of this innovative substrate permits the first observation of the Raman coherency on a macroscopic scale [2].

These Si NWs exhibit a huge aspect ratio arising as a perfect candidate for the realization of the first sensor based on Si luminescence at RT. The realization of a new class of label-free PL sensors based on Si NWs for protein and DNA is presented. These sensors are based on the PL quenching of the Si NWs after the selective capture of the analyte. In particular, we realized a sensor for C-reactive protein (CRP), which is crucial for heart-failure pathology. The availability of high sensitivity, low-cost and reliable CRP sensors is a priority demand in clinical diagnosis for cardiovascular diseases. Si NW sensors are fast, highly selective and offer a broad concentration dynamic range. Moreover, these sensors reach a fM sensitivity permitting a non-invasive analysis in saliva [3]. By changing the functionalization protocol, we realized a label- and PCR-free sensor capable to reveal few copies of Hepatitis B virus without amplification of the DNA and endowed with a strong selectivity.[4] All the adopted functionalization protocol are Si industry compatible and flexible for different biomarker and genome targets. Si NWs luminescent sensors pave the way towards new cheap optical label-free sensors for the primary health care diagnosis with a Si industrially compatible approach.

[1] *Light: Science & Applications***5**, page e16062 (2016)
[2] *Nature Photonics***11**, pages 170–176 (2017)
[3] *ACS Photonics*,**5** (2), pp 471–479 (2018)
[4]*ACS Sens.*, **3** (9), pp 1690–1697 (2018)

#306 - DARWINISM AND QUANTUM INFORMATION FLOW

Massimo Palma (I) - Università di Palermo

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Quantum Darwinism attempts to explain the emergence of objective reality of the state of a quantum system in terms of redundant information about the system acquired by independent non interacting fragments of the environment. We will consider three different scenarios to analyse the link between the emergence of Quantum Darwinism and the quantum information flow from the system to the environment, namely we first study a model of local interaction between a simple quantum system and a multi-mode environment that allows for a clear investigation of the interplay between information trapping and propagation in the environment and the emergence of quantum Darwinism we then analyse the unfolding oq quantum darwinism and its engineering by means of Zeno effect via collision models. We provide strong evidence of the correlation between non-Markovianity and quantum Darwinism in such models, thus providing strong evidence of a potential link between such fundamental phenomena.

#307 - EXPERIMENTAL STUDIES OF PERCOLATION PHENOMENA IN DISSIPATIVE RYDBERG GASES

Oliver Morsch (I) - INO-CNR and Dipartimento di Fisica

In my talk I will review our recent experiments on strongly driven dissipative Rydberg gases. Combining the facilitation mechanism (i.e., off-resonant excitation leading to the conditional excitation of a Rydberg atom in the presence of another Rydberg atom at a well-defined distance) with spontaneous decay, we realized a model for directed percolation. By varying the driving parameters we explored the phase transition between the absorbing (no Rydberg excitations) and the active state of the system. Finally, I will give an outlook on future experiments in which we plan to control dissipation and to realize a directed percolation model with partially coherent faciliation, for which the corresponding phase transition has been predicted to change from second order to first order.

#308 - ON QUANTUMNESS IN MULTI-PARAMETER QUANTUM ESTIMATION, CRITICALITY AND DISSIPATIVE PHASE TRANSITION

Angelo Carollo - University of Palermo

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We derive a measure of quantum-ness in quantum multi-parameter estimation problems. We can show that the ratio between the mean Uhlmann Curvature and the Fisher Information provides a figure of merit which estimates the amount of incompatibility arising from the quantum nature of the underlying physical system. This ratio accounts for the discrepancy between the attainable precision in the simultaneous estimation of multiple parameters and the precision predicted by the Cram\'er-Rao bound. We apply this measure to quantitatively assess the quantum character of phase transition phenomena in peculiar quantum critical models. We consider a paradigmatic class of lattice fermion systems, which shows standard closed quantum phase transition and dissipative non-equilibrium steady-state phase transitions.

#309 - QUANTUM RESOURCES FOR ENERGY STORAGE

Dario Ferraro - Università di Genova

Other Authors: Gian Marcello Andolina (Istituto Italiano di Tecnologia, NEST, SNS Pisa), Michele Campisi (Università di Firenze, INFN Firenze), Vittorio Pellegrini (Istituto Italiano di Tecnologia), Marco Polini (Istituto Italiano di Tecnologia)

Recently there has been a great interest on the possibility to exploit quantum-mechanical effects to increase the performance of energy storage. In this framework, we present a model of a Quantum Battery that can be engineered in solid-state architectures. It consists of N two-level systems coupled to a single photonic mode in a cavity. We demonstrate the emergence of a quantum advantage in the charging power on this collective model (“Dicke Quantum Battery”) with respect to the one in which each two-level system is coupled to its own separate cavity mode (“Rabi Quantum Battery”) [1]. Moreover, we discuss the model of a Quantum Supercapacitor. This consists of two chains, one containing electrons and the other one holes, hosted by arrays of double quantum dots. The two chains are in close proximity and embedded in the same photonic cavity, in the same spirit of the Dicke model. We find the phase diagram of this model showing that, when transitioning from the ferro/antiferromagnetic to the superradiant phase, the quantum capacitance of the model is greatly enhanced [2].

[1] D. Ferraro, M. Campisi, G. M. Andolina, V. Pellegrini, M. Polini, Phys. Rev. Lett. **120**, 117702 (2018).
[2] D. Ferraro, G. M. Andolina, M. Campisi, V. Pellegrini, M. Polini, arXiv:1902.06474.

#310 - THE MASTER EQUATION APPROACH FOR OPEN QUANTUM SYSTEMS IN THE ULTRASTRONG COUPLING REGIME

Alessio Settineri - Dipartimento di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra, Università di Messina

Other Authors: Vincenzo Macrí (2), Alessandro Ridolfo (4;2), Omar Di Stefano (2), Anton Frisk Kockum (5;2), Franco Nori (2;3), Salvatore Savasta (1;2) (1) Dipartimento di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra, Università di Messina, I-98166 Messina, Italy (2) Theoretical Quantum Physics Laboratory, Cluster for Pioneering Research, RIKEN, Saitama 351-0198, Japan (3) Physics Department, The University of Michigan, Ann Arbor, Michigan 48109-1040, USA (4) Dipartimento di Fisica e Astronomia Ettore Majorana, Universitá di Catania (Italy) (5) Department of Microtechnology and Nanoscience, Chalmers University of Technology, 412 96 Gothenburg, Sweden

The interaction among the components of a hybrid quantum system is often neglected when considering the coupling of these components to an environment. However, if the interaction strength is large, this approximation leads to unphysical predictions [1], as has been shown for cavity-QED and optomechanical systems in the ultrastrong-coupling regime. To deal with these cases, master equations with dissipators retaining the interaction between these components have been derived for the quantum Rabi model and for the standard optomechanical Hamiltonian. In this talk, we go beyond these previous derivations and present a general master equation approach for arbitrary hybrid quantum systems interacting with thermal reservoirs [2]. In particular, we decompose the system operators in terms of the dressed states of the hybrid quantum system and derive the master equation without performing the usual secular approximation.

Our approach can be applied to describe the dynamics of open hybrid systems with harmonic, quasi-harmonic, and anharmonic transitions. We apply our approach to study the influence of temperature on multiphoton vacuum Rabi oscillations in circuit QED. We also analyze the influence of temperature on the conversion of mechanical energy into photon pairs in an optomechanical system [2,3], which has been recently described at zero temperature [4]. We compare our results with previous approaches, finding that these can overestimate decoherence rates and underestimate excited-state populations.

[1] A. F. Kockum, A. Miranowicz, S. De Liberato, S. Savasta, and F. Nori, “Ultrastrong coupling between light and matter,” Nat. Rev. Phys. 1, 19–40 (2019).

[2] A. Settineri, V. Macrì, A. Ridolfo, O. Di Stefano, A. F. Kockum, F. Nori, and S. Savasta, “Dissipation and thermal noise in hybrid quantum systems in the ultrastrongcoupling regime,” Phys. Rev. A 98, 053834 (2018).
[3] A. Settineri, V. Macrì, L. Garziano, O. Di Stefano, F. Nori and S. Savasta "Conversion of Mechanical Noise into Correlated Photon Pairs: Dynamical Casimir effect from an incoherent mechanical drive" to appear in Phys. Rev. A
[4] V. Macrì, A. Ridolfo, O. Di Stefano, A. F. Kockum, F. Nori, and S. Savasta, “Nonperturbative dynamical Casimir effect in optomechanical systems: vacuum Casimir-Rabi splittings,” Phys. Rev. X 8, 011031 (2018).

#311 - HIGH-TEMPERATURE COHERENT TRANSPORT IN THE XXZ CHAIN IN THE PRESENCE OF AN IMPURITY

John Goold - Trinity College Dublin

Other Authors: Marlon Brenes (Trinity College Dublin), Eduardo Mascharenas (University of Strathclyde), Marcos Rigol (The Pennsylvania State University)

We study high-temperature spin transport through an anisotropic Heisenberg chain in which integrability is broken by a single impurity close to the center of the chain. For a finite impurity strength, the level spacing statistics of this model is known to be Wigner-Dyson. Our aim is to understand if this integrability breaking is manifested in the high-temperature spin transport. We focus first on the nonequilibrium steady state (NESS), where the chain is connected to spin baths that act as sources and sinks for spin excitations at the boundaries. Using a combination of open quantum system theory and matrix product operators techniques, we extract the transport properties by means of a finite-size scaling of the spin current in the NESS. Our results indicate that, despite of the formation of a partial domain wall in the steady state magnetization (and despite the Wigner-Dyson level spacing distribution of the model), transport remains ballistic. We contrast this behavior with the one produced by a staggered magnetic field in the XXZ chain, for which it is known that transport is diffusive. By performing a numerical computation of the real part of the spin conductivity, we show that our findings are consistent with linear response theory. We discuss subtleties associated with the apparent vanishing of the Drude in the presence of an impurity.

#312 - STATIONARY QUANTUM CORRELATIONS IN A SYSTEM WITH MEAN-FIELD PT SYMMETRY

Federico Roccati - Università degli Studi di Palermo - Dipartimento di Fisica e Chimica - Emilio Segrè

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A pair of coupled quantum harmonic oscillators, one subject to a gain one to a loss, is a paradigmatic setup to implement PT-symmetric, non-Hermitian Hamiltonians in that one such Hamiltonian governs the mean-field dynamics for equal gain and loss strengths. Through a full quantum description (so as to account for quantum noise) we show that when the system starts in any two-mode coherent state, including vacuum, there appear quantum correlations (QCs) without entanglement, as measured by the Gaussian discord. When the loss rate is above a threshold, once generated QCs no more decay. This occurs in a wide region of parameters, significantly larger than that where the full quantum dynamics is stable. For equal gain and loss rates, in particular, QCs decay in the exact phase (including the exceptional point) and are stable in the broken phase.

QUANTUM INFORMATION PHYSICS AND TECHNOLOGIES 3	BARBIERI/SANTORO
QUANTUM SIMULATIONS, SENSING AND METROLOGY	AMICO/MONTANGERO
PHYSICS OF AND WITH FREE ELECTRON LASERS	FEDERICO BOSCHERINI
MATTER IN EXTREME AND METASTABLE CONDITIONS	GIUSEPPE ANGILELLA
TOPOLOGICAL MATTER	LA MAGNA/SASSETTI

#313 - QUANTUM ANNEALING: A JOURNEY THROUGH DIGITALITALIZATION, QUANTUM CONTROL, AND HYBRID QUANTUM VARIATIONAL SCHEMES

Giuseppe Santoro (I) - SISSA

Other Authors: Glen B. Mbeng (SISSA), Rosario Fazio (ICTP)

Various optimization problems that arise naturally in science are frequently solved by heuristic algorithms.

Recently, multiple quantum enhanced algorithms have been proposed. One of the leading candidates, potentially promising for the implementation on near term devices, is the Quantum Approximate Optimization Algorithm (QAOA) introduced by Farhi et al. [arXiv:1411.4028]. I will give an overview of the algorithm and discuss its connection with Digitized Quantum Annealing and Quantum Control. I will then discuss recent numerical and theoretical results we have obtained for the quantum Ising chain problem to test the performance of the QAOA algorithm against standard Quantum Annealing.

#314 - PHOTONS AS A (SIMULATED) THERMAL MEDIUM

Marco Barbieri (I) - Università degli Studi Roma Tre

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Maxwell's demon has its place in the long list of fascinating conundrums in physics. A possible solution includes the act of erasing the information of the demon's register as the event generating entropy and saving the validity of the second law of thermodynamics. This simple but revolutionary connection has been stimulating over the last decade an intense effort towards understand thermal processes, especially those occurring out of equilibrium, taking into account informational figures. On the other hand, it is possible to obtain bounds on exchanged information based on the thermodynamics of the underlying physical processes.

In this talk, we will discuss how this cross fertilisation between thermodynamics and information can deliver new insights on quantum information, in particular when working with photonic quantum states. A first experiment illustrate how limits on the shared information, derived directly from Maxwell's example, are able to detect whether multipartite states enjoy non-classical correlations. In the second example, we will adopt figures inspired by thermodynamics for the characterisation of quantum measurements.

#315 - QUANTUM MEASUREMENT COOLING

Michele Campisi - Department of Physics and Astronomy, University of Florence, and INFN sezione di Firenze

Other Authors: Lorenzo Buffoni (Department of Information Engineering, University of Florence, via S. Marta 3, I-50139 Florence, Italy) Andrea Solfanelli (Department of Physics and Astronomy, University of Florence, and INFN sezione di Firenze, via G. Sansone 1, I-50019 Sesto Fiorentino (FI), Italy) Paola Verrucchi (Department of Physics and Astronomy, University of Florence, via G. Sansone 1, I-50019 Sesto Fiorentino (FI), Italy and Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, via Madonna del Piano 10, I-50019 Sesto Fiorentino (FI), Italy) alessandro Cuccoli (Department of Physics and Astronomy, University of Florence, and INFN sezione di Firenze, via G. Sansone 1, I-50019 Sesto Fiorentino (FI), Italy)

Invasiveness of quantum measurements is a genuinely quantum mechanical feature that is not necessarily detrimental: Here we show how quantum measurements can be used to fuel a cooling engine.

We illustrate quantum measurement cooling (QMC) by means of a prototypical two-stroke two-qubit engine which interacts with a measurement apparatus and two heat reservoirs at different temperatures.

We show that feedback control is not necessary for operation while entanglement must be present in the
measurement projectors. We quantify the probability that QMC occurs when the measurement basis is
chosen randomly, and find that it can be very large as compared to the probability of extracting energy (heat
engine operation), while remaining always smaller than the most useless operation, namely, dumping heat
in both baths. These results show that QMC can be very robust to experimental noise. A possible lowtemperature
solid-state implementation that integrates circuit QED technology with circuit quantum
thermodynamics technology is presented.

#316 - QUANTUM THERMODYNAMICS WITH SPIN QUBITS IN DIAMOND

Nicole Fabbri - LENS and CNR-INO

Other Authors: S. Hernández-Gómez (LENS and CNR-INO), S. Gherardini (LENS and SISSA), F. Poggiali (LENS and CNR-INO), F. S. Cataliotti (LENS and Univ. of Florence), A. Trombettoni (CNR-IOM DEMOCRITOS and SISSA), P. Cappellaro (MIT)

At the nanoscale, the energy transfer is well described through quantum fluctuation relations, which relate equilibrium properties of a system with the statistical analysis of out-of-equilibrium thermodynamics quantities. Open quantum systems, however, pose challenges due to the lack of operative quantum definitions of work and heat flux, and the limited practical access to information on the reservoir. Here, we have experimentally investigated quantum fluctuation relations, employing the spin qubit associated to a Nitrogen-vacancy (NV) center in diamond subject to repeated quantum projective measurements and a tunable connection to a heat reservoir, as a room-temperature quantum simulator of an open-quantum-system dynamics. With this toolbox, we verified for the first time the quantum exchange relation for an open quantum system.

#317 - HIGH TEMPERATURE COHERENT TRANSPORT IN XXZ IN THE PRESENCE OF AN IMPURITY

John Goold - Trinity College Dublin

Other Authors: Marlon Brenes, Trinity College Dublin Eduardo Mascarenhas, University of Strathclyde Marcos Rigol, Penn State

We study high-temperature spin transport through an anisotropic spin-1/2 Heisenberg chain in which integrability is broken by a single impurity close to the center of the chain. For a finite impurity strength, the level spacing statistics of this model is known to be Wigner-Dyson. Our aim is to understand if this integrability breaking is manifested in the high-temperature spin transport. We focus first on the nonequilibrium steady state (NESS), where the chain is connected to spin baths that act as sources and sinks for spin excitations at the boundaries. Using a combination of open quantum system theory and matrix product operators techniques, we extract the transport properties by means of a finite-size scaling of the spin current in the NESS. Our results indicate that, despite the formation of a partial domain wall in the steady state magnetization (and despite the Wigner-Dyson level spacing distribution of the model), transport remains ballistic. We contrast this behavior with the one produced by a staggered magnetic field in the XXZ chain, for which it is known that transport is diffusive. By performing a numerical computation of the real part of the spin conductivity, we show that our findings are consistent with linear response theory. We discuss subtleties associated with the apparent vanishing of the Drude in the presence of an impurity.

#318 - SINGLE-ATOM LASING AND SINGLE-PHOTON PUMP IN QUANTUM-DOT-BASED HYBRID DEVICES

Mattia Mantovani - Universität Konstanz

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Hybrid mesoscopic-QED devices which couple quantum dots to electromagnetic or mechanical resonators have received increasing interest in the last few years. They allow to tailor coherent interactions at the nanoscale, facilitating the exploration of new regimes of electron-photon interactions and heat-exchange mechanisms. Here, we analyze two setups in which single-electron tunneling events through quantum dots can drive harmonic oscillators into remarkable nonequilibrium states. We first consider a quantum dot with two spin-split levels, coupled to a harmonic resonator and embedded between two ferromagnetic contacts with opposite polarization [1]. A spin-polarized current injected in the dot induces single-atom lasing, whereby energy is pumped with close-to-unity efficiency into the resonator. This results in a breakdown of the usual rotating-wave approximation (RWA) employed for coherent spin-resonator interactions, without any requirement of ultrastrong light-matter coupling. Such RWA breakdown allows access to novel regimes of multistable lasing which are characterized by multi-peaked Fock distributions of the oscillator and are detectable with simple current measurements. Secondly, we examine a Cooper-pair-splitter setup consisting of two quantum dots, each coupled capacitively to a local resonator and a common superconductor. We demonstrate that the process of cross-Andreev reflection can be used to pump nonlocally single photons between both resonators, or to simultaneously cool them into their ground state [2]. Hence, such a system has potential applications ranging from coherent heat-control and cooling with single-photon precision to a microwave photon bus.

[1] M. Mantovani, A. Armour, W. Belzig, and G. Rastelli, Phys. Rev. B 99, 045442 (2019).
[2] M. Mantovani, W. Belzig, G. Rastelli, and R. Hussein, arXiv:1907.04308 (2019).

#319 - EXTRACTABLE WORK, THE ROLE OF CORRELATIONS, AND ASYMPTOTIC FREEDOM IN QUANTUM BATTERIES

Gian Marcello Andolina - Scuola Normale Superiore

Other Authors: Gian Marcello Andolina (Scuola Normale Superiore, IIT), Maximilian Keck(Scuola Normale Superiore), Andrea Mari(Scuola Normale Superiore), Michele Campisi (Department of Physics and Astronomy, University of Florence), Vittorio Giovannetti(Scuola Normale Superiore), Marco Polini(IIT)

We investigate a quantum battery made of N two-level systems, which is charged by an optical mode via an energy-conserving interaction. We quantify the fraction E(N) of energy stored in the B battery that can be extracted in order to perform thermodynamic work. We first demonstrate that E(N) is highly reduced by the presence of correlations between the charger and the battery or B between the two-level systems composing the battery. We then show that the correlation-induced suppression of extractable energy, however, can be mitigated by preparing the charger in a coherent optical state. We conclude by proving that the charger-battery system is asymptotically free of such locking correlations in the N \to \infty limit.

#320 - QUANTUM TECHNOLOGIES FOR FUTURE SCIENTIFIC RESEARCH

Simone Montangero (I) - Padova University

In this seminar, we briefly review the current status of some of the most promising applications of quantum technologies for future research. We present the challenges faced by quantum simulators, a class of quantum hardware dedicated to simulating highly interesting but hardly accessible physics: from models to study for high-Tc superconductors or topological systems, to critical systems, quantum chemistry or lattice gauge theories. Alongside, we present the tensor network methods, a classical numerical approach that promise to become a powerful tool accompanying future quantum simulations and computations, providing guidance, benchmarking and verification of the quantum simulation results. We review some of the latest achievements obtained: in particular, the first numerical and experimental quantum simulations of lattice gauge theories in regimes where Monte Carlo methods efficiency is hindered by the sign problem.

#321 - TOWARD A QUANTUM-ENHANCED STRONTIUM OPTICAL LATTICE CLOCK AT INRIM

Marco Tarallo (I) - INRIM

The new strontium atomic clock at INRIM seeks to establish a new frontier in quantum measurement by joining state-of-the-art optical lattice clocks and the quantized electromagnetic field provided by a cavity QED setup. The goal of our experiment is to apply advanced quantum techniques to state-of-the-art optical lattice clocks, demonstrating enhanced sensitivity while preserving long coherence times and the highest accuracy.

The first part of the talk will deal with current state-of-the-art in quantum-enhanced atomic clocks and their prospects to be achieved by two granted European projects, "Q-Clocks" from the QuantERA H2020 action, and "USQOS" from EMPIR fundamental action. In particular, the talk will describe three main research approaches feasible with our apparatus: the spin-squeezing approach to reduce the quantum projection noise from the atomic reference, the superradiant laser source to surpass technical noises (mirror thermal and seismic) in laser spectral purity generation, and finally cavity-enhanced spectroscopy towards a zero dead-time optical clock. These three lines of research can lead to optical clocks with 10-18 stability in few seconds instead of hours.

The second part of the talk will describe the progress of the experimental apparatus. The first building-block of our experiment was the realization of a sideband-enhanced cold atomic source of strontium atoms. We present a detailed study on enhancement and optimization of a cold strontium atomic beam flux from a two-dimensional magneto-optical trap (2D MOT) directly loaded from a collimated atomic beam by adding a sideband frequency to the cooling laser. Laser parameters of the 2D MOT and sideband beams were scanned for optimal settings for maximum atomic beam flux and compared with Monte Carlo simulations. When compared to a conventional 2D MOT with single laser frequency, we were able to obtain a 2.5 times enhancement of the atomic flux when the total laser power was 200 mW.

#322 - CONTINUOUS MEASUREMENTS FOR ADVANCED QUANTUM METROLOGY

Marco G. Genoni - Università degli Studi di Milano

Other Authors: Francesco Albarelli (University of Warwick, UK), Matteo A.C. Rossi (University of Turku, FL), Dario Tamascelli (Università degli Studi di Milano, IT), Matteo G.A. Paris (Università degli Studi di Milano, IT)

We present some recent results regarding the use of time-continuous measurements for quantum-enhanced metrology. In both cases we assess the estimation of a magnetic field along a known direction via time-continuous monitoring of an ensemble of two-level atoms (qubits).

First we consider an initial uncorrelated state and we show that, by continuously monitoring the collective spin observable transversal to the encoding Hamiltonian, one can exploit the spin-squeezing dynamically generated by the measurement and get Heisenberg scaling for the achievable precision.

In the second case, we consider an initial entangled GHZ state and independent noises acting separately on each qubit, responsible for degrading the scaling of the achievable precision from Heisenberg to standard quantum limited. We show that continuous monitoring of all the environmental modes responsible for the noise allows us to restore the desired Heisenberg scaling. We finally discuss the role played by the geometry of the noise affecting the qubits and the role of the efficiency of the time-continuous monitoring.

#323 - RÉNYI ENTROPY MEASURMENT WITH RYDBERG ATOMS

Simone Notarnicola - Università degli Studi di Padova

Other Authors: Simone Montangero (Università degli Studi di Padova)

Rydberg atoms are nowadays a very promising platform to perform quantum simulation of systems ranging from spin system to lattice gauge theories; there are a lot of proposals for experimental setups which may recreate many different systems and, on the other hand, very recent experimental achievements in which, for example, quantum phase transitions have been observed in chains of interacting Rydberg atoms. A crucial ingredient in the study of many transitions and phases of matter is the study of the entanglment, which is quantified through the entropy of the system. In my talk I would like to talk about an ongoing work whose aim is to set up a protocol for measuring the second-order Rényi entropy in Rydberg atoms systems.

#324 - STRONGLY INTERACTING MULTICOMPONENT SU(N) FERMIONS WITH CONTROLLED SYMMETRY BREAKING

Lorenzo Livi - Università degli Studi di Firenze

Other Authors: Leonardo Fallani (Università degli Studi di Firenze) Jacopo Catani (Università degli Studi di Firenze) Lorenzo Franchi (Università degli Studi di Firenze) Daniele Tusi (Università degli Studi di Firenze) Daniel Benedicto Orenes (Università degli Studi di Firenze)

We report on the experimental investigation of a strongly interacting gas of fermionic ^{173}Yb ultracold atoms in a 3D optical lattice with controllably-broken SU(3) symmetry.

SU(N) symmetric interactions naturally emerges in the ground state of fermionic Yb due to the electronic and nuclear properties of alkaline-earth atoms. We explicitly break the SU(N) symmetry by exploiting two-photon Raman processes coupling the internal degrees of freedom of the atomic ground state. In particular, we address the case in which the Raman coupling affects only two states of a three component spin-mixture and demonstrate that the interplay between strong interactions and the external Raman field favours the localization of the atoms in the lattice, reducing the number of double occupancies. Exploiting a spin-resolved doublons detection, we have further investigated this insulating phase demonstrating the flavour selectivity of its properties.

#325 - INDISTINGUISHABILITY-ENABLED COHERENCE FOR QUANTUM METROLOGY

Alessia Castellini - Università di Palermo

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#326 - THE EUROPEAN XFEL: NEW SCIENCE OPPORTUNITIES, START OF USER OPERATION AND FIRST RESULTS.

Sakura Pascarelli (I) - European XFEL

In the past decade we have seen very important developments in the field of accelerator based X-ray user facilities, with the advent of 4th generation synchrotron sources and MHz rate free electron lasers.

The first hard X-ray free-electron laser, LCLS (US) became operational in 2009 andover the last decade four additional hard X-ray FELs have begun user operation - SACLA (Japan), PAL-FEL (Korea), Eu-XFEL (Germany) and SwissFEL (Switzerland). Among these, the Eu-XFEL is the first hard XFEL powered by a superconducting linear accelerator, which enables MHz rate pulse generation.

A specificity of XFELs is their very short pulse duration (10-100fs) opening new scientific opportunities to probe matter at the atomic scale, with chemical selectivity and bulk sensitivity, and on the relevant timescales. Ultrashort, high intensity X-ray pulses from FELs are also providing a totally new approach to structural determination with X-rays, where useful structural information from very small, “radiation sensitive” or “dynamic” crystals is acquired before radiation damage sets in.

After many years of construction, user operation at the Eu-XFEL has finally begun. In the Fall of 2017, two hard X-ray instruments FXE (devoted to studying extremely fast processes) and SPB/SFX (for investigating biomolecules and biological samples) opened to external users. Before the end of 2018, the two soft X- ray instruments SQS (Small Quantum Systems) and SCS (Spectroscopy and Coherent Scattering) followed. Finally, two additional hard X-ray instruments are presently welcoming first user groups: HED for studying matter under extreme pressures and temperatures, and MID for investigating nanostructures or irregularly ordered materials such as glass, liquids and biological substances.

In this talk I will first briefly introduce the present performance of the facility in terms of electron and photon beam characteristics and operation modes. I will thenreport first results from early user experiments, and comment on some important challenges ahead.

#327 - MARIX: CONCEPTUAL DESIGN REPORT OF A MULTI-DISCIPLINARY ADVANCED RESEARCH INFRASTRUCTURE FOR THE GENERATION AND APPLICATION OF X-RAYS

Luca Serafini (I) - INFN-Milano

Other Authors: on behalf of MariX-CDR collaboration

The need of a fs-scale pulsed, MHz-class repetition rate, X-ray source for time-resolved fine analysis of matter (spectroscopy and photon scattering) in the linear response regime is addressed by the conceptual design of a facility called MariX, outperforming current X-ray sources based on FELs or Synchrotrons for the declared scope. MariX is based on the original design of a two-pass two-way superconducting linear electron accelerator, equipped with an arc compressor, to be operated in CW mode (1MHz). MariX provides FEL emission in the range 0.2-8 keV with 10^8 photons per pulse using a 1.5 GeV Linac. The accelerator complex includes an early stage that supports an advanced inverse Compton source of very high-flux hard X-rays (up to 10^13 monochromatic X-ray photon beams) of energies up to 180 keV that are well adapted for large area radiological imaging, realizing a broad science program and serving a multidisciplinary user community, covering fundamental science of matter and application to life sciences, including health at preclinical and clinical level. MariX is designed to represent a new research infrastructure for Northern Italy, and in particular for the Milan metropolitan area and the new Scientific Campus of University of Milan in the post-Expo area (and its Milan Innovation District, MIND). MariX CDR has been recently completed and published at www.marix.eu.

#328 - TRACING FRAGMENTATION DYNAMICS UPON ABSORPTION OF VERY INTENSE X-RAY PULSES

Patrik Grychtol - European XFEL

X-ray free-electron lasers (XFELs) have opened up unprecedented possibilities in different scientific areas. Key features of FEL radiation are the very short pulse duration and the high number of photons per pulse, leading to extreme intensities under which hitherto unknown effects in X-ray matter interaction are revealed. When isolated molecules absorb an intense, femtosecond X-ray pulse, a complex interplay of multiple inner-shell photo absorptions, Auger decays, and nuclear motion takes place. All processes happen on timescales similar to the pulse duration, thus giving rise to effects such as resonantly-enhanced ionization, leading to extremely high charge states. A detailed understanding of the atomic response on the femtosecond timescale is crucial for the interpretation of many XFEL experiments.

The Small Quantum Systems (SQS) instrument at soft X-ray branch of the European XFEL is dedicated to the investigation of nonlinear phenomena and ultrafast dynamics of gas-phase atoms, molecules and nanoparticles. A wide range of experimental techniques for spectroscopic investigations using electrons, ions and photons, as well as various sample delivery systems are available for users. The design of the three experimental chambers has been optimized to take advantage of the high repetition rate and to enable various types of coincidence methods. User operation started in November 2018.

In one of the first user experiments at the SQS instrument, we have investigated the charge rearrangement and the fragmentation dynamics upon absorption of very intense soft X-ray pulses in polyatomic molecules. Of particular interest were molecules containing a single heavy atom that acts as a localized absorber due to the strongly increased absorption cross section. Under typical experimental conditions at SQS, extremely high charge states have been observed in isolated heavy atoms, for example, up to 42 charges in a xenon atom. In a heavy-atom containing molecule, the charge is initially located on the heavy atom, but can spread to the other atoms in the molecule very quickly, thus charging up the complete molecule, which subsequently undergoes Coulomb explosion. Its fragmentation can be experimentally observed by means of 3d ion momentum imaging in a so-called reaction microscope (REMI). Under ultra-high vacuum conditions, several ions (and/or electrons) originating from the same molecule can be detected in coincidence, and mass spectra, kinetic energies, and relative angles between ions can be determined, thus providing a complete picture of the rich fragmentation dynamics of this molecule after absorption of a very intense X-ray pulse.

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#329 - TIME RESOLVED PHOTOELECTRON CIRCULAR DICHROISM OF FENCHONE AT FERMI

Salvatore Stagira - Politecnico di Milano - Dipartimento di Fisica

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Chirality plays a fundamental role in nature. A chiral molecule is defined as one whose configuration is not superimposable on its mirror image. Two mirror images of the same chiral compound are called enantiomers, or optical isomers, since they can be easily distinguished by making them interact with circularly polarized light sources. In spite of having the same chemical structure, most enantiomers show very different chemical properties when interacting with other chiral species, which is the reason why the study of chirality has been a subject of deep investigation in biology, chemistry and pharmaceutics. However, the ultrafast dynamics of chiral compounds is mostly unexplored.

One of the more promising investigation techniques for studying the time-dependent dynamics of a chiral compound is time-resolved photo-electron circular dichroism (TR-PECD). In conventional PECD, a circularly polarized pulse ionizes a randomly oriented optical isomer. The dichroism of the sample emerges from a strong forward-backward asymmetry of the angle-resolved photoemission along the propagation direction of the ionizing pulse.

Recently, the relaxation dynamics of a photoexcited chiral sample have been tracked with PECD from the electronically excited states of molecules, providing the first demonstration of the sensitivity of TR-PECD to ultrafast chiral dynamics [1,2]. We extended this approach by performing PECD on photoexcited fenchone at the carbon K-edge, to merge the chemical sensitivity of core excitation with the chiral sensitivity of circularly polarized light. Indeed, huge chiral asymmetry in the angular distribution of photoelectrons ejected from carbonyl C 1s core orbitals of fenchone has been previously reported [3]. To this end, the FERMI light source offers unique properties, being the only free-electron laser (FEL) providing both circularly polarized XUV pulses up to the Carbon K-edge and a jitter-free external laser for time-resolved pump-probe experiments.

We probed the ultrafast chiral dynamics occurring in fenchone after excitation with a linearly polarized pulse at 400 nm wavelength (*pump*). A circularly polarized FEL pulse at 300 eV (*probe*) was used to ionize the molecule, and the circular dichroism of the photo-electron angular distribution was acquired with a velocity map imaging spectrometer. From the PECD measurements at different pump-probe delays, the chiral asymmetry parameter b_1 of the photoionized electrons at a binding energy of 292.5 eV was recorded. This result represents the first observation of chiral femtosecond dynamics probed with core-level excitation.

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#330 - DYNAMIC CHARGE TRANSFER BETWEEN PLASMONIC NANOPARTICLES AND CERIUM OXIDE

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The coupling of wide band gap oxides with suitable plasmonic nanoparticles (NPs) has shown to be effective in providing materials with a light absorption range extending over the full solar radiation spectrum. This represents a promising strategy to obtain efficient functional materials, which convert solar into chemical or electric energy, relevant for a wide range of applications, like sensors, photocatalysts or photovoltaic devices. The localized surface plasmon resonance (LSPR) decay, occurring on femtosecond time scales, involves a relevant energy transfer to the oxide, which may lead to modifications of the material properties on much longer time scales. A clear understanding of the mechanisms for plasmonic energy transfer in well-controlled systems is essential for a knowledge-driven optimization of this important class of functional materials. Among wide bad gap oxides, cerium oxide represents an extremely interesting material with well-established applications in automotive, and with an emerging relevance in hydrogen-related technologies. The importance of cerium oxide is ascribed to its ability to quickly form, fill and transport oxygen vacancies, linked to possibility for the Ce cations to reversibly switch between the 4+ and the 3+ oxidation states.

We have recently shown that a high absorbance in the visible range can be obtained by embedding Ag NPs in a cerium oxide matrix [1]. By fast transient absorption spectroscopy (FTAS) measurements, performed at EuroFEL Support Laboratory (EFSL – CNR-ISM), we identified a long-living excited state induced by LSPR decay, and we tentatively ascribed it to a transient occupation of 4f levels [1]. The state has a lifetime beyond 500 ps [1] and it is expected to have an influence on the material redox properties. However, the limited time resolution and the lack of chemical selectivity of the FTAS technique did not allow to access the modifications occurring at the ultrashort time scales, where a LSPR decay related feature dominates the FTAS spectra, hindering the possibility to clearly determine the mechanisms for plasmonic energy transfer. To overcome this drawback a pump-probe XAS experiment at the EIS-TIMEX beamline at FERMI using FEL2 has been planned. The first preliminary results show a clear variation in the Ce $N_{4,5}$ absorption edge after LSPR excitation, compatible with a dynamic charge transfer from the Ag NP to the oxide matrix. The obtained results are very promising in view of an experiment aimed at following the dynamics of LSPR-induced charge injection with sub-picosecond time resolution. Moreover, they demonstrate the possibility to apply FEL-related techniques to functional materials.

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#331 - MEGAHERTZ X-RAY MICROSCOPY AT EUROPEAN X-RAY FREE ELECTRON LASER

Patrik Vagovic - European XFEL

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We demonstrate X-ray phase contrast microscopy performed at the European X-ray Free-Electron Laser sampled at 1.128 MHz rate for the first time. We have applied this method to image stochastic processes induced by an optical laser incident on water-filled capillaries with micrometer scale spatial resolution. This study opens up new perspectives for imaging of irreversible stochastic processes not accessible via visible light imaging or with less intense X-ray sources. At hard X-Ray MHz rate XFEL facilities and this method enables the observation of stochastic object motion at high velocities on the order of m/s to several km/s.

#332 - HIGH-INTENSITY TERAHERTZ AND MID-INFRARED RADIATION: PRODUCTION AND OPPORTUNITIES IN CONDENSED MATTER RESEARCH

Stefano Lupi - INFN and Department of Physics, Sapienza University of Rome

Terahertz (THz) and Mid-Infrared (MIR) radiation, ranging from 0.5 meV to 1 eV, are in resonance with most of the fundamental excitations in condensed matter, allowing to measure, in steady-state linear-response spectroscopy, both their characteristic energy and lifetime. Recently, the developing of new high-intensity, sub-fs pulsed radiation sources emitting in the THz-MIR spectral region, has open a new scenario for condensed matter, allowing not only to excite those excitations but also to modulate and control their behavior in time and frequency.

This is particular important in Quantum Materials, where exotic excitations like Dirac and Weyl electrons, charge-phonons, spinons, skyrmions, Higgs and Goldostone modes, with a complex texture of spin, lattice and electronic degrees of freedom, affect their low-energy transport and electrodynamics.

Here, we present some experimental results recently obtained [1,2], discussing also new THz and MIR facilities planned or already existing in Italy.

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#333 - TRANSFORMATIONS IN MATERIALS SCIENCE: REACTIONS, NUCLEATION, AMORPHISATION, PHASE TRANSITIONS

Antonino Marco Saitta (I) - Sorbonne University

Other Authors: Fabio Pietrucci (Sorbonne University)

Computational approaches are nowadays a full, self-standing branch of materials science, both for their quantum-based ("*ab initio*") accuracy, and for their multiscale extent. In this talk I will present an overview of our computational materials science (CMS) research at Sorbonne University. I will start with fundamental questions, such as the topological-based definition of global coordinates capable to describe and predict, at the *ab initio* level, transformations thermodynamics, kinetics and mechanisms in materials. I will show how, introducing a novel space of generalized
coordinates that capture changes in the topology of the interatomic network, we are able to systematically
track transitions among liquid, amorphous, and crystalline forms throughout the whole phase diagram of
water, including the nucleation of crystals above and below the melting point. Our approach, based on
molecular dynamics and enhanced sampling or free energy calculation techniques, is not specific to water
and could be applied to very different structural phase transitions, paving the way towards the prediction of
kinetic routes connecting polymorphic structures in a range of materials.

#334 - SUB-NANO CONFINED MATTER AT HIGH PRESSURES

Mario Santoro - CNR-INO and LENS

I will talk about a very intriguing research field, joining high pressure science of simple molecular systems to the amazing world of zeolites. On a pure physical ground, confining dense, inhert simple systems at high pressures, at the Angstrom scale, in zeolites, produces novel and exotic sub-nanophases of these systems. Indeed, I will present results on recently obtained dense sub-nanophases of rare gases and of N_2, O_2, H_2 and H_2O, where these systems tend to form disordered/glassy confined structures and also, in the case of O_2, weak chemical clusters such as O_4. I will then present on several novel compounds obtained by reacting dense simple carbon bearing molecular systems at GPa or tens of GPa, strongly confined in the sub-nanopores of zeolites. The reaction products are polymer/zeolite nanocomposites, of 1D type in some cases, and they have remarkable interest for fundamental science, and also for potential applications in mechanics, electronics, photonics and energy storage. Investigations were performed by using diamond anvil cells, optical spectroscopy, and X-ray diffraction, and also classical and DFT simulations.

#335 - AB INITIO SPECTROSCOPY OF WATER UNDER ELECTRIC FIELD

Giuseppe Cassone - Czech Academy of Sciences

Other Authors: Jiri Sponer (Czech Academy of Sciences), Sebastiano Trusso (CNR-IPCF Messina), Franz Saija (CNR-IPCF Messina)

Whereas a boundless literature exists on the spectroscopy of water in disparate conditions [1,2], infrared (IR) and Raman spectra of water subjected to electric fields have never been reported so far. Based on state-of-the-art *ab initio* molecular dynamics simulations, here we present IR and Raman spectra of bulk liquid water under the effect of static electric fields beneath the molecular dissociation threshold (***i.e.***, up to 0.30 V/Å [3,4]). A contraction of the entire frequency range is recorded upon increasing the field intensity both in the IR and in the Raman spectra. Whilst the OH stretching band is progressively shifted toward lower frequencies – indicating a field-induced strengthening of the H-bond network – all the other bands are up-shifted by the field. The order-maker action of the field emerges also from the increase of the water tetrahedral order. The kosmotropic effects carried by the field render the water structure more and more “ice like” as the field strength is increased.

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#336 - INFRARED STUDY OF THE PRESSURE-INDUCED METALLIZATION IN BULK 2H-MOTE2

Elena Stellino - Dipartimento di Fisica e Geologia, Università degli studi di Perugia

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Among Transition Metal Dichalcogenides (TMDs), 2H-molybdenum-based compounds have been intensively investigated since their semiconducting nature and band gaps in the optical region make them interesting for a wide range of electronic and optoelectronic applications. Additionally, a strong dependence of the electronic structure on the number of layers have been observed; in particular, a crossover from an indirect to a direct gap occurs when the crystal sample is reduced down to mono-layer, indicating that the inter-layer coupling plays a key role in determining the physical properties of these systems. The application of pressure, which mainly acts on the inter-layer distance, is thus a powerful and clean tool to tune and study their electronic properties.

Bulk 2H-MoTe2 is a semiconductor with an indirect band-gap of 1.0 eV, which becomes direct (1.1 eV) in the mono-layer case. This system is of particular interest since, compared to the most widely studied MoS2 and MoSe2 with band-gaps in the visible region, its band-gap energy allows optoelectronic devices also in the near infrared range.

The effects of the applied pressure on bulk 2H-MoTe2 have been studied in a number of experimental and theoretical works. While the lattice structure does not appreciably change at least up to 50 GPa, the band gap closes above 10 GPa and, consequently, the crystal undergoes a semiconductor to semimetal transition.

We herein report the first infrared absorption measurements devoted to the study of the pressure dependence of the metallization process in 2H-MoTe2. Transmission measurements on bulk samples were conducted at ambient temperature at the SOLEIL synchrotron for pressures up to about 20 GPa by using diamond anvil cells. Experiments in the mid-near infrared region were performed at the SMIS beamline to obtain information on the pressure dependence of the band-gap. In the far infrared region, measurements at the AILES beamline were aimed at identifying the signature of the transition to the metallic state, i.e. the increase of the absorption intensity due to the increase of the free electron density.

On the basis of these independent experiments, we found a metallization pressure range between 12 and 14 GPa, which is well consistent with previous theoretical and experimental results. For the metallic phase, on the basis of the Drude model, we propose a simple method that relates the integral of the FIR absorption to the free electron density n, allowing us to experimentally estimate the rate of increase of n above metallization.

Density Functional Theory computations were also performed to calculate the electronic density of states at different pressures from 10 to 20 GPa. An independent estimate of the rate of increase of n was thus obtained, which results to be well compatible with the experimental one.

#337 - MULTIPHONON ANHARMONICITY OF MGO

Paola Giura - Sorbonne Univeristé - IMPMC

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Anharmonic lattice dynamics is at the center of an intense research activity largely driven by the significant advances in the theoretical treatement of phonon-phonon and spin-phonon interactions. Remarkably, in a litterature abundantly dominated by calculations, a direct experimental validation of the thoretical methods is still missing.

In this work we report infrared and inelstic x-ray scattering masurements together with desity funtional perturbation theory (DFPT) calculations of the MgO single crystal lattice dynamics as a function of temperature. More specifically we analyze the effects of multiphonon interactions on the energy and width behavior of the optical phonon modes. Our results clarly show the signatures of anharomic effects in the phonon-phonon self energy measured by infrared spectroscopy as well as anomalies in the longitudinal phonon lifetime measured by inelastic x-ray scattering. More important, guided by the remarkable agrement between our advanced DFPT calculations and the experimental results, all the peculiarities of the ionic collective dynamics of MgO find a clear explanation by well defined multiphonon scattering process.

The results obtained shed light on the anharmonic phenomena governing the collective dynamics of MgO with genral consequences for ionic systems and alkali halides. They also highlight the importance of the correct treatement of anharmonic contributions to the thermodynamic properties of solids and notably to the thermal conductivity.

#338 - OUT OF EQUILIBRIUM DYNAMICS IN TOPOLOGICAL SYSTEMS

Maura Sassetti (I) - Dipartimento di Fisica, Università di Genova

Topological states of matter are presently one of the most exciting topic in condensed matter physics. They strongly differ from standard materials, classified in terms of symmetry breaking and local observables, since they exhibit topological global properties, robust against deformations. This makes them extremely promising for several applications ranging from single electron control, spintronics, to quantum computation. In this talk I will first review and introduce these novel materials [1]. Later I will focus on two key topological systems: the quantum Hall and quantum spin Hall, addressing the problem of how to create and manipulate robust single particle excitations, even in presence of interactions. I will show how the topological properties of edge states allows to test dynamical quantum transport at the single particle level. In this context, the stability and coherence of single-particles injected into the edge states of a fractional quantum Hall bar [2,3], and into interacting helical channels of a quantum spin Hall system [4] will be discussed.

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#339 - QUANTUM PUMPING AND LOCALIZATION PROPERTIES IN DISORDERED FLOQUET SYSTEMS

Matteo Wauters - SISSA

Other Authors: Giuseppe E. Santoro (SISSA, ICTP), Angelo Russomanno (ICTP), Lorenzo Privitera (University of Würzburg)

We investigate the topological phase transition induced by disorder in a periodically driven one-dimensional model displaying quantized topological transport. We show that, while instantaneous eigenstates are necessarily Anderson localized, the periodic driving plays a fundamental role in delocalizing Floquet states over the whole system, henceforth allowing for a steady state nearly-quantized current. Remarkably, this is linked to a localization/delocalization transition in the Floquet states of a one-dimensional driven Anderson insulator, which occurs only when the periodic driving describe a topologically non-trivial loop in the parameter space of the model. As a consequence, the Floquet spectrum becomes continuous in the delocalized phase, in contrast with a pure-point instantaneous spectrum.

#340 - TOPOLOGICAL TERMS VS TOPOLOGICAL STATES IN SPIN MODELS WITH LADDER DIMERISATION

Cristian Degli Esposti Boschi - CNR-IMM, Sezione di Bologna

Other Authors: Elisa Ercolessi (Dipartimento di Fisica e Astronomia dell'Università di Bologna & INFN, Sezione di Bologna), Greta Ghelli (Dipartimento di Fisica e Astronomia dell'Università di Bologna), Giuseppe Magnifico (Dipartimento di Fisica e Astronomia dell'Università di Bologna & INFN, Sezione di Bologna)

We analyze the possible existence of topological phases in two-legged spin ladders considering a staggered interaction in both chains. When the staggered interaction in one chain is shifted by one site with respect to the other chain, the model can be mapped, in the continuum limit, into a nonlinear sigma model plus with a so-called topological term which is nonvanishing even if the number of legs is two.

This suggests a quantum phase transition that is explored numerically, using a DMRG approach, by considering energy gaps, surface correlations as well as nonlocal correlators and entanglement indicators such as entropy and degeneracy of reduced density matrix levels. This characterisation indicates the appearance of a topological phase (an analogue of Mott-Haldane transition) with genuine multipartite entanglement, and provide insights in the role of topological field-theoretic terms vs topological states in quasi 1d quantum systems.

#341 - INVESTIGATION OF HYBRID JOSEPHSON JUNCTIONS FOR TOPOLOGICAL APPLICATIONS

Matteo Carrega - CNR Nano and Scuola Normale Superiore

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Hybrid superconductor/semiconductor devices constitute a powerful platform where intriguing topological properties can be investigated.

Here we present Josephson junction devices formed by a high-mobility InAs quantum-well bridging two Nb superconducting contacts. We demonstrate supercurrent flow with transport measurements, high critical temperature of 8.1 K, and critical fields of the order of 3T. Modulation of supercurrent amplitude can be achieved by acting on two side gates.

Low-temperature measurements reveal well-developed quantum Hall plateaus, showing clean quantization of Hall conductance and demonstrating the potential of hybrid devices to investigate the coexistence of superconductivity and Quantum Hall effect. Moreover, we present a different, fully tunable, hybrid semiconductor/superconductor device, in which the width, area, and supercurrent of the two arms of a SQUID-like geometry can be independently controlled with high precision.

We demonstrate wide tunability from a SQUID with narrow arms to a Fraunhofer pattern in an extended JJ by electrostatic means. These results pave the way for new device architectures with potential topological applications.

#342 - SIMULATING TOPOLOGICALLY PROTECTED TRANSPORT IN NOVEL QUANTUM SPIN HALL INSULATORS

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We report a full first-principles simulation of topologically protected transport at the edge of novel quantum spin Hall insulators.

With input from newly developed computational 2D materials databases [1,2], containing thousands of 2D materials and forming the ideal starting point for the investigation of unexplored topological materials, we focus on new interesting candidates to achieve large-gap quantum spin Hall insulators [3].

We then explore the electronic band structure of such candidates in different nanoribbon geometries, highlighting the emergence of robust metallic states whose eigenvalues cross the region of bulk gap, and investigate the robustness of their transport properties in the framework of non-equilibrium Green's function formalism.

Contrary to what is usually expected for time-reversal invariant topological insulators, simulations

show that an impurity at the edge can spontaneously acquire a magnetic moment, therefore violating time-reversal symmetry and leading to a strong suppression of edge transport.
Our results, which are in agreement with recent theoretical predictions based on the Kane-Mele-Hubbard model [4], shed light on a previously underestimate mechanism that may realistically affect 2D topological insulators, whose quantized conductance is indeed often difficult to attain in experiments.

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#343 - UHLMANN NUMBER IN TRANSLATIONAL INVARIANT SYSTEMS

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The Chern insulators are 2D topological insulators which display non-trivial topological phases, characterised by the Chern number, a topological invariant which depends only on the ground-state band structure of the model.
In systems at thermal equilibrium, as for any mixed state, the Chern number cannot be used, as the latter is only defined only for pure state systems.
The Uhlmann approach provides a way of generalising to the mixed state scenario concepts such as topology and geometry.
In our work we show that through this approach one can introduce novel quantities, such as the mean Uhlmann curvature or the Uhlmann number, which are able to capture distinctive topological properties of Chern insulators at finite temperature.
We will show how these quantities do not display a temperature driven phase transition, but instead they describe a distinct cross-over transition from a zero-temperature topological behaviour to a trivial high-temperature one.
To quantitatively assess this cross-over transition we define a suitable cross-over temperature, and show how the latter is governed by a universal critical scaling in proximity of the topological phase transition.
Despite its mathematical abstract definition, the Uhlmann approach can be readily related to experimentally accessible quantities, such as the dynamical conductivity, or more generally, the dynamical susceptibility.
Indeed, the Uhlmann number can be seen as a straightforward generalisation of the Chern number, and we will introduce a generalised TKNN relation, that links the Uhlmann number to the dynamical conductivity.

#344 - QUANTUM SPIN HALL QUANTUM POINT CONTACTS

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Other Authors: Christoph Fleckenstein (Wuerzburg Universitaet), Bjoern Trauzettel (Wuerzburg Universitaet)

Quantum spin Hall systems are potential candidates for spintronics, quantum spintronics, and quantum computation applications. In the talk I will consider in particular the possibility to engeneer fractional charges[1], odd requency superconductivity[2], anoumalous conductance quantization[3], and even parafermionic bound states[4] in set ups involving constrictions between helical edges and, in some cases, superconductors.

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#345 - COMPARATIVE STUDY OF ELECTRONIC BAND STRUCTURE OF PB(SN)-BASED TOPOLOGICAL INSULATORS

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Topological insulators (TIs) have emerged as a novel quantum state of matter. The Dirac-like surface state (topological surface state: TSS) and the peculiar spin-texture play an essential role in manipulating spin-polarization and spin-current of TI-based devices [1,2]. A fine tailoring of TSS electronic properties has been attempted but with strong modifications of the surface states. One other critical point is that future topological based devices will most likely involve surfaces that are exposed to ambient environment. An innovative approach that allows to design TIs with tunable electronic states, *unaffected* by contaminants exposure, relies on Pb-based ternary chalcogenides. In contrast to the binary compounds, the crystal structure of ternary/quaternary compounds is formed by alternating quintuple- (QL) and septuple-layer (SL) blocks. By means of scanning tunnelling microscopy (STM) and angle-resolved photoemission spectroscopy (ARPES) measurements supported by density functional theory (DFT) on $PbBi_4Te_7$ and $PbBi_6Te_{10}$ we proved coexisting TSSs, deriving from different surface terminations, displaying distinct electronic band dispersion, and Dirac point energies [3,4]. Recently, we also proved that a tailoring of the TSSs is made possible by the replacement of heavy atoms by lighter isoelectronic ones, as predicted by theory [5,6]. In this context, we will present a systematic electronic band investigation of this novel class of ternary/quaternary TIs, $A^{IV}Bi_4Te_{7-x}Se_x$ (A^{IV}= Sn, Pb; x=0, 1), by means of ARPES measurements and DFT calculations. Finally, we show that the electronic structure of the investigated systems is barely affected by contaminants exposure.

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Posters

#P001 - PROTEIN AGGREGATES FOR WATER PURIFICATION

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Water pollution is the contamination of water bodies including lakes, rivers, oceans and it is a leading global risk factor for illness and death for people, plants and living organisms. A principal source of water pollution is industry, from which increasing amounts of toxic pollutants are released including heavy metals such as cobalt, lead and copper. Today various technologies for purifying contaminated water can be applied, a lot of them being typically expensive, ion specific and characterised by low efficiency. For these reason, the search of new biocompatible materials with increased capabilities is strongly needed.

Protein aggregates have already revealed their potential as environmentally friendly, biocompatible, flexible materials for different application ranging from scaffold for tissue engineering to drug delivery.

In peculiar conditions, proteins may destabilise their structure and undergo different association processes leading to amyloid like aggregates. These highly ordered structures stabilised by H-bonds include fibrils, spherulites and particulates. By suitably varying solution conditions it is possible to tune aggregate size and morphologies as well as their physicochemical (hydrophobicity, hydrophilicity, swelling/deswelling properties) and mechanical properties. Amyloid fibrils have already revealed their potential for applications in water purification as fundamental components of carbon based filter membranes used for separating water from heavy metals. Here we present an experimental study where particulates are tested as new tuneable biomaterials for metal adsorption. Particulates are considered a generic state for protein aggregation they are perfectly spherical aggregates whose diameter ranges from hundreds nanometers to few microns. They can be readily formed at high temperature in water solutions at pHs close to the isoelectric point and have never been related to pathologies.

We used spectroscopy and microscopy methods to characterize the aggregates formation, structure and morphologies. Inductively coupled plasma Optical Emission Spectroscopy (ICP – OES) and Differential Pulse Anodic Stripping Voltammetry (DP-ASV)techniques are used to evaluate uptake/release of metal ions in different conditions as a function of time and of adsorbate – adsorbent ratio in kinetic and thermodynamic experiments. The most used kinetic and isotherm equations were used to fit experimental data in order to obtain information about adsorption mechanism.

Changing aggregation conditions and in turn molecular properties of aggregates, it is possible to highlight peculiar structural features essential for metal binding/adsorption. This knowledge can be used to develop efficient biomaterials for removing toxic heavy metal from wastewater, also, to exploit them for several cycles of purification with minimal reduction in performance.

#P002 - SPONTANEOUS INTERFACIAL FRAGMENTATION OF INKJET PRINTED OIL DROPLETS AND THEIR ELECTRICAL CHARACTERIZATION

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This work presents the fabrication of femtoliter-scale oil droplets by inkjet printing based on a novel mechanism for the spontaneous fragmentation at the interface with an immiscible water phase and the electrical characterization of the resulting immersed “daughter” droplets. [1] In particular, picoliter-scale fluorinated oil droplets impact on surfactant laden water phase at moderately high Weber number (10^1), and are subjected to spreading and capillary instabilities at the water/air interface which ultimately lead to rupture in smaller sized droplets, according to reported models for macroscale droplets systems - [2] the emerging fragmentation results in “daughter” droplets having volumes of about 10-30 % with respect to the initial droplet volume. Remarkably, the picoliter scale downscaling leads to a novel surfactant-driven fragmentation due to the low Bond number (around 10^{-4}-10^{-5}), meaning that droplet immersion is dependent on surface tension forces and not on gravitational forces. In fact, the non-ionic Polyoxyethylene (20) sorbitan monolaurate was observed to permit the droplet immersion in the water phase only if spiked in the water phase at concentrations equal or higher than its critical micellar concentration (i.e. around 0.003% v/v). The resulting oil “daughter” droplets are characterized by a chip with integrated microelectrodes, permitting to extract number, velocities and diameter distribution (peaked at about 3 μm) employing electrical impedance measurements. In accordance with reported models, the electrical characterizations show that the droplets have volumes in the femtoliter scale and are subjected to inertial focusing. [3] This work can be considered an important advancement for understanding the effects of downscaling on fragmentation phenomena at immiscible interfaces, leading to a knowledge platform for a tailored oil droplets fabrication applicable for drug encapsulation, pharmaceutic preparations, and thin-film wrapping around droplets. [4]

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#P003 - ON THE EFFECT OF DOWNSCALING IN INKJET PRINTED LIFE-INSPIRED COMPARTMENTS

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The fabrication of size-scalable liquid compartments is a topic of fundamental importance in synthetic biology, aiming to mimic the structures and the functions of cellular compartments. Here, inkjet printing is demonstrated as a customizable approach to fabricate aqueous compartments at different size regimes (from nanoliter to femtoliter scale) revealing the crucial role of size in governing the emerging of new properties. At first, inkjet printing is shown to produce homogenous aqueous compartments stabilized by oil-confinement with mild surfactants down to the hundreds of picoliter scale [1]. Raster Image Correlation Spectroscopy allows to monitor few intermolecular events by the involvement of protein-binding assays within these compartments [2]. Subsequently, in order to reduce droplet size at values below the nozzle size, a theoretical model from Eggers et al. [3] is experimentally reproduced permitting to obtain femtoliter-scale aqueous droplets from picoliter-scale microchannels [4]. As a remarkable difference to picoliter scale droplets, downscaling at the femtoliter-size triggers the spontaneous formation of molecularly crowded shell structures at the water/oil interface stabilized by a mixture of biocompatible surfactants. The shells have typical thickness in order of hundreds of nanometers, in accordance with theoretical models [5]. Molecular crowding effects in these systems are tested by using fluorescence lifetime imaging under the phasor plot approach [6], revealing different characteristic lifetimes of specific probe molecules in the confined volumes with respect to bulk solutions. The femtoliter-scale compartments autonomously trigger the formation of unique features (e.g., up-concentration, spatial heterogeneity, molecular proximity) that are mediated by the intermolecular interactions in these novel environments, ultimately permitting to mimic the native conditions of sub-cellular scale compartments. The crowding conditions in femtoliter-scale droplets do not to affect the conformation variation of a model DNA hairpin in presence of molecular triggers and of a CYP2E1-catalyzed enzymatic reaction. Our results can be a first step towards the fabrication of size-scalable *lab-on-a-chip* compartments mimicking sub-cellular environments.

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#P004 - CROSSOVER IN ELECTRON-GAS RELAXATION DYNAMICS VS EXCITING PHOTON ENERGY IN EUV-EXCITED ALUMINIUM

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We report a time-resolved study of the relaxation dynamics of Al films excited by ultrashort intense free-electron laser (FEL) extreme ultraviolet pulses. The system response was measured through a pump-probe detection scheme, in which an intense FEL pulse acted as the pump, while a time-delayed ultrafast pulse probed the near-infrared (NIR) reflectivity of the Al film. The pump pulse wavelength was varied in the range 18 – 42 nm. Remarkably, following the intense FEL excitation at the shortest wavelength, the reflectivity of the film exhibited no detectable variation for hundreds of femtoseconds, after which it decreases. Following recent theoretical calculations of the EUV-excited electron dynamics, the delayed NIR-reflectivity evolution is interpreted invoking the formation of very-long-living non-thermal hot electron distributions in Al after exposure to intense EUV pulses. With increasing wavelength of the EUV pump pulse the reflectivity decreases with shorter delay and becomes essentially instantaneous at 42 nm. This evidence for a crossover in the electron gas relaxation dynamics suggests that the NIR reflectivity, due to excitations around the Fermi level, starts to be affected only when the hot electrons thermalize to the valence band.

#P005 - MAPPING OF LIGHT EMITTING DEFECTS IN ZNO NANORODS UNDER DIFFERENT THERMAL ANNEALING

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In the last few years, ZnO nanostructures have received a growing interest for potential application in light emitting devices, sensing and optoelectronics. Among the different synthesis processes,

Chemical Bath Deposition (CBD) is a fast and low-cost technique which allows to efficiently grow a large amount of nanorods (NRs) without the need of high vacuum or high temperature processes.
In this paper, we report on the synthesis and characterization of ZnO nanorods obtained by CBD and the effects of thermal annealing on the luminescence features.
For the NR growth a Si substrate was spin coated with an ethanol solution containing ZnO nanoparticles, acting as seeds, and then immersed in a solution of 25 mM zinc nitrate hexahydrate [$Zn(NO_3)_2 \cdot 6H_2O$] and 25 mM hexamethylenetetramine [$C_6H_{12}N_4$] (HMTA) at a temperature of 90 °C. After the growth, ZnO NRs were annealed in furnace under different ambients (O_2 or Ar) at 600°C for 1h.
A comprehensive structural, chemical and optical characterization was conducted by a Scanning Electron Microscope (SEM) equipped with an Energy Dispersive X-Ray Spectroscope (EDX) and a Cathodoluminesce (CL) system. Scanning Electron Microscopy allowed us to distinguish the occurrence of two families of ZnO NRs: (i) ZnO NRs grown on the seeded substrate and (ii) ZnO NRs grown in solution (by spontaneous homogeneous nucleation).
In particular, we measured a mean length of about 740 ± 50 nm for NRs belonging to the first family, while the NRs grown in solution reach a length of few μm. The EDX analyses show us the characteristic X-Ray peaks of ZnO, demonstrating the absence of spurious elements after the annealing under different ambients. Finally, the CL spectrum of as-grown ZnO NRs shows a sharp peak in the UV (wavelength of 384 nm) and a broad band in visible range (~590 nm) which are associated, respectively, to carriers recombination in correspondence to near band gap and deep level defect states. After the annealing, the UV peak position is unchanged while a red shift is noted in the visible range for both O_2 and Ar ambient annealing; moreover a strong quenching was observed after treatment in Ar. In addition, thecombination of CL and SEM maps let us to observe that the UV emissions is mainly associated to a ZnO NR core while the visible one is associated to superficial defects states.
In conclusion, this experiment suggests that light emission can be tuned in the visible range by varying the annealing conditions and allowing to engineer ZnO NRs for future applications in optics. This work was done within the framework of the "Materials and Nanostructures Laboratory" course of the Master Degree in Physics at University of Catania.

#P006 - INVESTIGATION OF BORON DIFFUSION FOR P+ EMITTER FORMATION ON N-TYPE SILICON

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This work reports on boron diffusion processes for emitter formation on the front side of n-type mono crystalline silicon based solar cells. Diffusion processes are carried out in a tube furnace using preform source as boron dopant source. Three parameters are varied in this study: drive-in temperature, drive-in duration and temperature ramp-up rate. It is found that sheet resistance measured by four point probe (4pp) decreases from 93 Ohm/sq to 24 Ohm/sq as drive-in temperature increases from 850°C to 950°C, it decreases also from 57 Ohm/sq to 38 Ohm/sq as drive-in duration increases from 20 min to 40 min. Active boron dopant profiles measured by electrochemical capacitance voltage (ecv) exhibit surface concentrations below the solid-solubility limit of boron in silicon for all the studied emitters, the maximum surface concentration of 1.3×10^{20} atm./cm^3 is reported on emitter formed at 950°C. The Hall Effect measurement method is used for measuring sheet resistance and sheet carrier concentration.

#P007 - SYNTHESIS AND CHARACTERIZATION OF WOX NANOSTRUCTURES BY LOW-COST METHOD FOR SENSING APPLICATIONS

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Tungsten oxide (WOx) is a transition metal oxide with wide ranging applications, going from ceramics and paints to smart windows.With the advent of nanotechnologies, the synthesis of WOx nanostructures has become increasingly prominent, with a plethora of advantages in sensing and catalysis applications. Indeed, nanostructuring of WOx can enhance the performance of this important functional material and provides it with unique properties that do not exist in its bulk form, with application not only in electrochromic devices, but also for photocatalysis, sensing or recently also solar cells.

It was shown that WOx can be obtained in a range of crystal phases (amorphous, triclinic, monoclinic, hexagonal, orthorhombic), each one with different properties and field of applications. The crystal phase depends on the specific WOx nanostructure and the way by which it is obtained. Investigating the synthesis techniques of nanostructured WOx is hence very important for understanding its fundamental properties as well as its practical applications.

In this work we investigated the realization of WOx nanostructures by low cost electrodeposition methods (combination of pulsed and continuous potentiostatic conditions). The advantage of this processing method is that it is possible to produce nanocrystalline WO3 films at room temperature which are chemically more stable than their amorphous counterparts without any significant loss of electrochromic efficiency or kinetics. The growth parameters (growth time, solution concentration, applied bias, pulse time, ect.) were varied in order to obtain very thin layers and to properly control their self-assembling to form small and low-density well-defined nanostructures. A comparison between continuous and pulsed electrodeposition is performed, evidencing the effect of short, high potential pulses in the particle nucleation process and their following growth with respect to lower voltage continuous deposition. The thermal evolution under post-growth annealing in air or nitrogen atmosphere of the obtained materials is also investigated.

*Keywords:*tungsten oxide, nanostructure, electrodeposition

#P008 - MECHANICAL SPECTROSCOPY OF LIALH4

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The dynamic elastic modulus and internal friction of cold consolidated mixtures of Al and $LiAlH_4$ powders have been measured. On heating, $LiAlH_4$ decomposes into three steps:

(1) $3LiAlH_4 \Rightarrow Li_3AlH_6 + 2Al + 3H_2$ with a 5,3% mass H_2 release

(2) $Li_3AlH_6 \Rightarrow 3LiH + 1{,}5H_2 + Al$ 2,6% with a mass H_2 release

(3) $LiH + Al \Rightarrow LiAl + (½)H_2$ 2,6% with a mass H_2 release

These decomposition reactions occurring in $LiAlH_4$ during a thermal run have been detected as dynamic elastic modulus anomalies and internal friction peaks. These measures prove the effectiveness of mechanical spectroscopy for the study of alanate and provide complementary informations to calorimetric and x-ray diffraction ones.

#P009 - MECHANICAL SPECTROSCOPY OF LIALH4

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Dynamic elastic modulus and internal friction of cold consolidated mixtures of Al and $LiAlH_4$ powders have been measured. Specimens are prepared mixing $LiAlH_4$ powders with Aluminum and then cold consolidating under a uniaxial pressure of about 1 Gpa. The three decompositions occurring in $LiAlH_4$ during a thermal run:

(1) $3LiAlH_4 > Li_3AlH_6 + 2Al + 3H_2$
(2) $Li_3AlH_6 > 3LiH + 1{,}5H_2 + Al$
(3) $LiH + Al > LiAl + (½)H_2$

have been detected as internal friction peaks and dynamic elastic modulus spikes, proving the usefullness of mechanical spectroscopy for the study of alanate.

#P010 - MECHANICAL SPECTROSCOPY OF LIALH4

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The $LiAlH_4$ decompositions with Hydrogen release as a function of temperature have been studied by means of Mechanical Dynamic Spectroscopy, proving the effectiveness of mechanical spectroscopy for the study of alanate. The Hydrogen release occurs into three steps:

(1) $3LiAlH_4 > Li_3AlH_6 + 2Al + 3H_2$ 5,3% mass H_2 release
(2) $Li_3AlH_6 > 3LiH + 1{,}5H_2 + Al$ 2,6% mass H_2 release
(3) $LiH + Al > LiAl + (½)H_2$ 2,6% mass H_2 release

the first at 440-450 K, the second at 480-490 K and the third at 645-670 K, in agreement with values reported into the literature. All decomposition are detected as damping and dynamic elastic modulus anomalies and are complementary to calorimetric and thermogravimetric data.

#P011 - OPTIMIZATION OF TRANSMISSION SEM OBSERVATIONS OF POLYMERIC NANOCOMPOSITES THROUGH VIDEO AMPLIFIER SETTINGS

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Polymeric systems are part of a growing class of materials that appear interesting for their application in several fields as biomedicine, agronomy, flexible electronics, photonics and solar cells[1–3]. In particular, polymer nanocomposites, thanks to the inclusion of nanofillers (Si nanowires, metal-oxide nanoparticles, etc.) are designed to enhance the material properties depending on their distribution, size and composition. The soft nature of many polymers imposes the use of low-energy and non-destructive techniques for morphological and chemical characterization. Scanning Electron Microscope (SEM) can provide both morphological and chemical characterization of such systems thanks to the combination of Secondary Electron imaging and X-ray analyses (EDX). This combined approach has allowed to localize the nanofiller inside the polymeric matrix. Moreover, the implementation of a solid-state detector for transmitted electrons allows also performing Dark and Bright Field images providing atomic number contrast[4]. However, such images can give rise to artefacts, misleading the size and shape evaluation of such polymeric systems depending on video amplifier settings. The influence of the latter one on Transmission SEM (TSEM) observation of chitosan-based nanocomposites is reported. Moreover, we will demonstrate how small variations in both *brightness* and *contrast* can help in distinguishing pure polymeric systems from the nanocomposite, even at low nanofiller concentration. Simultaneous EDX mapping with nanometric resolution further confirm this aspect.

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#P012 - POROUS SILICON LIGHT EMITTING MICROPARTICLES FOR NANOMEDICINE

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Porous silicon (pSi) is a sponge-like nano structured material with peculiar properties, such photoluminescence (PL) in the visible range and large porosity, which are very interesting in perspective of biomedical application, since they allow to use this material as a drug delivery carrier, traceable by imaging. pSi microparticles are produced by anodization etching and sonication of crystalline silicon wafers and successively stabilized for years in ethanol by a light driven carboxyl functionalization.

For biomedical application, pSi microparticles have to be dispersed in an aqueous material, such as PBS. This step quenches completely the PL of the microparticles due to their oxidation. We used two approaches to avoid the degradation and preserve the pSi microparticles properties in biological solution: we covered the porous material with both organic and inorganic coating.

In the first case, we covalently attached organic polymers (i.e. chitosan and PEG, having an average positive and negative surface charge, respectively) and we stabilized the optical properties for several months. In the second case, to reduce the covering layer thickness, we coated the pSi surface by ALD (atomic layer deposition) technique, which allowed to create a thin and uniform TiO_2 layer that stabilizes the optical and structural properties for over 6 months.

We tested this system as a drug carrier, and we used Cbi (a precursor of B2 vitamin) as a test drug. We firstly observed that the drug molecule was not chemically modified by the interaction with the microparticles and then that, in particular for negatively charged particles, a large amount of Cbi could be loaded into the pores and subsequently released with a very slow rate.

We tested the biocompatibility of the pSi microparticles by evaluating the effect of the coated microparticles on human dendritic cells (DCs) through in-vitro tests. For this purpose, DCs were incubated with various pSi microparticle up to 100 µg/mL concentrations and we observed no toxicity effect on the cells neither before nor after the coating. We performed ELISA tests to evaluate the possible activation of the immune response system and release of immunomodulatory cytokines (i.e. IL-6, IL-12 and TNF-alpha). With this intention, we incubated DCs with several concentrations of microparticles, as well as with the well-known bacterial immune cells activator lipopolysaccharide (LPS), as a positive control. We observed no cell activation, but attention has to be paid in an already immune activated system, since the microparticles could potentiate the cytokine release induced by LPS (priming effect). We also verified that the optical properties were maintained inside the cells, by two photon experiments.

With these results, we could conclude that coated pSi microparticles have the chance to be a promising tool in NanoMedicine.

#P013 - TUNING THE OPTICAL PROPERTIES OF FLAME-SYNTHESIZED CARBON NANOPARTICLES

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Carbon-based nanomaterials (CNPs) have attracted considerable interest because of their unique electronic, optical and mechanical properties. Among them, CNPs have become increasingly popular mainly due to their photoluminescence (PL) properties which make them ideal for bio-medical imaging or drug-delivery in addition to light-emitting devices because of their low toxicity, environmental friendliness, low cost and relatively simple synthesis processes.

There are many routes for the synthesis of CNPs divided into top-down nano-cutting methods and bottom-up organic approaches. The first one includes laser ablation, arc discharge, chemical and electrochemical oxidation of large carbon structures; recently, starting from the pioneering work of Liu et al. [1], also the so called “candle soot” turned out to be an excellent precursor for the synthesis of CNPs for a variety of applications [2].

A wide set of studies indicates that the constituents of CNPs in flames are mainly PAHs of moderately size [3, 4]. Furthermore, there is a large body of evidence indicating a change in the electronic and optical properties of CNPs during their early stages of nucleation and growth [5] and recently, Liu et al. [6] demonstrated quantum dots behavior of the CNPs, in the particle range 4-23 nm, directly produced and collected from flames. Therefore, carbon particle nucleation and growth in flames can be exploited as a bottom up process for CNPs through direct sampling CNPs from a well-controlled flame reactor.

In this work particle size has been measured on-line in aerosol phase by a differential mobility analyzer. Particles with different average sizes have been sampled and characterized for the first time by scanning tunneling microscopy/spectroscopy (STM/STS). The electronic properties, i.e., density of states and energy band gap, of flame-formed nanoparticles measured by STS have been correlated to nanostructure determined by Raman spectroscopy and the UV-visible absorption spectra and optical band gap determined by Tauc analysis.

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#P014 - KINETIC UNCERTAINTY RELATION

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We start from a recent theorem of microscopic thermodynamics, pictorially called thermodynamic uncertainty relation (TUR), which forms part of the more general framework of thermodynamic inequalities that arise from the handling of microscopic processes in a non-equilibrium state. More specifically, the above-mentioned theorem puts a bound on the ratio between the average rate of the an out of equilibrium current and the generalized diffusivity (proportional to the variance of the current) times the entropy production rate. However, it was showed that this thermodynamic relation can be obtained in a very general way, namely using a mathematical object called the Kullback-Leibler divergence that, for some particular cases, can be linked to entropy production. We will hence use the latter to obtain a new non-equilibrium inequality for systems modelled by continuous time Markov chains: in fact, performing a simple perturbation on the system's dynamic (namely a linear rescaling of the transition rates) we calculate the Kullback-Leibler divergence that arises from this procedure and show that it is proportional to the dynamical activity of the system, namely the average total number of jumps that the system performs in a given time interval. This final result has been called kinetic uncertainty relation (KUR). Finally we investigate the differences between the TUR and the KUR and analyse the regimes in which they give tighter constraints.

#P015 - OPTICAL COATINGS BASED ON NANO-COMPOSITE DIELECTRIC OXIDES FOR GRAVITATIONAL WAVE DETECTORS

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The first direct observation of gravitational waves was performed by Laser Interferometer Gravitational-wave Observatory (LIGO) on September 14th, 2015 [1]. Being the expected gravitational wave signals extremely weak, the reduction of the noise in the most sensitive frequency band (50-300 Hz) where the first signals have been detected, represents the highest modern challenge of the presently operating detectors (Virgo, LIGOs, Kagra). To date, the predominant noise in the frequency range of interest is due to the thermal noise of the highly reflective optical coatings of cavity mirrors. The design of such mirrors in currently operating interferometers is based on the alternance of two materials with high and low refractive index and thickness equal to a quarter of wavelength $\lambda/4$. Such design can be optimized with respect to the thermal noise, for example, by reducing the thickness of the material with higher optical losses [2,3]. Here, we report a study of innovative reflective optical coatings, based on dielectric oxides (TiO_2, SiO_2, ZrO_2, NbO_2,…), replacing homogeneous layers with stratified nano-composites. As already reported in the literature [4], the main advantage of this strategy is the inhibition of crystallization upon annealing. Indeed, while on the one side the annealing process is necessary to relax intrinsic material stress/strain, to guarantee smooth surfaces and interfaces, and to set-up the correct material stoichiometry, on the other hand it induces the formation of crystallites, which will work as scattering centres for the light, with a consequent blow up of optical losses and thermal noise. Starting from TiO_2, we have combined it with ZrO_2 and SiO_2 in nano-layered structures (by using a Argon plasma-assisted Electron Beam evaporator) , to study crystallization temperature and morphology at different annealing temperatures, through X-Ray diffractometry (XRD), small-angle X-ray scattering (SAXS) and scanning probe microscopy (SPM) techniques.

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#P016 - BIOINSPIRED MATERIALS AND DEVICES: NANOPORES AND NANOPOCKET

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Nature frequently uses self-assembly to orchestrate recognition events. The regulation of recognition events in nature via dynamic and reversible self-assembly of building blocks has inspired the emergence of supramolecular architectures with similar biological activity. Processes of molecular recognition and self-assembly direct the way in which relatively simple building blocks recognize each other, associate and form ordered one-, two-, and three-dimensional nanostructures and macroscopic objects with nanoscale order. The organization of the building blocks into ordered structures is based on specific recognition that is facilitated by a combination of many different non-covalent interactions. This report aims to highlight the diversity of self-assembled nanostructures constructed from mono-disperse synthetic building blocks; with a particular focus on their design, self-assembly, functionalization with bioactive ligands and effects thereof on the self-assembly, and possible applications. Over the past decade, substantial progress has been made in constructing molecular hosts that emulate protein pockets. D,L-Alternating peptides spontaneously folds and assemble producing well-ordered nanostructured under physiological conditions. Thus, the self-assembly properties of these peptides have been exploited for generating bioinspired nanostructures. Here we investigated short D,L-alternating sequences (6,7,8 residues) that show a strong preference to form a turn of β-helical structures. The folded and hemicyclic structures were extensively characterized based on multiple techniques such as one- and two-dimensional NMR, X-ray crystallography and AFM of multilayer LB film, as well as theoretical calculations. As a results a variety of reliably folded, modifiable scaffold can be constructed. The well-defined crescent hemicyclic conformations contain internal cavities having multiple introverted amide oxygen atoms. The availability of these porous molecules has supplied a new class of nanosized building blocks that provide the opportunity of creating the next generation nanostructures capable of presenting multiple functional groups, forming various pores and channels, and finally, developing functionalized matrix.

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#P017 - APPLICABILITY OF A NEW SULFONATED PENTABLOCK COPOLYMER MEMBRANE AND MODIFIED GAS DIFFUSION LAYERS FOR LOW-COST WATER SPLITTING PROCESSES

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Polymer electrolyte membrane (PEM) water electrolysis is one of the most promising technologies for hydrogen production due to its relatively high compactness, simple system, low operating temperature and high efficiency. Moreover, the as produced hydrogen is very clean and the system is well suitable to couple with energy renewable sources. The durability and costs of PEM electrolysers are still the two main barriers for their commercialization. Usually, the membrane is an insulator ionomer characterized by high proton conductivity, low permeability to hydrogen and oxygen, chemical, mechanical and thermal stability, long lifetime, low cost and the capability to be implemented into membrane electrode assemblies (MEAs). Although its high cost, Nafion® isthe most used one due to its high cell performance and long lifetime. Anyway, high performance membranes cheaper than the fluorinated membranes are required.In this study, Nexar™, a sulfonated pentablock copolymer (s-PBC: tBS–HI–sS : S–HI–tBS), has been investigated in a water electrolysis cell and its performance is compared with Nafion itself. Its block architecture structure results in a cheaper polymer with controlled swelling and good mechanical properties in the hydrated state. Nexar™ polymer has been tested as a more economical and efficient alternative to Nafion® membrane for proton exchange membrane (PEM) electrolysis cells. Furthermore, we have studied a new methodology for *modification of gas diffusion layers (GDL) by depositing Pt and TiO_2 nanoparticles at the cathode and anode side, respectively, and a protective polymeric layer on their surface, allowing the improvement of the contact with the membrane. Morphological, structural, and electrical characterization were performed on the Nexar*^{TM} *membrane and on the modified GDLs. The use of modified GDLs positively affects the efficiency of the water electrolysis process. Furthermore, Nexar*^{TM} *showed higher water uptake and conductivity with respect to Nafion*$^{\circledR}$*, resulting in an increased amount of current generated during water electrolysis. In conclusion,we show that Nexar*^{TM} *is an efficient and cheaper alternative to Nafion*$^{\circledR}$ *as the proton exchange membrane in water splitting applications and we suggest a possible methodology for improving GDLs' properties. These results meet the urgent need for low-cost materials and processes for hydrogen production.*

#P018 - AGAROSE/K-CARRAGEENAN-BASED HYDROGEL FILMS WITH NATURAL EXTRACTS FOR THE HEALING OF CUTANEOUS WOUNDS

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Hydrogels are 3D hydrophilic networks that can hold significant amounts of water within their structure, without dissolving in water. They can offer a combination of favorable properties, including high absorbency of biological fluids, biocompatibility, biodegradability, stimuli-responsiveness, high storage capacity and release ability of small and large therapeutic molecules.

The hydrogel films designed for wound dressing may accomplish several functions, playing an important role in the healing processes. They can absorb and retain the wound exudates, stimulating fibroblast proliferation and keratinocyte migration and promoting re-epithelialization. Furthermore, they can incorporate and release bioactive molecules allowing a faster healing process.

In the past years, the materials used to design hydrogel films for wound dressing were synthetic polymers, but more recently natural polymers have been employed as main components of hydrogel dressings for their active involvement in the wound healing process and new tissue regeneration.

The components of the films here proposed are agarose (1.0% w/w) and increasing amount of k-carrageenan (0.5, 1.0 and 1.5% w/w) mixed with glycerol (3% and 5% w/w) used as plasticizer agent, in order to obtain an optimal combination of softness and conformability. During preparation, the polymers were added of natural extracts obtained by *Cryphaea heteromalla* (Hedw.) D. Mohr, a bryophyte species living in the Mediterranean area. The films have been characterized in terms of dynamic rheological properties and ability to absorb fluids. Furthermore, their biocompatibility has been tested in vitro in NIH 3T3 fibroblast cell model.

#P019 - TOWARDS BALLISTIC DEVICES BASED ON GRAPHENE HETEROJUNCTIONS WITH NITRIDE SEMICONDUCTORS

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The heterogeneous integration of two dimensional (2D) materials with group III-Nitride semiconductors (III-N) has been the object of increasing interest in the last years, as it can open the way to novel applications in optoelectronics and high-power/high-frequency electronics [1,2]. Recently, graphene (Gr) junctions with AlGaN/GaN heterostructures have been proposed as a key building block to realize a Gr-Base Hot Electron Transistor (GBHET), i.e., a vertical device relying on the ballistic transport of hot electrons across an atomically thin Gr electrode [3-5]. Such a device concept holds great promise for operation at ultra-high frequencies, i.e. in the THz regime.

In this work, two complementary approaches for fabricating Gr/III-N heterostructures have been explored, i.e. (i) the transfer of Gr grown by chemical vapour deposition (CVD) on catalytic metals [6]; (ii) the direct non-catalytic CVD growth of Gr on AlN and AlGaN/GaN templates on different substrates (Si, SiC, sapphire), as well as on bulk AlN [7].

The morphological and structural properties of the Gr/III-N heterostructures were extensively investigated by the combination of several characterization techniques, including AFM, XRD, STEM/EELS, XPS, LEED, Raman. Furthermore, vertical current transport across the interfaces was investigated by electrical measurements on properly fabricated test patterns and local electrical analyses by CAFM [6]. Finally, the experimental information were compared with ab-initio DFT calculations of the Gr/III-N electronic properties.

The main processes for GBHET fabrication have been developed and characterized, such as Ohmic contacts on Gr and AlGaN/GaN 2DEGs, and the atomic layer deposition (ALD) of ultra-thin high dielectrics (Al_2O_3) on Gr [8,9]. Finally, prototypes of GBHET transistors based on Gr/AlGaN/GaN heterostructures have been fabricated, and their electrical characteristics have been compared with theoretical predictions in the case of ballistic transport through the Gr base layer.

These results are important advances towards the assessment of a Gr/Nitrides hybrid technology for future high frequency electronics.

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#P020 - KERATIN-POLYVINYLPYROLIDONE-CINNAMON ESSENTIAL OIL ELECTROSPUN NANOFIBERS AS NATURAL-BASED SMART WOUND DRESSINGS

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The last years a lot of research is dedicated to the deeper understanding of the wound healing process. Systems that can actively control the spatial and temporal profile of drug release have been shown to be beneficial for wound treatment. Innovative smart wound dressings should possess biocompatibility, in order to avoid any toxicity toward the wound tissues and they should be able to accelerate the healing process, while at the same time maintaining the wound bed clean, acting as a shield against further infections. Ideally, wound healing dressings should be resorbed by the wound bed, in order to avoid repeated injury upon removal.

Keratin is the most abundant structural protein of the epithelial cells and one of the most important biopolymers, presenting suitable features for cell attachment and growth.The abundance and the natural biocompatibility of keratin make it an ideal material for a range of applications in bioengineering, including wound healing. Furthermore, the incorporation of natural bioactive substances into keratin-based materials lead to the release of the substance in a controlled way, ameliorating the healing process. Such bioactive substances include essential oils, that are well-known for their biological properties and their encapsulation in polymeric matrices has been generally investigated. Amongst them, cinnamon essential oil has been shown antimicrobial and antioxidant activities and its beneficial activity has been proved in a range of applications, ranging from cosmetics to medicines.

Based on the above, wool-extracted keratin was combined with polyvinylpyrrolidone and different concentrations of cinnamon essential oil to create aqueous emulsions for subsequent green electrospinning, in order to obtain a biocompatible composite material with controlled release of active compounds of the essential oil. The morphology, physicochemical properties and stability of the electrospun nanofibrous matrices containing cinnamon essential oil were thoroughly investigated. Notable is the fact that the matrices containing cinnamon essential oil showed enhanced mechanical properties. The electrospun composite mats were shown to be biocompatible, exhibiting strong antioxidant activity. Furthermore, the composites were shown to present enhanced antibacterial activity against Gram (+) (*Staphylococcus aureus*) and Gram (-) (*Escherichia coli*, *Pseudomonas aeruginosa*) bacterial strains, qualifying the material as a potential smart wound dressing.

#P021 - TOPOLOGICALLY-INDUCED ATOM-PHOTON BOUND STATES

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Formation of atom-photon bound states is typical in coupled-cavity arrays interacting with quantum emitters.

Here, considering a coupled-cavity array with staggered inter-cavity couplings, i.e. a photonic SSH, we show that a bound state appears also when the atomic energy lies in the energy gap.

This bound state possesses the topological properties of the edge state of the cavity.

Due to these properties, when two atoms are coupled to the cavity in the weak coupling regime, an effective long-range and decoherence-free interaction between the atoms arises.

#P022 - ELECTRICAL CHARACTERIZATION OF FLAME-SYNTHESIZED CNP AND CNP/TIO2 THIN FILMS

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Incipient carbon nanoparticles, CNP, formed by incomplete hydrocarbon combustion are composed of polycyclic aromatic hydrocarbons [1,2] and exhibit a quantum dot behavior [3], which make them ideal for a wide range of applications.

Flame synthesis offers a continuous and low-cost process for producing inorganic nanoparticles, such as TiO2, with fine control of cristallinity and phase. Likewise, carbon nanoparticles, CNPs, with tailored size and optical and electronic properties can be produced by optimizing the flame process. The assembly of nanoparticles into a uniform thin film with precise control over chemical and physical properties poses a significant challenge. Thermophoretic sampling relies on the thermophoretic forces driving the particles in the hot flame towards a cold substrate inserted in the flame and can be used to produce nanostructured, self-assembled films that can lead to novel applications.

In this work, CNP and CNP/TiO2 nanoparticles have been produced in premixed ethylene-air flames and thin films have been realized by thermophoretic deposition on silicon substrates with gold interdigitated electrodes.

Scanning mobility particle sizer furnished the particle size distribution and Raman and optical spectroscopy chemico-physical and structural information.

The electrical characterization of the films was conducted by measuring the IV characteristics which shows a good linearity in the interval [-5 V, 5 V] whereas non-linear phenomena appear for wider voltage ranges and hysteresis phenomena are also observed in carbon/TiO2 films. Impedance spectroscopy was used to investigate the films with respect to their microstructure. This method is indeed particularly useful for nanostructured films with inter-grain and grain-edge impedances and capacities. Finally, noise spectral density at low and very low frequency was measured to investigate the electron transport. The main source of noise is of thermal type for the carbon material, whereas carbon/TiO2 film shows a Fliker type, 1/f noise, consistent to a larger amount of localized states responsible for trapping/detrapping processes of charge carriers and charge fluctuations during the conduction process.

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#P023 - FACILE SYNTHESIS OF POROUS NI OXIDE FILM FOR SENSING APPLICATIONS

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Among the most promising metal oxide nanostructures, Ni-based ones are widely studied for potential application in sensing and catalysis application, due to their low-cost fabrication and high performances. Various forms of Nickel Oxides have been adopted in sensing probes, for instance, hollow microspheres, nanoparticles, nanoflakes, nanowires, and nanosheets. Nanowalls are an ideal three-dimensional (3D) nanostructure composed of nanosheet arrays that are vertically aligned on a substrate. They exhibit excellent physical and chemical properties due to their open geometry, high porosity, large surface area, and a substantial framework structure. In this work, NiO nanowalls are obtained through Chemical Bath Deposition (CBD) on Si substrates followed by thermal annealing at 350°C. The surface morphology and thickness of samples have been characterized by scanning electron microscopy (SEM). All the samples are characterized by an open nanoporous film, partially covered by porous NiO nanospheres grown by homogenous nucleation during the CBD and landed on the film. A strategy for optimization of NiO nanowalls film for large area application is pursued by reducing the density of the NiO nanospheres. Moreover, the synthesis of the porous NiO film has been modified for application in sensing fields.

#P024 - INDIVIDUAL AND ENSEMBLE LIFETIMES OF HIGH-LYING RB RYDBERG STATES

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Rydberg atoms have become a versatile tool for atomic physics, quantum optics and quantum information in recent years. Their strong van-der-Waals and dipole interactions and long lifetimes make them ideally suited, *e.g.*, to creating large optical nonlinearities and to simulating the dynamics of many-body systems. For high-lying Rydberg states, however, transitions between neighbouring

Rydberg states induced by black-body radiation [1] become an important process that can strongly affect the experimental outcomes.

In order to study those processes for Rydberg states with principal quantum number n>60, for which state-selective field ionization becomes difficult to apply, we use a hybrid method involving state-selective depumping via a fast-decaying intermediate state [2], and field ionization. This allows us to measure both the individual lifetime of an individual target Rydberg state and that of the ensemble of Rydberg states populated via black-body radiation.

We find that for Rydberg S states the individual lifetimes agree well with theoretical predictions up to n=90, but deviate substantially for higher n (we also find large deviations for smaller n when the background electric field in our experimental cell, of order 200 mv/cm, is not sufficiently compensated). The ensemble lifetimes agree with a numerical model including all possible black-body induced transitions and essentially approximate the target state lifetime at zero temperature. For Rydberg D states, we find large deviations from the theoretical predictions between n=60 and n=90. Possible reasons for the deviations in the S and D states are currently under investigation, including modifications of the Planck formula for the black-body spectrum [3] due to the finite sizes of the surrounding structures (cell, external supports), which are of the same order of magnitude (several centimetres) as the wavelength of the relevant transitions in the microwave region.

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#P025 - QUANTUMNESS AND MEMORY OF AN OPEN QUBIT UNDER CLASSICAL CONTROL

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Hybrid quantum-classical systems constitute a promising architecture for useful control strategies of quantum systems by means of a classical device. Here we provide a comprehensive study of the dynamics of various manifestations of quantumness with memory effects, identified by non-Markovianity, for a qubit controlled by a classical field and embedded in a leaky cavity. We consider both Leggett-Garg inequality and quantum witness as experimentally-friendly indicators of quantumness, also studying the geometric phase of the evolved (noisy) quantum state. We show that, under resonant qubit-classical field interaction, a stronger coupling to the classical control leads to enhancement of quantumness despite a disappearance of non-Markovianity. Differently, increasing the qubit-field detuning (out-of-resonance) reduces the nonclassical behavior of the qubit while recovering non-Markovian features. We then find that the qubit geometric phase can be remarkably preserved irrespective of the cavity spectral width via strong coupling to the classical field. The controllable interaction with the classical field inhibits the effective time-dependent decay rate of the open qubit. These results supply practical insights towards a classical harnessing of quantum properties in a quantum information scenario.

#P026 - RHEOLOGICAL PROPERTIES OF COMPOSITE SOFT COLLOIDS IN THE MICROCHANNEL

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The concept of creating magnetic filaments (semiflexible polymer-like chains of magnetic nanoparticles permanently crosslinked with polymers) has existed for many decades. The advantage of such magnetic supramolecular polymers is that they can be used as an alternative to nanoparticles in magnetic fluids to obtain a desired and easily controlled response. The shape and size of filaments allow filtration and mixing in systems which size does not exceed hundreds of nanometers. In this contribution, using Langevin dynamics simulations, first we focused on solutions of filaments, the magnetic nanoparticles in which are not only interacting via dipole-dipole potential, but also via short-range attractive forces (Lennard-Jones type). Such filaments tend to aggregate in dense spherical droplet-like clusters. The resulting composite soft colloid is placed in the microchannel, where its behavior in the shear flow is investigated, varying a wide range of system parameters. The thickness of the channel varies from the one comparable to the size of the nanocomposite magnetic particle to that of 10 radii of gyration. Two values of the magnetic interaction intensity are selected, that correspond to two regimes: the dipole energy is comparable to the thermal one, and the dipole energy is several times higher than the thermal energy. We also studied several shear-rates. We find the relationship between magnetic forces, central attraction and shear-rates at which the cluster deforms but does not break and eagerly follows the flow. This way we study the possibility of transport-based applications based on the soft colloids made through self-assembly of magnetic filaments.

#P027 - ORDERED ADSORPTION AND DEMETALLATION OF ZINC-PHTHALOCYANINE ON AL(100)

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In recent years, thin films of organic molecules have attracted increasing interest. Among them, thin films of metal-phthalocyanines (MPcs) deposited on solid state substrates are of importance. MPcs can absorb light in the visible range and this makes MPc heterostructures particularly useful for optoelectronic applications, like solar energy conversion or organic-light-emitting diodes (OLEDs) production. In all areas of utilization, the electronic and structural properties of those complex structures play a crucial role. They depend, not only on the intrinsic properties of the constituents, but also on the molecule-molecule and molecule-solid interaction.

In this work zinc-phtalocyanine (ZnPc) molecules were thermally deposited on Al(100) surface. The chemical and electronic properties and the ordering of the molecular films were investigated by combining photoemission spectroscopy (PS) and low energy electron diffraction (LEED).

As for CuPc/Al(100) [1], at low coverage (1 ML), a sizable charge transfer from the substrate to the molecules is observed, this indicating a strong interaction at the organic-inorganic interface. However, this does not prevent diffusion of the molecules and ordering on the substrate. LEED patterns clearly show a (5x5) reconstruction, characteristic of flat-lying molecules forming a long-range-ordered structure with square unit cell. The degree of ordering (i.e. the average domain size) is increased when the substrate is held above 100 C during the deposition. As a consequence of the thermal treatment the zinc atom (held in the ZnPc central cavity) is removed and diffuses into the aluminum substrate. This chemical modification does not affect π-conjugation leaving the molecular structure intact.

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#P028 - COMPACT MODULES FOR DIGITAL HOLOGRAPHIC MICROSCOPY IN MICROFLUIDICS: FEATURES AND DESIGN SOLUTIONS FOR POINT OF CARE DIAGNOSTICS

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The development of Lab-on-a-Chip (LoC) devices has experiences a steady growth in the last years. Their diffusion is promoted by the introduction of accurate and cheap technologies to fabricate microfluidic platforms and to control and manipulate fluids and micro-particles. At the same time, the research community is striving to transfer more and more of the functionalities of a modern analysis laboratory on LoC platforms. One of the most promising applications of these compact systems is the possibility to introduce point-of-care diagnostics in low-resource settings, where adequate instruments, costly facilities, and clinical laboratories for accurate analysis are still missing. Clearly, the possibility to observe the samples inside the LoC platforms is fundamental to fully express the diagnostic potentialities of these devices. In particular, a suitable imaging system should satisfy different needs: high-throughput data collection, label-free imaging, quantitative measurements and compactness. The first three requirements are necessary to obtain statistically relevant and informative data from biological samples.In this framework, Digital Holography (DH) microscopy is an interesting technique, able to provide quantitative phase information of the samples by label-free image acquisition. However, standard DH setups do not conform to the requirements of compactness and portability.

In this work, we present a compact module that reproduced the interferometric setup needed in off-axis DH microscopy on a commercial LoC. Thanks to the inscription of a diffraction grating onto the chip surface, it is possible to split a single incoming wave in an object and reference beam. We have investigated different configurations, positioning the grating parallel and orthogonal to the sample flow inside the channel. We have shown that the amplitude and quantitative phase imaging features of DH, as well as its flexible focusing capabilities, are preserved in the proposed module. Moreover, we have highlighted how the two configurations suit different needs. Then, we have presented a fully integrated version of the module, obtained by printing a polymer lens onto the chip. The resulting pocket module is well suited to point-of-care diagnostic application, thanks to its improved compactness and portability. As an exemplary case of use, we tested a spatio-temporal scanning acquisition modality to yield high-throughputcounting and 3D tracking of Red Blood Cells. We further improve our system portability by using a compact coherent source, namely a laser diode. Our work thus show that it is possible to realize a compact and cost-effective imaging module for high-throughput screening of fluid samples, which, among other applications, could be used to increase the diagnostic capabilities in resource-limited settings.

#P029 - 1/F CRITICAL CURRENT NOISE IN SHORT BALLISTIC GRAPHENE JOSEPHSON JUNCTIONS

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Short ballistic graphene Josephson junctions sustain superconducting current with a non-sinusoidal current-phase relation up to a critical current threshold. The current-phase relation, arising from proximitized superconductivity, is gate-voltage tunable and exhibits peculiar skewness observed in high-quality graphene-superconductors heterostructures with clean interfaces. These properties make graphene Josephson juncions promising sensitive quantum probes of microscopic fluctuations underlying transport in two-dimensions. We demonstrate that fluctuations with 1/f power spectrum of the critical current of a short ballistic graphene Josephson junction directly probe carrier density fluctuations of the graphene channel induced by carrier traps in nearby oxides. Tunability with the chemical potential, close to and far from the charge neutralty point, and temperature dependence of the noise amplitude are clear fingerprints of the underlying material-inherent processes. These results provide also relevant figure of merits in view of the envisaged implementation of coherent quantum circuits in hybrid quantum information architectures.

#P030 - CROSSOVER FROM FAST TO SLOW DYNAMICS IN A LONG RANGE INTERACTING ISING CHAIN

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Quantum many body systems with long range interactions are known to have a lot of fascinating properties that can be detected experimentally which are however hard to describe theoretically. In this paper we present a cluster mean field method and three different applications to the dynamics of quantum Ising chains with power law interactions. First we derive the equilibrium phase diagram as a function of the power law exponent. Then we will study the steady state attained after a linear quench of the transverse field showing the emergence of three regimes: the quench regime, the intermediate regime and the annealing one. To conclude we will show that the method is affected by finite size problems whenever we use it to investigate non uniform spin configurations.

#P031 - FABRICATION OF AUPD NANOPARTICLES ON TRANSPARENT AND CONDUCTIVE SUBSTRATE BY LASER DEWETTING OF BIMETALLIC FILMS

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The generation of metallic nanostructures on surfaces is a thrust in materials science from scientific viewpoint and technological applications in areas such as catalysis, photonics, plasmonics, solar cells, etc. [1]. In particular, bimetallic nanoparticles (NPs) are attracting a large interest due to the possibility to largely tune their properties by the control of the relative composition, in addition to size and shape [1-4]. In this framework, AuPd alloys are frequently used as catalysts since Pd is an excellent catalyst whose activity and selectivity can be significantly enhanced by the addition of Au [1-4]. Furthermore, recently, AuPd NPs are attracting large interest due to the synergic effect of the two combined metals, being Au an excellent plasmonic material, and Pd an excellent catalytic material.

Starting from these considerations, in this work we report on a simple, versatile, cost-effective methodology to produce AuPd NPs directly on a transparent and conductive substrate. In particular, the AuPd NPs are formed on Fluorine-doped tin oxide (FTO)/glass by nanosecond-pulsed laser irradiation induced dewetting process of deposited AuPd bimetallic films. We report on the effect of the surface topography of the substrate on the dewetting process and, so, on the final mean size of the NPs. In fact, we used two supporting FTO substrates differing in the surface topography: we used a FTO layer which is un-intentionally patterned since it is formed by FTO pyramids randomly distributed on the glass slide. We used, also, an additional FTO substrate, presenting, as result of a chemical etching, a higher roughness The results concerning the size of the obtained AuPd NPs show that the substrate topography strongly impacts on the dewetting process, driving the NPs formation and determining their sizes, for AuPd film thickness above a critical value. Below this critical value, the NPs obtained on the two different substrates present, instead, similar sizes. In this last case, then, the dewetting process is not influenced by the substrate topography since the film does not interact with the substrate topography. These results are quantified and discussed by the description of the substrate topography effect on the excess of chemical potential driving the dewetting process.

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#P032 - COMPUTER SIMULATION OF THE STRUCTURE AND CARGO RELEASE PROPERTIES OF SIMPLE AND CORE-SHELL NANOGELS CREATED BY RANDOM POLYMER CROSSLINKING UNDER CONFINEMENT

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Colloidal gel particles consist of a diluted network of crosslinked polymers—*i.e.*, a gel structure—with characteristic sizes ranging from few tens to 100 nanometers, in the case of the smallest particles (nanogels), and up to 100 micrometers in the case of largest ones (microgels). Thanks to a set of unique properties derived from their internal structure and size, including high porosity and very strong structural response to external stimuli, these soft particles are one of the most interesting building blocks of smart materials [1].

The great potential of nanogel and microgel particles has stimulated the development of numerous techniques for their synthesis and experimental characterization, with an increasing degree of control on their size and response [2]. However, the complexity of these systems still represents a challenge for their theoretical modeling. Most purely analytical models disregard their internal polymer network structure, using continuum descriptions that can not capture accurately detailed properties, especially in case of particles with complex structural inhomogeneities. In principle, the precise topology of their internal polymer network could be incorporated into computer simulation models, but such topologies can not be fully resolved experimentally with available methods. On the other hand, lengths and time scales involved in their synthesis and responsive behavior are still too costly for fully atomistic descriptions. Therefore, most computer models are based on coarse-grained representations, with strong approximations and/or top-down descriptions of their internal structure. Only very recently first steps towards more realistic representations of their internal structure in computer models have been taken [3].

Among such recent computer models there is the one we introduced for colloidal gel nanoparticles synthesized by random crosslinking of polymer precursors confined in emulsion nanodroplets [4]. With this model we study the effects of degree of crosslinking and droplet confinement on the internal structure of the resulting nanogel particles, comparing the cases of single-step and two-step crosslinking of core-shell systems. The impact of the internal structure on the diffusion and escape of small tracer particles within the nanogels is also studied. This is relevant for the use of these materials as drug delivery systems.

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#P033 - ELECTRICAL PROPERTIES OF OHMIC CONTACTS AND GATE DIELECTRICS ON CUBIC SILICON CARBIDE

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Cubic silicon carbide (3C-SiC) is often regarded as a good material for power electronics. However, compared to the mature hexagonal polytype (4H–SiC), 3C-SiC technology still suffers from the influence of the material quality. In this context, metallizations and dielectrics are important building blocks of 3C-SiC power devices (e.g., diodes, MOSFETs), which deserve to be investigated.

This work reports on the development and characterization of Ohmic metallizations and gate dielectrics on 3C-SiC layers grown on Si(111) substrates.

The Ohmic contact formation was achieved both on n-type and p-type type 3C-SiC, employing annealed Ni and Ti/Al/Ni layers annealed at 950°C. The 3C-SiC layers were epitaxially grown onto Si substrates by MOCVD. Circular TLM (C-TLM) structures were used for electrical characterization of the contacts and of the 3C-SiC layers. The formation of different phases at the interface and/or in uppermost part of the reacted metal layer (e.g., Ni_2Si, Al_3Ni_2, TiC,...) was correlated with the changes of the electrical and morphological properties of the contacts. The specific contact resistance was in the range 10^{-3}-10^{-5} Ω cm^2 , depending on the doping level of the 3C-SiC.

Several structural and morphological analyses (XRD, AFM, TEM) have been used to get information on the microstructure of the metal layers, correlating phases formation with electrical behavior of the contacts.

On the other hand, the electrical properties of thermally grown SiO_2 layers were studied by means of I-V and C-V analyses of MOS capacitors. The thermal SiO_2 growth rate resulted to be dependent on the different surface roughness. A rate of approximately 25 nm/h have been calculated. Moreover, a high density of positive charge have been detected, independently of the roughness. The sample having the smooth surface, subjected to Chemical Mechanical Polishing, showed an improved dielectric breakdown field.

The electrical measurements allowed to estimate values of interface state density in the order of 4-8×10^{12} cm^{-2}eV$^{-1.}$ A negative shift of the flat band voltage was observed in the MOS capacitors, likely due to the presence of positive charged donor states in the material.

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#P034 - FULLY INKJET PRINTED 2D MATERIAL FIELD-EFFECT HETEROSTRUCTURES FOR WEARABLE AND TEXTILE ELECTRONICS

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olution processing of graphite and other layered materials provides low-cost inks based on two-dimensional (2d) material enabling printed electronic devices [1]. Fully inkjet printed active heterostructures based on 2d materials have been demonstrated on polyethylene-terephthalate (PET) and textile using graphene and hexagonal-boron nitride (h-BN) inks, achieving a field effect mobility of $\mu \sim 91 \pm 29$ cm^2 V^{-1} s^{-1} [2]. However, the complexity of the layered arrangement and the lack of suitable *p*-type and *n*-type semiconducting 2d material inks has impeded the fabrication of active high on/off ratio (> 10) field-effect devices with fully-printed 2d heterostructures [3]. In this work, we demonstrate fully inkjet printed 2d material active heterostructures using MoS_2 and h-BN inks, and use them to fabricate all inkjet printed flexible *p*-type field effect transistors (FETs) on textile, reaching a field effect mobility of $\mu \sim 14 \pm 29$ cm^2 V^{-1} s^{-1} and on/off ratio of 10^4 on polyester fabric, at low operating voltages (< 5 V) The devices maintained their performance even under ~4% tensile strain and showed stable operation for periods up to 2 years, indicating the two-fold role of the h-BN layer as a flexible dielectric and encapsulant. The viability of our process for printed and flexible electronics is demonstrated by fully inkjet printing electronic circuits, such as reprogrammable volatile memory cells, complementary inverters, and OR logic gates with graphene/h-BN and MoS_2/h-BN FETs.

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#P035 - ESTIMATING SPECIES RICHNESS AND MACRO-PATTERNS FROM LOCAL PRESENCE-ABSENCE DATA

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Biodiversity provides support for life, vital provisions, regulating services and has pos- itive cultural impacts. It is therefore important to have accurate methods to measure biodiversity, in order to safeguard it when we discover it to be threatened. For practical reasons, biodiversity is usually measured at fine scales whereas diversity issues (e.g. conservation) interest regional or global scales. Moreover, biodiversity may change across spatial scales. It is therefore a key challenge to be able to translate local information on biodiversity into global patterns.

In addition, many databases give no information about the abundance of a species within an area, but only its occurrence in each of the surveyed plots. Here we present an analytical framework to infer species richness and abundances at large spatial scales in biodiversity-rich ecosystems when species presence/absence information is available on various scattered samples (i.e. upscaling).

This framework is based on the scale-invariance property of the negative binomial. Our approach allows to infer and link within a unique framework important and well- known biodiversity patterns of ecological theory, such as the Species Accumulation Curve (SAC), the Relative Species Abundance (RSA) as well as a new emergent pattern, the Relative Species Occupancy (RSO). Our estimates are robust and accurate, as confirmed by tests performed on both in silico-generated and real forests. Expanding the ability to upscale species richness and obtain abundance distributions from presence-absence data is of fundamental importance in many contexts, where abundance information are not available or trustable. This is particularly true for microbial or marine (e.g. plankton) ecological data obtained from metagenomics and 16S ribosomal gene sequences. The use of sequence-based taxonomic classification of environmental microbes has exploded in recent years and these approaches are becoming a standard method for characterizing the biodiversity of both prokaryotes and eukaryotes. Thanks to advance in high throughput sequencing we begin to be able quantifying the vast number of microbes in our environments, expanding our knowledge on microbial diversity. However, large fractions of the sequence reads remain unclassified and also species abundance estimated have a very high uncertainty. Thus, being able to estimate species richness and abundance distributions from species occurrence data may lead to a big step-forward in the taxonomic classification of microbial ecosystems.

#P036 - MONOLITHIC LITHIUM NIOBATE CHIP FOR LAB-ON-A-CHIP APPLICATIONS

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Since the growing interest in Lab-On-a-Chip (LOC) application, the integration of multiple stages on the same platform was one of the main challenge. The purpose of this work is to present lithium niobate ($LiNbO_3$) as an effective monolithic substrate for multifunctional integrated LOC. $LiNbO_3$ is an electro-optic material well known in the field of integrated optical devices, thanks to its unique combination of optical and structural properties. Recently lithium niobate has been also proposed as candidate for application in opto-microfluidic technology, thus combining the tools typical of microfluidics with the potentialities offered by this material, such as piezoelectricity for acoustofluidic stage or photorefractivity for photovoltaic tweezers.

Nevertheless, its application in Microfluidic always required a matrix, where combine the interesting features of $LiNbO_3$ and coupling it with standard stage of LOC, like microfluidic circuitry and integrated optical probe. Herein, we will present the first device with an optical probe and a microfluidic circuit integrated in the same monolithic substrate of lithium niobate. We combine the well-known application of $LiNbO_3$ in the field of integrated optics to realize Ti-waveguide coupled with a cross-shape microfluidic channel.Two waveguide are realized on the two side of the microchannel: one for the illumination, one for the collection of the transmitted light across the channel. Both waveguide are self-aligned and their output/input are exposed on the microfluidic channel. The technique used for the channel realization consisted in engraving by means of a circular saw. The engraved geometry allows the chip to work both in a mono-dispersed configuration, and also either as T-junction or as cross-junction droplet generator. In particular, the device aims to generate droplet and to perform on-site optical sensing processes such as those required in chemical and biological analysis, using a monolithic highly integrated chip. Indeed this opto-fluidic platform were tested for different optical investigation of droplet content and properties: index of refraction, pH using indicators, shape, length and curvature. Thus paving the way for the realization of a multifunctional and highly integrated LOC in lithium niobate, combing the studied core building block (droplet generator and optical sensor) with the numerous applications in Microfluidic.

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NOCENTE MASSIMO	#172	PLASMA PHYSICS 2	02 WED
NOTARNICOLA SIMONE	#323	QUANTUM SIMULATIONS, SENSING AND METROLOGY	04 FRI
OSSI PAOLO	#027	PHYSICS TECHNOLOGIES FOR HEALTH	30 MON
OSSI PAOLO	#264	NANOPHOTONICS AND PLASMONICS	03 THU
PACE SIMONA	#082	LOW-DIMENSIONAL MATERIALS 3	01 TUE
PACILE' DANIELA	#008	LOW-DIMENSIONAL MATERIALS 1	30 MON
PAGLIARULO VITO	#072	CULTURAL HERITAGE 1	01 TUE
PALIVAN CORNELIA	#254	BIOPHYSICS, BIOMEDICINE AND MODELING 3	03 THU
PALMA MASSIMO	#306	OPEN QUANTUM SYSTEMS	03 THU
PALMISANO LEONARDO	#195	MATERIALS FOR ENVIRONMENTAL APPLICATIONS 2	02 WED
PAOLONI DANIELE	#289	ORGANIC ELECTRONICS	03 THU
PAPAGNO MARCO	#345	TOPOLOGICAL MATTER	04 FRI
PASCARELLI SAKURA	#326	PHYSICS OF AND WITH FREE ELECTRON LASERS	04 FRI
PASQUALE DIGREGORIO	#193	OUT OF EQUILIBRIUM STATISTICAL PHYSICS 2	02 WED
PASQUALE STEFANIA	#126	CULTURAL HERITAGE 2	01 TUE
PASQUALI LUCA	#288	ORGANIC ELECTRONICS	03 THU
PASTORE MARIACHIARA	#047	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 2	01 TUE

PELLEGRINO FRANCESCO MARIA DIMITRI	#273	QUANTUM FLUIDS OF ATOMS AND LIGHT	03 THU
PEPE FRANCESCO	#151	QUANTUM INFORMATION PHYSICS AND TECHNOLOGIES 1	02 WED
PERALI ANDREA	#293	SUPERCONDUCTIVITY 2	03 THU
PEREIRA CARDOSO CLAUDIA MARIA	#080	LOW-DIMENSIONAL MATERIALS 3	01 TUE
PETRELLI ISABELLA	#067	OUT OF EQUILIBRIUM STATISTICAL PHYSICS 1	01 TUE
PEZZI ORESTE	#104	PLASMA PHYSICS 1	01 TUE
PIATTI ERIK	#248	SUPERCONDUCTIVITY 1	03 THU
PICCININ SIMONE	#046	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 2	01 TUE
PICCITTO GIULIA	#191	OUT OF EQUILIBRIUM STATISTICAL PHYSICS 2	02 WED
PICONE ANDREA	#003	LOW-DIMENSIONAL MATERIALS 1	30 MON
PIETRALUNGA SILVIA MARIA	#016	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 1	30 MON
PISANELLO FERRUCCIO	#157	PHYSICS MEETS THE BRAIN: BIOPHYSICAL APPROACHES TO THE NEUROSCIENCE	02 WED
POLIMENO PAOLO	#266	NANOPHOTONICS AND PLASMONICS	03 THU
POLITI GIUSEPPE	#074	CULTURAL HERITAGE 1	01 TUE
POLVERINI EUGENIA	#187	BIOPHYSICS, BIOMEDICINE AND MODELING 2	02 WED
PONTIROLI DANIELE	#090	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 3	01 TUE
PRANDO GIACOMO	#235	STRONGLY CORRELATED SYSTEMS AND SPINTRONICS 1	03 THU
PRESTIPINO SANTI	#274	QUANTUM FLUIDS OF ATOMS AND LIGHT	03 THU
PRIVITERA LORENZO	#249	SUPERCONDUCTIVITY 1	03 THU
PRIVITERA STEFANIA	#241	NOVEL SEMICONDUCTORS AND APPLICATIONS 3	03 THU
PROFETA GIANNI	#292	SUPERCONDUCTIVITY 2	03 THU
PRONTERA TANIA	#285	ORGANIC ELECTRONICS	03 THU
PUGLISI ROSARIA A.	#086	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 3	01 TUE
PUTTI MARINA	#247	SUPERCONDUCTIVITY 1	03 THU
QUARTA GIANLUCA	#120	CULTURAL HERITAGE 2	01 TUE
RAPISARDA MATTEO	#284	ORGANIC ELECTRONICS	03 THU
RICCO GALLUZZO FABIO	#091	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 3	01 TUE
RICCO' MAURO	#087	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 3	01 TUE
RIDOLFO ALESSANDRO	#219	QUANTUM INFORMATION PHYSICS AND TECHNOLOGIES 2	03 THU
RIGHI GIULIA	#199	MATERIALS FOR ENVIRONMENTAL APPLICATIONS 2	02 WED
RIPANTI FRANCESCA	#014	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 1	30 MON
ROCCATI FEDERICO	#312	OPEN QUANTUM SYSTEMS	03 THU

ROMAGNOLI MARCELLO	#052	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 2	01 TUE
ROMANO VITTORIO	#174	ADVANCED COMPUTATIONAL METHODS 2	02 WED
RONDA LUCA	#260	BIOPHYSICS, BIOMEDICINE AND MODELING 3	03 THU
RONTANI MASSIMO	#076	LOW-DIMENSIONAL MATERIALS 3	01 TUE
ROSA ANGELO	#180	BIOPHYSICS, BIOMEDICINE AND MODELING 2	02 WED
ROSENBERG MARGARET	#058	ACTIVE AND SOFT MATTER AND FLUIDS 2	01 TUE
ROSSELLA FRANCESCO	#138	NANOSTRUCTURES AND NANOTECHNOLOGIES 1	01 TUE
ROSSINI DAVIDE	#271	QUANTUM FLUIDS OF ATOMS AND LIGHT	03 THU
ROSTAMI HABIB	#265	NANOPHOTONICS AND PLASMONICS	03 THU
RUFFINO FRANCESCO	#227	NANOSTRUCTURES AND NANOTECHNOLOGIES 3	03 THU
RUGGERI FRANCESCO SIMONE	#258	BIOPHYSICS, BIOMEDICINE AND MODELING 3	03 THU
RUSSO ROBERTO	#085	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 3	01 TUE
SAITTA ANTONINO MARCO	#333	MATTER IN EXTREME AND METASTABLE CONDITIONS	04 FRI
SALA ALESSANDRO	#002	LOW-DIMENSIONAL MATERIALS 1	30 MON
SANCATALDO GIUSEPPE	#186	BIOPHYSICS, BIOMEDICINE AND MODELING 2	02 WED
SANTORO GIUSEPPE	#313	QUANTUM INFORMATION PHYSICS AND TECHNOLOGIES 3	04 FRI
SANTORO MARIO	#334	MATTER IN EXTREME AND METASTABLE CONDITIONS	04 FRI
SANZARO SALVATORE	#017	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 1	30 MON
SARTORI PAOLO	#098	ACTIVE AND SOFT MATTER AND FLUIDS 3	01 TUE
SASSETTI MAURA	#338	TOPOLOGICAL MATTER	04 FRI
SATTA ALESSANDRA	#071	CULTURAL HERITAGE 1	01 TUE
SAVASTA SALVATORE	#272	QUANTUM FLUIDS OF ATOMS AND LIGHT	03 THU
SBRAGAGLIA MAURO	#092	ACTIVE AND SOFT MATTER AND FLUIDS 3	01 TUE
SCALESE SILVIA	#127	MATERIALS FOR ENVIRONMENTAL APPLICATIONS 1	01 TUE
SCANDURRA ANTONINO	#030	PHYSICS TECHNOLOGIES FOR HEALTH	30 MON
SCANDURRA ANTONINO	#243	NOVEL SEMICONDUCTORS AND APPLICATIONS 3	03 THU
SCHIATTARELLA CHIARA	#183	BIOPHYSICS, BIOMEDICINE AND MODELING 2	02 WED
SCHILIRO' EMANUELA	#145	NOVEL SEMICONDUCTORS AND APPLICATIONS 1	01 TUE
SCHILIRO' EMANUELA	#006	LOW-DIMENSIONAL MATERIALS 1	30 MON
SCHIRO' GIORGIO	#255	BIOPHYSICS, BIOMEDICINE AND MODELING 3	03 THU
SCIUTO ALBERTO	#178	ADVANCED COMPUTATIONAL METHODS 2	02 WED
SCIUTO ALBERTO	#245	NOVEL SEMICONDUCTORS AND APPLICATIONS 3	03 THU
SCUDERI MARIO	#278	STRONGLY CORRELATED SYSTEMS AND SPINTRONICS 2	03 THU

SENGUPTA DIPANJAN	#050	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 2	01 TUE
SERAFINI LUCA	#327	PHYSICS OF AND WITH FREE ELECTRON LASERS	04 FRI
SERVIDIO SERGIO	#170	PLASMA PHYSICS 2	02 WED
SETTINERI ALESSIO	#153	QUANTUM INFORMATION PHYSICS AND TECHNOLOGIES 1	02 WED
SETTINERI ALESSIO	#310	OPEN QUANTUM SYSTEMS	03 THU
SHAIDU YUSUF	#176	ADVANCED COMPUTATIONAL METHODS 2	02 WED
SHIROKA TONI	#253	SUPERCONDUCTIVITY 1	03 THU
SICILIANI DE CUMIS MARIO	#304	PHOTONIC MATERIALS AND DEVICES	03 THU
SILVESTRELLI PIER LUIGI	#111	ADVANCED COMPUTATIONAL METHODS 1	01 TUE
SMECCA EMANUELE	#015	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 1	30 MON
SPAGNOLO BERNARDO	#064	OUT OF EQUILIBRIUM STATISTICAL PHYSICS 1	01 TUE
SPERA MONIA	#146	NOVEL SEMICONDUCTORS AND APPLICATIONS 1	01 TUE
STAGIRA SALVATORE	#329	PHYSICS OF AND WITH FREE ELECTRON LASERS	04 FRI
STELLA GIUSEPPE	#122	CULTURAL HERITAGE 2	01 TUE
STELLINO ELENA	#336	MATTER IN EXTREME AND METASTABLE CONDITIONS	04 FRI
SUKUL PRASENJIT PRASAD	#303	PHOTONIC MATERIALS AND DEVICES	03 THU
TAFURI FRANCESCO	#218	QUANTUM INFORMATION PHYSICS AND TECHNOLOGIES 2	03 THU
TARALLO MARCO	#321	QUANTUM SIMULATIONS, SENSING AND METROLOGY	04 FRI
TERRACINA ANGELA	#132	MATERIALS FOR ENVIRONMENTAL APPLICATIONS 1	01 TUE
TERRASI ANTONIO	#011	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 1	30 MON
TIRIBOCCHI ADRIANO	#021	ACTIVE AND SOFT MATTER AND FLUIDS 1	30 MON
TOCCHIO LUCA FAUSTO	#239	STRONGLY CORRELATED SYSTEMS AND SPINTRONICS 1	03 THU
TOMADIN ANDREA	#262	NANOPHOTONICS AND PLASMONICS	03 THU
TORELLI PIERO	#133	NANOSTRUCTURES AND NANOTECHNOLOGIES 1	01 TUE
TORRE IACOPO	#267	NANOPHOTONICS AND PLASMONICS	03 THU
TORRISI FELICE	#039	LOW-DIMENSIONAL MATERIALS 2	01 TUE
TORTORA LUCA	#073	CULTURAL HERITAGE 1	01 TUE
TOTANI ROBERTA	#049	MATERIALS AND DEVICES FOR RENEWABLE ENERGY 2	01 TUE
TRAVERSO ZIANI NICCOLO	#344	TOPOLOGICAL MATTER	04 FRI
TRIGONA CARLO	#124	CULTURAL HERITAGE 2	01 TUE
TRIOLO CLAUDIA	#140	NANOSTRUCTURES AND NANOTECHNOLOGIES 1	01 TUE
TROVATO ANTONIO	#184	BIOPHYSICS, BIOMEDICINE AND MODELING 2	02 WED
URRU ANDREA	#109	ADVANCED COMPUTATIONAL METHODS 1	01 TUE
URSO MARIO	#031	PHYSICS TECHNOLOGIES FOR HEALTH	30 MON
URSO MARIO	#244	NOVEL SEMICONDUCTORS AND APPLICATIONS 3	03 THU

USSIA MARTINA	#198	MATERIALS FOR ENVIRONMENTAL APPLICATIONS 2	02 WED
VAGOVIC PATRIK	#331	PHYSICS OF AND WITH FREE ELECTRON LASERS	04 FRI
VALLETTA ANTONIO	#211	NOVEL SEMICONDUCTORS AND APPLICATIONS 2	02 WED
VANNUCCI LUCA	#342	TOPOLOGICAL MATTER	04 FRI
VENDITTI GIULIA	#250	SUPERCONDUCTIVITY 1	03 THU
VENUTI VALENTINA	#075	CULTURAL HERITAGE 1	01 TUE
VERANDA MARCO	#171	PLASMA PHYSICS 2	02 WED
VERDINI ALBERTO	#286	ORGANIC ELECTRONICS	03 THU
VERONESI STEFANO	#226	NANOSTRUCTURES AND NANOTECHNOLOGIES 3	03 THU
VINAI GIOVANNI MARIA	#240	STRONGLY CORRELATED SYSTEMS AND SPINTRONICS 1	03 THU
VITALI DAVID	#148	QUANTUM INFORMATION PHYSICS AND TECHNOLOGIES 1	02 WED
WAUTERS MATTEO	#339	TOPOLOGICAL MATTER	04 FRI
ZALTRON ANNAMARIA	#095	ACTIVE AND SOFT MATTER AND FLUIDS 3	01 TUE
ZANOTTO SIMONE	#268	NANOPHOTONICS AND PLASMONICS	03 THU
ZEN ANDREA	#206	NANOSTRUCTURES AND NANOTECHNOLOGIES 2	02 WED
ZIMBONE MASSIMO	#216	NOVEL SEMICONDUCTORS AND APPLICATIONS 2	02 WED
ZUCCARELLO FRANCESCA	#103	PLASMA PHYSICS 1	01 TUE