INDEX

THE MATERIALS SCIENCE DEPARTMENT

http://www.mater.unimib.it/

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Mail	**Secretariat: lucia.rodolfi@unimib.it**
Director	**Prof. Marco Martini - Prof. Alessandro Abbotto** **(since 1/11/2018)**
ISI-CRUI Sectors	**Chemistry, Physical Chemistry, Chemical Physics Spectroscopy, Instrumentation Engineering, Analytical Sciences, Optics and Optometry, Organic Chemistry, Polymer Science, Materials Science, Physics, Condensed Matter, Applied Physics**

ABOUT US
The Department was established in 1997 on the initiative of a group of physicists and chemists of the Università degli Studi di Milano. It is linked to the Materials Science Degree Courses and Doctorate, to the Degree Courses in Optics and Optometry and to the Degree Courses in Chemical Science and Technology.

The main research fields are:

- materials for environment and energetics
- materials for photonics and microelectronics
- materials in cultural heritage
- nanomaterials and nanomedicine
- optometry
- organic and polymeric materials

The Department offers an interlinked system of services, consisting in vocational guidance support, help desk for didactics and student career, Socrates-Erasmus desk, office for stages in private high-tech companies, advanced scientific analyses for private customers.

STRATEGIC GOALS

General goals of the Materials Science Department include competitive Research & Development and Advanced Training, both in basic and applied research, in the field of new materials and their industrial applications.

Theoretical and experimental studies are carried out in several fields such as ionic conductors, electrochemistry, molecular electronics, laser, molecular modelling, insulator oxides, non-linear optics, polymers, semiconductors, sensors, organic and inorganic synthesis, superconductors, luminescence, glass, optical fibres. Beside the main spectroscopic and electrical characterization techniques, advanced materials analysis is achieved by means of many experimental techniques like AFM, STM, ESR, FIB, NMR and a number of other advanced optical, magnetic and electrical instrumentations.

The research activities are also devoted to specific application fields like new materials and techniques for energetics, environment and cultural heritage.

Research is carried out within the framework of national and international projects, leading to a great number of high level publications and patents.

The educational project aims at forming young professionals highly qualified in both physics and chemistry, able to fit their knowledge to the contemporary requirements of the related labour market. Milano-Bicocca University is in fact located in an area where highly specialized high-tech companies are abundant, offering stimulating employment opportunities in consolidated applications (nanotechnology, elastomers, polymers, insulators, semiconductors, ceramics) as well as in innovative materials (optical fibres, ionic conductors, superconductors, organic and inorganic semiconductors, materials for non linear optics, micro and opto-electronics, radiation detectors).

Degrees in Materials Science and in Chemical Science and Technology include a basic degree (Laurea, three years), followed by a possible two-year specializing course (Laurea Magistrale).

The three-years course of Optics and Optometry gives interesting professional opportunities.

Finally, rich opportunities for post-lauream courses and research are offered by the Doctorate in Materials Science and Nanotechnologies.

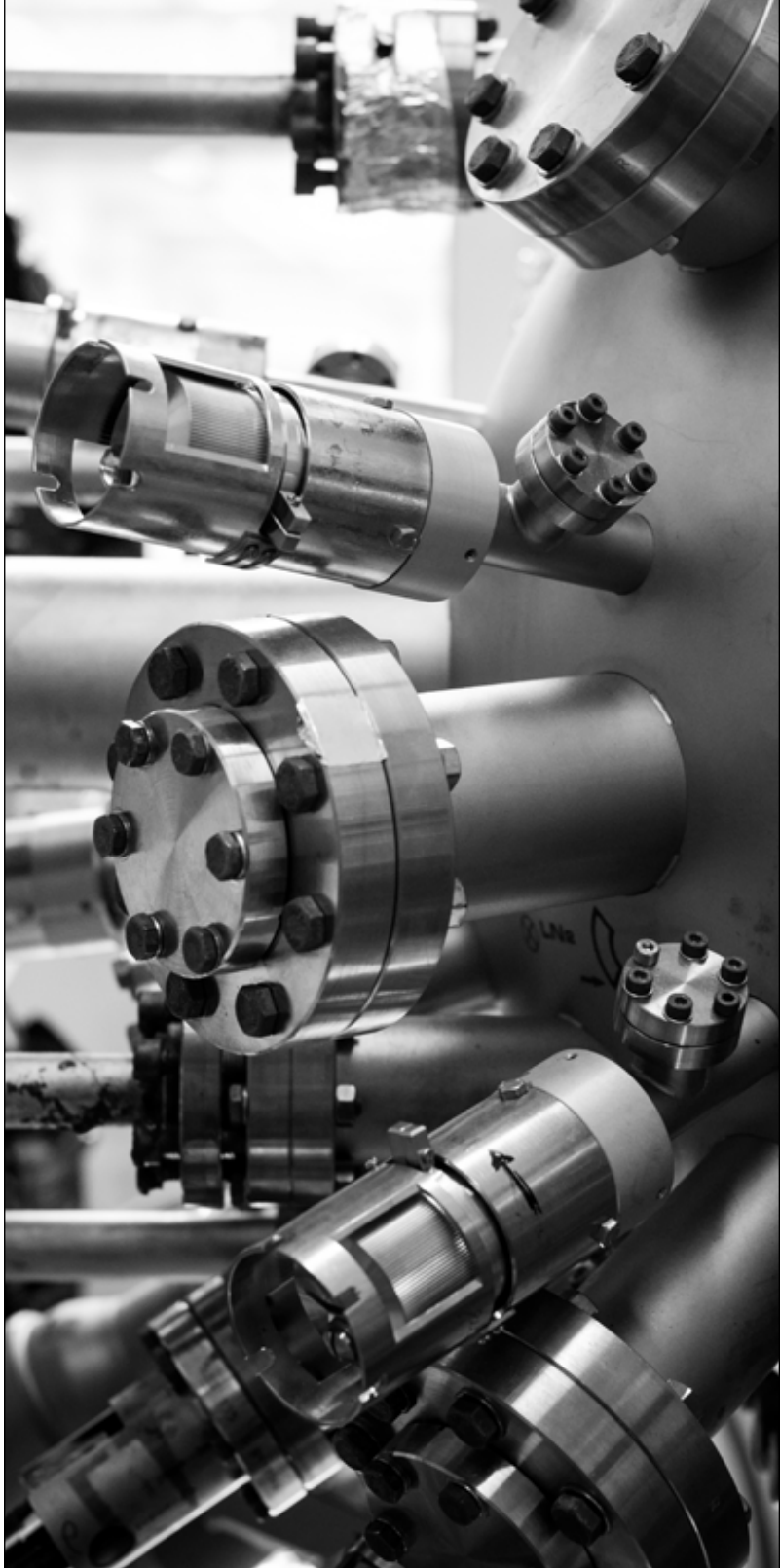
BOARDING

Until October 2018 / *since November 2018*

DIRECTOR
Marco Martini */ Alessandro Abbotto*

DEPUTY DIRECTOR
Antonio Papagni */ Anna Vedda*

Angiolina Comotti, Massimiliano D'Arienzo, Alberto Paleari, Luisa Raimondo, Lucia Rodolfi, Adele Sassella, Anna Vedda / *Simona Binetti, Angela Bracco, Alberto Paleari, Antonio Papagni, Giorgio Patriarca, Lucia Rodolfi, Adele Sassella, Roberto Scotti*



TEACHING

Until October 2018 / *since November 2018*

Chemical Science Courses coordinator:

Alessandro Abbotto / *Simona Binetti*

Materials Science Courses coordinator:

Alberto Paleari

Optics and Optometry Course coordinator:

Antonio Papagni / *Adele Sassella*

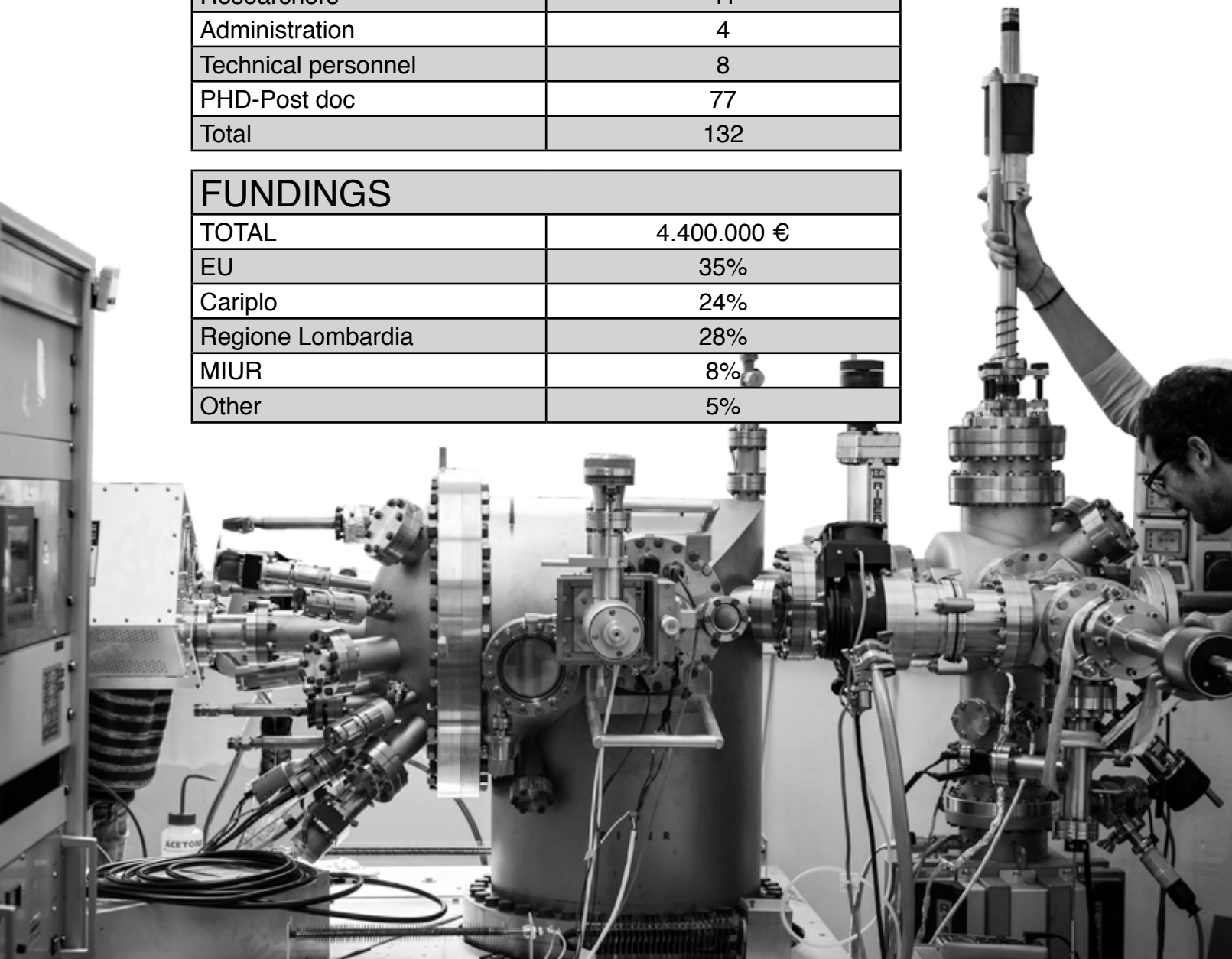
Doctorate coordinator:

Marco Bernasconi

NUMBERS

PERSONNEL	#
Emeritus	2
Researchers	41
Administration	4
Technical personnel	8
PHD-Post doc	77
Total	132

FUNDINGS	
TOTAL	4.400.000 €
EU	35%
Cariplo	24%
Regione Lombardia	28%
MIUR	8%
Other	5%



Research (in alphabetic order)

Materials for energy and environment

Maurizio Acciarri, Simona Binetti, Dario Narducci. **Photovoltaics, thermoelectrics and carbon dioxide capture**

Gian Paolo Brivio. **Theory and computations of adsorbate interfaces**

Angiolina Comotti. **Porous materials: design, synthesis, structural characterization and switchable molecular dynamics**

Massimiliano D'Arienzo, Barbara Di Credico, Roberto Scotti. **Chemistry of inorganic and hybrid materials**

Cristiana Di Valentin. **Theory of 2D and 0D materials: bidimensional layers and nanoparticles**

Massimo Moret. **Crystal growth and characterization: study of polymorphism**

Gianfranco Pacchioni, Sergio Tosoni. **Theory of oxide surfaces, interfaces, and supported clusters**

Materials for microelectronics and photonics

Marco Bernasconi. **First principles simulations of materials for microelectronics**

Emiliano Bonera, Fabio Pezzoli. **Optical spectroscopy of semiconductors**

Sergio Brovelli, Francesco Meinardi, Angelo Monguzzi. **Advanced spectroscopy of functional nanomaterials**

Marco Fanciulli. **Materials and spectroscopies for nanoelectronics and spintronics**

Mauro Fasoli, Alberto Paleari, Anna Vedda. **Oxide nanostructures and silica-based materials for optical technology**

Leo Miglio, Francesco Montalenti. **Modeling and simulations of semiconductor heteroepitaxy**

Stefano Sanguinetti. **Fabrication and study of semiconductor quantum nanostructures**

Adele Sassella. **Organic molecular films and heterostructures**

Materials in cultural heritage

Anna Galli, Marco Martini, Emanuela Sibilia. **Dating and characterization of ancient materials. Materials science and cultural heritage**

Mathematics

Veronica Felli. **Singular elliptic equations: asymptotic analysis, unique continuation, spectral stability for singularly perturbed problems**

Organic and polymeric materials

Alessandro Abbotto. **Organic and hybrid materials and devices for solar fuels, artificial photosynthesis, and photovoltaics**

Luca Beverina. **Functional dyes and pigments for photonics, electronics and optoelectronics**

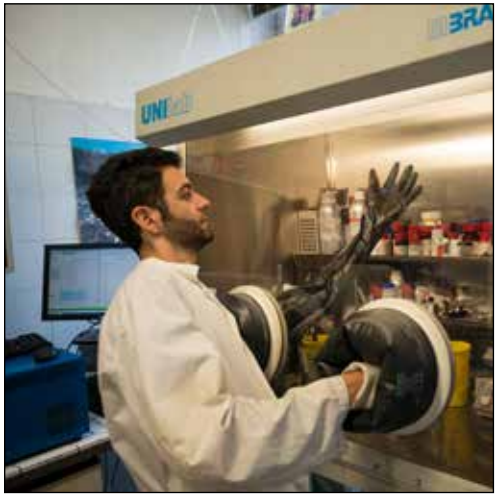
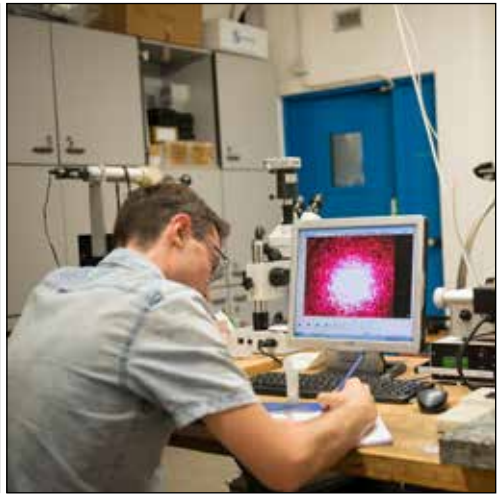
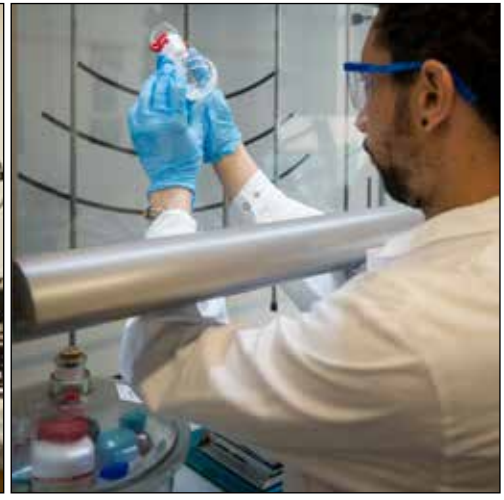
Antonio Papagni. **Organic molecular systems for II order non-linear materials, low energy emitters and organic semiconductors**

Roberto Simonutti. **Synthesis and characterization of novel polymeric nano-structures**

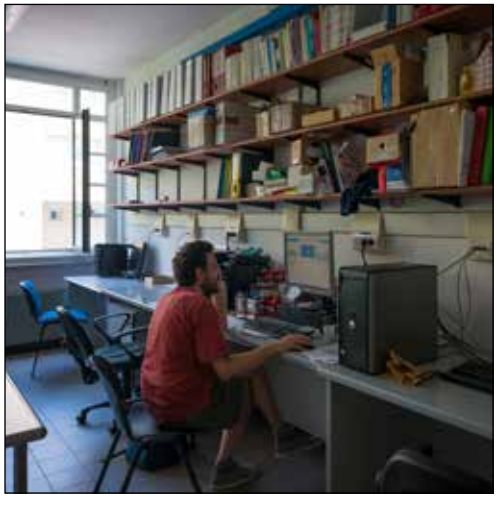
Silvia Bracco, Piero Sozzani. **Generation of nanospaces for polymerization and gas capture**

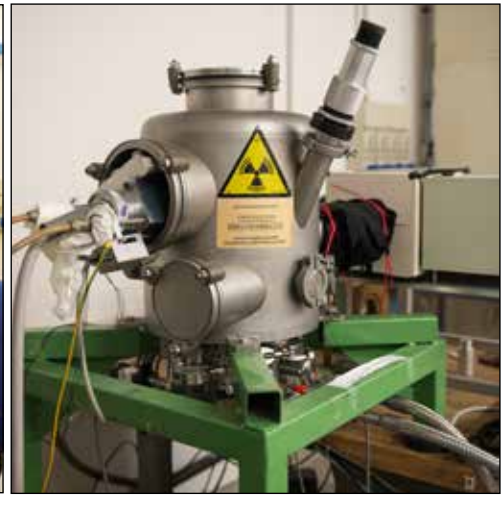
Optics and optometry

Silvia Tavazzi. **Optics and optometry**







Photovoltaics and thermoelectrics

MAURIZIO **A**CCIARRI, **S**IMONA **B**INETTI, **D**ARIO **N**ARDUCCI

NANOTECHNOLOGY FOR THERMOELECTRICITY

Thermoelectricity is a way to convert heat into electricity without the use of any movable part. As such, thermoelectric generators are suitable, especially when miniaturized, to harvest low-temperature heat and to make it available as electric power to distributed sensor networks or to other portable devices. Bottom-up and top-down nanotechnology has played a major role in the enhancement of the efficiency of thermoelectric materials. Over the last decade we have developed methods to obtain silicon nanowires and nanolayers, and to enhance bulk thermoelectric properties by controlled precipitation of second phases in nanocrystalline silicon thin films. Research on thermoelectrics is currently oriented along two main lines, namely (a) silicon-based thermoelectric integrated devices working in the medium temperature range to supply electric power to wireless devices and (b) the development of novel mixed organic-inorganic nanocomposites to harvest body heat in portable (wearable) sensors.

SILICON FOR SOLAR CELLS

The properties of defects in silicon have been studied for more than twenty-five years with substantial contributions to today knowledge of the mc-Si solar cells. Since 1990, the group has been involved in many European Renewable Energy Projects. Recently, under the realistic assumption that Si-wafer based PV modules will dominate the market in the coming decade, we have focused on the characterization of low price and high quality solar grade silicon feedstock and on new initiatives to build high efficiency tandem solar cell coupled with perovskite or DSSC solar cells.

INORGANIC SEMICONDUCTOR THIN FILMS FOR PHOTOVOLTAICS

In collaboration with a small company we have recently developed a new, original method for chalcogenide thin film (CIGS) deposition on glass and flexible substrates, like plastic foils. This system is based on an innovative hybrid sputtering-evaporation approach combining the advantages of both growth techniques. First of all, such a growth apparatus allows to effectively controlling the metal compositional ratios also in an industrial process on large area substrates, as they only depend on the amount of metals deposited during the sputtering step. Furthermore, the implementation of an evaporation step allows the achievement of metal ratio in-depth profiles typical of three-stage grown CIGS layers. Last but not least, both the use of single metal targets and the extremely controlled nature of the sputtering deposition (which occurs in a Se vapours-free zone) allow a reduction of the costs. In the last few years, a possible alternative to CIGS PV thin film where more abundant and less expensive elements like Zn and Sn are used in place of In and Ga, namely Cu_2ZnSnS_4 (CZTS), was considered, too. Two main growth methods are under investigation and testing: sputtering process and chemical methods (i.e. dip coating, spray pyrolysis).

Theory and computations of adsorbate interfaces

GIAN **P**AOLO **B**RIVIO

The main interest of the group is focused on developing and interpreting first-principle investigations of the electronic properties of novel low dimensional materials. The Group is a core node partner of the “European Theoretical Spectroscopy Facility”(ETSF). This network, comprising 68 Universities and research Laboratories, aims at advancing computational spectroscopy. We make use and contribute to quantum codes both for the supercell geometry and for low dimensional systems within the density functional theory (DFT) framework. Our results are relevant to basic knowledge and to device implementations, such as photovoltaics and nanoelectronics.

ULTRAFAST PROCESSES OF ELECTRON TRANSFER RATES OF A CORE EXCITON

Charge transfer rates at metal/organic interfaces affect the efficiencies of devices for organic based electronics and photovoltaics. A study of electron transfer rates, which take place on the femtosecond timescale, is often difficult, especially since in most systems the molecular adsorption geometry is unknown. Here, we use X-ray resonant photoemission spectroscopy to measure ultrafast charge transfer rates across bipyridine/graphene deposited as single layer or bilayer on a Ni surface. We demonstrate that a bi-directional charge transfer across the molecule/metal interface is enabled upon creation of a core hole in the molecule by X-ray absorption. Results are confirmed by DFT calculations.

FEMTOMAGNETISM OF CORE EXCITED FUNCTIONALIZED GRAPHENE

Chemisorption and physisorption properties of aromatic molecules on graphene have been worked out by DFT. We found that chemisorbed moieties magnetize graphene in the ground state while physisorbed ones do not. However, when core excited by radiation such molecules show an opposite behavior in the femtosecond range. Consequently, physisorbed pyridine is magnetic for the time duration of the core-hole lifetime. This effect opens up new possibilities for switching on and off information in the fs times.

SPECTROSCOPIC AND OPTICAL PROPERTIES OF POTASSIUM DOPED PTCDA ON METALS

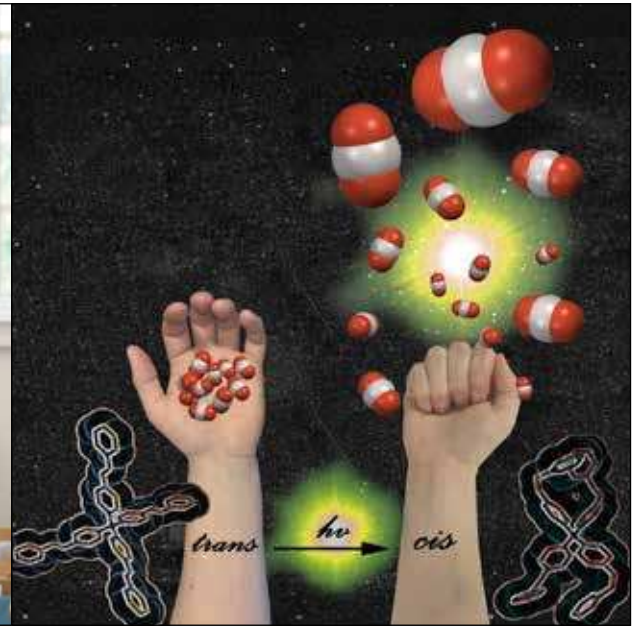
Alkali metal atoms are a simple yet efficient n-type dopant of organic semiconductors such as those formed by PTCDA molecules. With a joint theoretical effort between this Group and that of E. Zojer (TU Graz) following the experiments performed at the Group of T. Fritz (Jena Univ.), with the help of TDDFT calculations we show a very good agreement between measurements and theory for the electronic and optical properties of PTCDA layers on Ag surfaces at different K stoichiometry.

Porous materials: design, synthesis, structural characterization and switchable molecular dynamics

ANGIOLINA **C**OMOTTI

The research activity deals with the generation of frameworks containing one-, two- and three-dimensional confined spaces with uniform and precisely engineered geometries to create new environments for capture of chemical entities. The study is focused on new materials with nanoscale architectures for storage of important gases, such as methane and hydrogen, considered as clean fuels. Additionally, carbon dioxide and other pollutants are removed from nitrogen and hydrogen by selective sequestration in pores. The construction of stable and robust covalent organic and hybrid frameworks with 3D periodic motifs can increase separation, capture and storage of small gas molecules, especially molecular hydrogen. These frameworks can arrange sites and receptors into arrays, for interacting with the targeted gas species. The adsorption properties of the novel materials are superior in many instances to the existing ones and yielded patents for applications in gas storage and purification. Characterization methods of the porous structures and of the confined gases/vapors is currently achieved by X-ray diffraction techniques: advanced experiments using synchrotron-light and neutron sources are currently performed at various European facilities, such as at ESRF (Grenoble) and Elettra (Trieste). In particular, the synchrotron XRD experiments enable the in-situ observations of the gas arrangement as well as adsorption kinetics. Additionally, the dynamics of gases and vapors in the confined state and the identification of weak interactions will be studied in depth by advanced solid state NMR spectroscopy.

A challenging issue is the dynamics of nanoporous solids. The research activity is focused on the insertion of molecular rotors in the building blocks of the porous materials, giving access to the control of rotary motion by chemical and physical stimuli. The combination of porosity with ultra-fast rotor dynamics is investigated in molecular crystals, covalent organic frameworks and MOFs by complementary techniques, which were proved to be sensitive to motion at regimes ranging from 104 to 1011 Hz. Remarkably, the rotor dynamics can be switched on and off by guest absorption/desorption, showing a change of material dynamics, which, in turn, produces modulated physical responses. Novel fluorinated dipole-bearing molecular rotors can be inserted on porous architectures, realizing ordered arrays of fast dipolar molecular rotors. The extremely rapid re-orientation in solids is challenging and enables the fabrication of ferroelectric switches, as revealed by dielectric measurements. The combination of pore-structure and dipolar rotors can be exploited for stimulated guest release.
A series of flexible molecular crystals made by azobenzene tetramers, that form porous molecular crystals in their trans configuration is pursued. The efficient trans $\longrightarrow$ cis photo-isomerization of the azobenzene units converts the crystals into a non-porous phase but crystallinity and porosity are restored upon Z $\longrightarrow$ E isomerization promoted by visible light irradiation or heating. The photo-isomerization enables reversible on/off switching of optical properties as well as the capture of CO_2 from the gas phase.


trans
hv
cis

Chemistry of inorganic and hybrid materials - NanoMat@Lab

MASSIMILIANO **D'A**RIENZO, **B**ARBARA **D**I **C**REDICO, **R**OBERTO **S**COTTI

NANOSTRUCTURED MATERIALS FOR CATALYSIS, PHOTOCATALYSIS AND ENERGY STORAGE

The research aims at the synthesis by soft-chemistry methods of morphology-controlled oxide nanoparticles (e.g. TiO_2 , ZnO, MoO_3) and tuneable porous systems (macro/mesoporous silica or Metal Organic Frameworks, MOF), and at the study of their (photo)catalytic mechanism (formation and interfacial reactivity of paramagnetic defects) by spectroscopic and spectromagnetic techniques. In particular, the possibility of tailoring size, anisotropy and surface functionalities of these systems by employing catalysts (acid or bases), soft templates (e.g. amphiphilic surfactants), capping molecules or particular solvents, has been exploited for the modulation of the inorganic-organic interfaces. This play a crucial role in determining their properties and implementation for the development of advanced hybrid materials commonly utilized for water/air depollution, CO_2 photoconversion in renewable fuels and Na-ion batteries.

INORGANIC NANOFILLERS FOR MULTIFUNCTIONAL POLYMER NANO-COMPOSITES

The research focus on the preparation by bottom-up approaches of oxides (mainly ZnO and SiO_2) nanoparticles and polysilsesquioxanes (PSQ) with controlled morphological and surface features, employed in a wide range of applications (i.e. automotive, high performance dielectrics, gas-barrier). In particular, since 2008, these materials have been exploited by our group, in collaboration with other academic and industrial partners (i.e Pirelli Tyres, SAES Getters), for the preparation of novel polymer nanocomposites mainly utilized in tires application. In this context, the results of the activity have provided a relevant scientific and technological impact, leading to the production and implementation of a material developed in the NanoMat@Lab in the industrial plant. Currently, the group is working on the application of these designed fillers in other multifunctional nanocomposites (conductive composites for low-k or high-k materials, O_2 barrier coatings) where, besides a peculiar functionality, remarkable mechanical strength, low deformability and high thermal stability are required.

FACILITIES

Two fully equipped laboratories for inorganic synthesis: solvothermal reactors, furnaces for thermal treatment up to 1600°C, Schlenk lines, mixing reactors with impeller, centrifuges
Bench-scale plants for UV and Vis-light photocatalytic test;
Total Organic Carbon analyzer (TOC) Shimadzu TOC-V CSH for liquid and gas samples;
XRPD Diffractometer (Rigaku);
Scanning Electron Microscopy (SEM, TESCAN VEGA 5136XM with EDAX GENESIS 4000XMS probe);
Thermal analysis (TGA) up to 1400°C connected with MS station;
Bruker ESR spectrometer equipped with liquid N_2/He Cryostat.

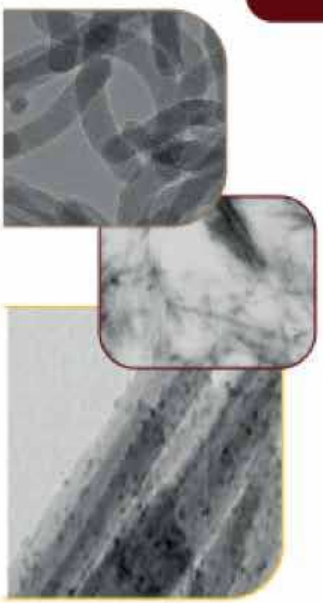
The NanoMat@Lab Unimib aims at the synthesis by soft-chemistry and at the characterization of inorganic pure and hybrid materials for energy saving

Shape and Controlled Anisotropic NPs
(TiO_2, SiO_2, SnO_2, ZnO, CuO)

2D Layered Nanomaterials
(MoS2, WS2,) **and Clays**
(e.g. sepiolite fibers)

Poly Silsesquioxanes
(POSS)
Molecules

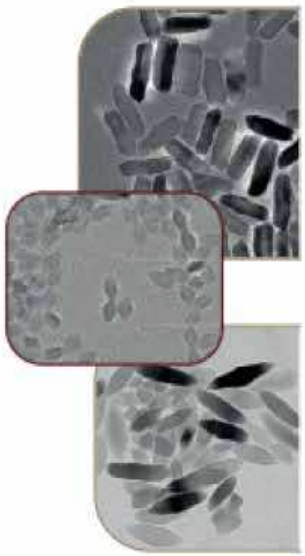
Selected Polymers: thermoplastics, elastomers & thermosettings



Material Preparation by Colloidal Methodes
(furnaces, autoclaves, dip-coating, spin-coating)

Structural & Morphological Characterization
(XRD, DLS, SEM, TGA-MS, ESR spectroscopy)

Functional Characterization
(TOC analyzer, DMA, Electrochemical Characterizations)



Application 1
Photocalytic and Catalytic Materials

Application 2
Polymer Nanocomposites for tires

Application 3
Materials for Li or Na ion batteries

Application 4
Nanocomposites for low-k and high-k materials

Chemistry of inorganic and hybrid materials - NanoMat@Lab

CRISTIANA **D**I **V**ALENTIN

COMPUTATIONAL NANOMEDICINE

Emerging semiconducting metal oxide nanostructures (nanospheres, nanotubes, thin films) with photocatalytic or magnetic properties are currently opening totally new horizons in nanomedicine (e.g. novel photodynamic therapies, a new class of contrast agents, magnetically guided drug delivery). We investigate shape and size dependent properties, we screen potentially efficient linkers for anchoring surfaces and binding biomolecules. We tether various kinds of biomolecules (from oligopeptides and oligonucleotides to small drugs) to the activated surface according to the desired functionality. The assembled bioinorganic systems may also be labeled with fluorescent markers and contrast agents.

COMPUTATIONAL ELECTROCHEMISTRY AND FUEL CELLS

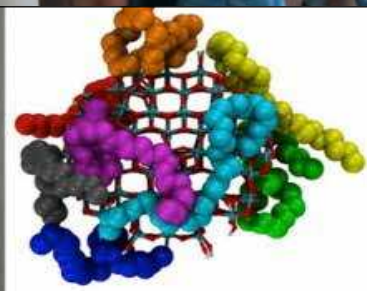
We use electronic structure calculations to design novel electrode materials for electrochemical devices and fuel cells, which are as efficient as or even more capable than precious and environmental unfriendly metal electrodes. Gibbs free energies of reaction in an aqueous environment for the all the steps of reduction (at the cathode) or of oxidation (at the anode) are computed, for example, for the oxygen reduction reaction (ORR) or for methanol oxidation reaction (MOR), respectively. Details of the reaction mechanisms and accurate cell onset- or over-potentials can be derived from the Gibbs free energy diagrams. The latter are computational quantities that can be directly compared to experimentally obtained cell overpotentials.

CATALYSIS UNDER COVER (2D LAYERS)

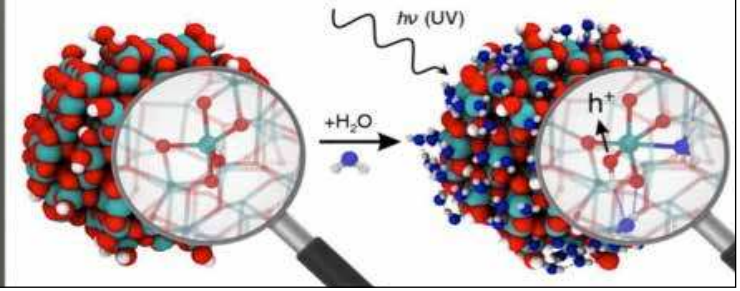
The catalysis "under cover" is a recent and emerging field of research (see review article by X. Bao and co. in Nature Nanotech. 2016, 11, 218), focusing the attention on the chemical reactivity taking place in the confined zone between two interfacing materials. Typically, at least one of materials is 2D, e.g. graphene, h-BN or MoS_2. A number of examples of enhanced reactivity have now been reported in the literature, where the chemical process is favored if taking place between the two exposed surfaces. Still very little is known on the mechanism of this special type of catalysis and on the true role played by the two surfaces. Is the space confinement effect a sufficient reason for the enhanced reaction rate or are surface atoms actually involved in the reaction steps? Are defects and impurities also active in the promotion of chemical reactions?

GRAPHENIC NANOSTRUCTURES FROM MOLECULAR PRECURSORS

Combining density functional theory calculations with scanning tunneling microscopy and X-ray spectroscopic techniques (from our experimental partners) we investigate novel approaches for surface-assisted preparation of graphene-based nanostructures (nanoribbons, nanobowls, etc) by means of Ullmann coupling polymerization and dehydrogenation reactions of polyaromatic molecules.



nanoQlab



Theory and computations of adsorbate interfaces

RICCARDO **R**UFFO

Since the birth of the Department, the group is active in fields of Energy Storage and Production, Gas Sensing, and characterization of Organic Molecular or Polymeric Materials. Group facilities comprise a fully equipped electrochemical lab with several potentiostats-galvanostats, two multichannel systems for long time testing, two semi-automatic glove boxes at N_2 or Ar, a climatic chamber to control temperature and humidity, optical fibers coupled with UV-visible spectrophotometer for in-situ spectroelectrochemistry, and a quartz crystal electrochemical microbalance. Furnaces, thick/thin film applicators, and standard chemical equipments are available for chemical synthesis and electrode formulations.

MATERIALS FOR ENERGY STORAGE AND PRODUCTION

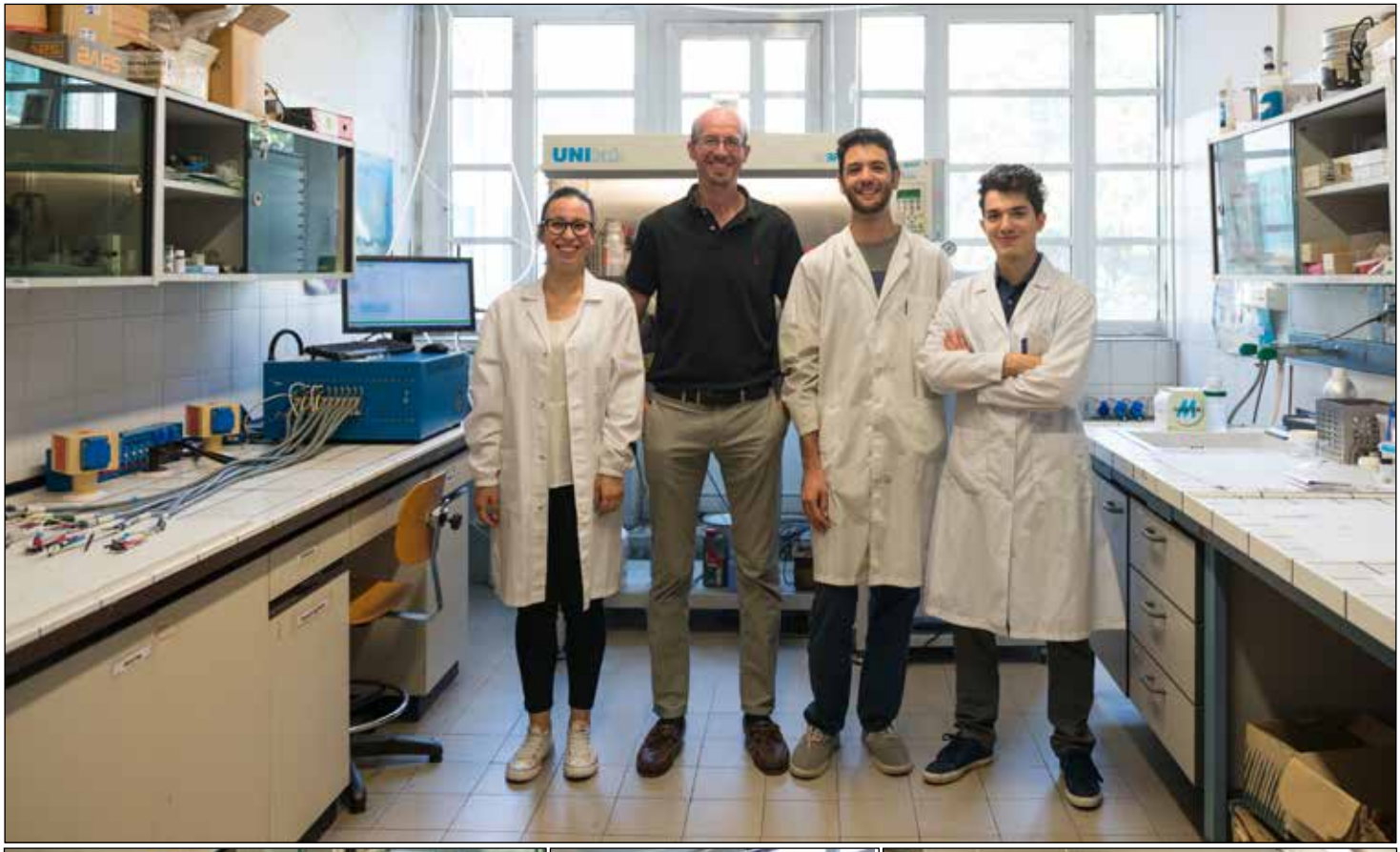
This research line is devoted mainly to the investigation of electrode and electrolyte materials for rechargeable batteries and solid oxide fuel cells. Materials are produced by our team or in collaboration with national and international research groups. The electrical and electrochemical characterizations, carried out using standard techniques such as impedance spectroscopy, DC Hebb Wagner conductivity measurement, cyclic voltammetry, potential spectroscopy, galvanostatic cycling, are performed with the aim to investigate the correlation among structural, morphological features and functional properties.

MATERIAL FOR GAS SENSORS

Potentiometric or amperometric solid state electrochemical gas sensor are investigated and realized to determine the composition of CO/CO_2 or H_2/H_2O gas mixtures and the concentration of CO or H_2O or SO_2 in air as well as Cl_2 or O_2 or CO_2 in nitrogen and air. Moreover, nanostructured thin film semiconductor gas sensors of pure or noble metal doped semiconductors prepared via sol gel or dip coating technique, were used as sensing elements to determine low concentration of reducing gas (CO). The experimental measurements pointed out the strong correlation among the electrical properties, the point defects, the amount of doping level, and the morphology.

MATERIAL FOR ORGANIC OPTOELECTRONICS

Since ten years, the group collaborate with organic chemistries of the department to characterize dye molecules, tiophene and pyrrole based monomers, and poly-tiophene based polymers for electro-optic applications (solar cells and electrochromic devices). The systems are characterized respect to their electrochemical and spectroelectrochemical properties in solution or in solid state (as thin film). The electronic properties, the energy levels, and the electro-optical characteristic are correlated to the chemical structure and to the film morphology. Redox mechanisms in conducting polymers are also investigated.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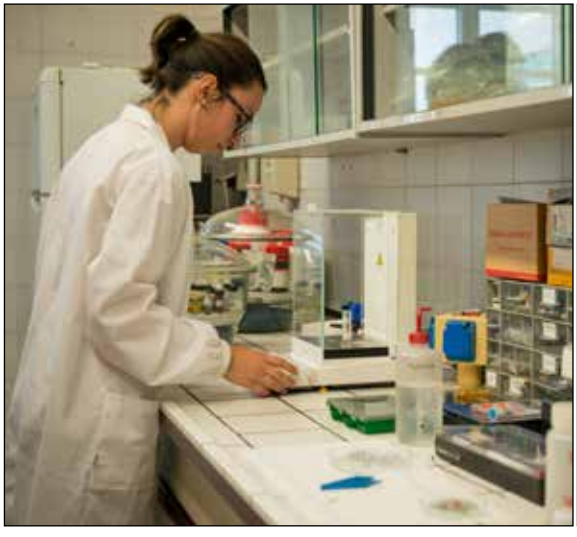



BRAUN

Theory and computations of adsorbate interfaces

MASSIMO MORET

Growth and characterization of crystals is a mandatory step in many fields of science and technology. Growth of crystals involves complex surface chemical processes and therefore study of surface reactivity is a key point to optimize crystal growth as well as the interactions of crystals with natural or artificial environments.

The research activities are mainly devoted to crystal growth from solution (flexible coordination polymers, MOFs, inorganic solids for catalysis, composite crystalline systems, amino acids), study of sorption processes at the crystal/solution interface in natural and artificial environments and (e.g. doping of crystals or setting of cements/plasters in the presence of organic additives).

Growth of crystals (solution, solvothermal methods, sublimation, physical vapor transport) is complemented with ex-situ SPM, single crystal X-ray diffraction and hot stage optical microscopy. Theoretical modelling with Periodic Bond Chain analysis, electron density partitioning of crystal space with Hirshfeld surfaces, PIXEL calculations of electron density, topological analysis of solids are further steps towards the detailed analysis of packing modes and intermolecular interactions in crystals and rationalization of physical properties.

Due to its academic and practical relevance, the phenomenon of polymorphism, usually an undesired occurrence in crystal growth trials, is a central point of interest. Study of thermodynamic and kinetic factors affecting occurence of polymorphism include exploitation of temperature, pressure, impurities/additives, nucleating substrates, conformational space of molecules, isotopic replacement.

FACILITIES

• Single crystal X-ray diffractometer with temperature control from ca. 80 to 490 °K
• Termostatted crystallizers for crystal growth from solution, sublimation, vapor deposition
• Metallographic and stereoscopic microscopes equipped with analizer/polarizer, DIC Nomarski prism, frame grabber for time lapse imaging, heating/freezing stage from 90 to 870 °K.

Theory of oxide surfaces, interfaces, supported clusters

GIANFRANCO **P**ACCHIONI, **S**ERGIO **T**OSONI

The understanding of the structure-properties relationship is of fundamental importance for the design of new materials. In our group various models are employed to study the electronic structure of inorganic and ceramic materials in combination with highly accurate quantum-mechanical techniques. Particularly important is the role of theory in the study of point defects, impurities in solids, active sites or functional groups on surfaces, phenomena like atomic and molecular chemisorption, ultrathin films, supported clusters, light-matter interactions, and for the interpretation of various spectroscopies, IR and Raman, X-ray absorption and photoemission, EPR and NMR, optical transitions, STM etc.

OXIDE SURFACE AND THIN OXIDE FILMS

Ultrathin oxide films grown on metal supports represent a new class of materials with unprecedented properties. Our activity is directed towards the determination of their electronic and structural properties: work function changes, presence of nanoholes or regular arrays of adsorption and reactive sites, etc.

SUPPORTED CLUSTERS

Metal nanoclusters as models of supported catalysts. We study the interaction and stabilization of the metal clusters at specific sites of the support like oxygen vacancies and other defects. We investigate the possible electronic modification of metal clusters on ultrathin insulating films due to electron tunneling phenomena from the metal support (charging, change in shape and reactivity, etc.). We also study the reactivity of supported clusters in elementary steps of catalytic reactions.

DEFECTS AND DOPANTS IN OXIDES

Nature of point defects in oxide materials for photocatalysis, photoelectrochemistry, microelectronics, fiber optics etc., in particular amorphous and crystalline TiO_2, ZnO, WO_3, SiO_2, alkaline earth oxides. The activity is directed toward the determination of stability, structure, and spectral properties of intrinsic and extrinsic point defects (vacancies, metal and non-metal dopants, codopants, hydroxyl groups, trapped electrons, etc.) and their interplay through charge transfer processes. Particular attention is devoted to the study of optical absorption for activation in the visible region and of electron spin resonance spectra for identification of paramagnetic centres.

OXIDE SEMICONDUCTORS AND HETEROJUNCTIONS

Heterojunctions between semiconductors (notably oxides) are a class of materials attracting growing attention in the field of photocatalysis. This research line aims at the accurate description of the band alignment, charge transfer phenomena, and charge carrier separation at the junction by means of state-of-the-art DFT calculations.

MAIN FACILITIES

- Total computing power of 960 AMD Opteron cores in local facilities.
- Access to CINECA supercomputing centre facilities via an institutional account financed by the University as well as via peer-reviewed scientific proposals.

Theoretical modelling and *ab-initio* simulation of material properties

MARCO **B**ERNASCONI

PHASE CHANGE MATERIALS FOR DATA STORAGE

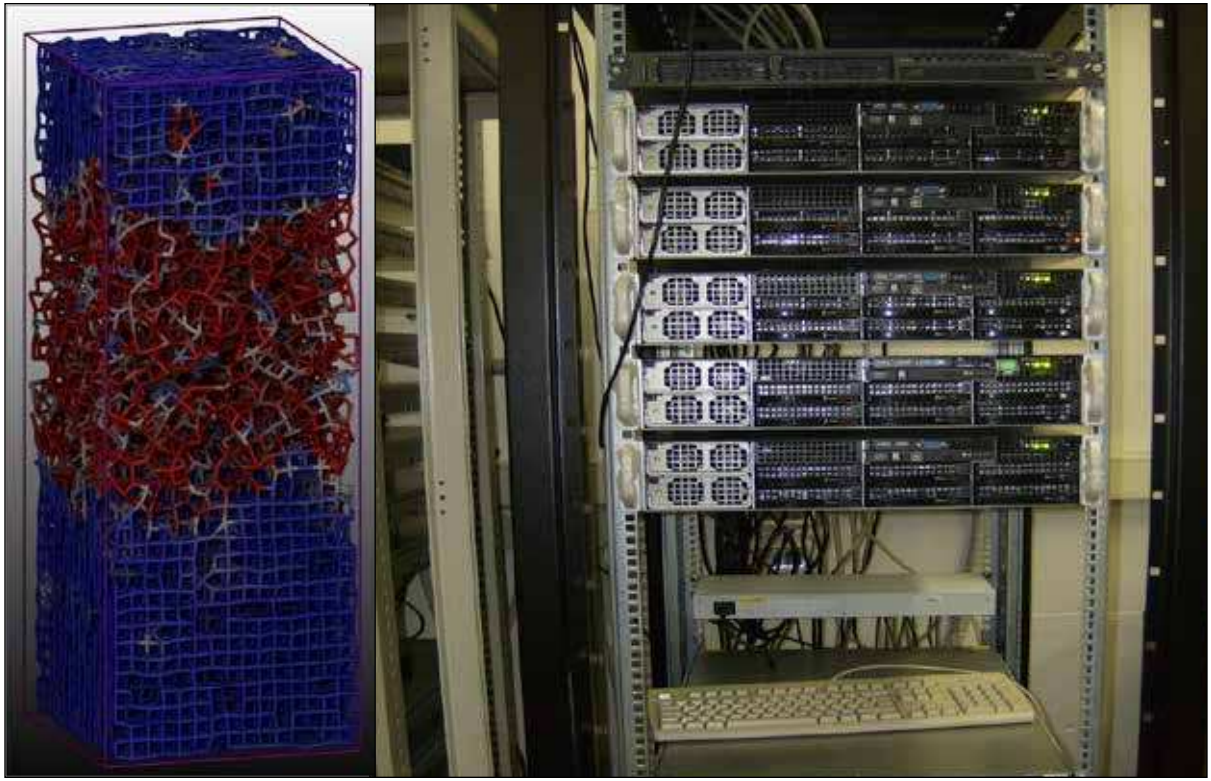
Phase change materials ($Ge_2Sb_2Te_5$ and related telluride alloys) are attracting an increasing interest worldwide for applications in optical disks (DVDs) and in a novel non volatile electronic memory, the phase change memory cell. Both applications rely on a fast (10-100 ns) and reversible transformation between the crystalline and amorphous phases induced by heating. The two states of the memory can be discriminated thanks to the large contrast in electronic conductivity and optical reflectivity between the two phases.

On the basis of density functional molecular dynamics simulations, we investigate the structural, dynamical and electronic properties of the amorphous and crystalline phases of materials in this class aiming at establishing correlations between the composition of the alloy and the electronic and optical functional properties exploited in the devices. The models of amorphous phases (300-500 atoms) are generated by quenching from the melt within ab-initio molecular dynamics simulations.

Large scale molecular dynamics simulations are also performed by means of interatomic potentials generated by fitting a large DFT database with Neural Network methods. The Neural Network potential allows simulating several thousand atoms for tens of ns to study thermal transport at the nanoscale, microscopic mechanisms responsible for the crystalization and the properties of nenowires.

SURFACE PHONONS AND TOPOLOGICAL INSULATORS

Some chalcogenide compounds of interest for phase change applications belong to the class of topological insulators, i.e. they are bulk insulators with a non trivial topology of the electronic bands which induces the formation of topologically protected metallic electronic bands at the surface. On the basis of density functional perturbation theory, we study the surface phonons and the electron-phonon interaction of materials in this class.



Optical spectroscopy and fabrication of semiconductors and semiconductor quantum structures

EMILIANO **B**ONERA, **F**ABIO **P**EZZOLI

Our research is mainly devoted to the experimental study of the optical properties of both group IV and group III-V semiconductors and quantum structures of interest for micro- and opto-electronics. Most of our research is carried out in within the L-NESS interuniversity Centre.

SiGe HETEROSTRUCTURES

SiGe alloys are of fundamental and applicative interest due to their structural, chemical and electronic characteristics, for applications in microelectronics and photonics.

1. Using Raman and photoluminescence we study the correlations between growth conditions and system properties. We analyse the effects of strain, composition and dimensionality on the vibrational and electronic properties of the heterostructures.
2. The vibrational properties of SiGe nanostructures, mainly quantum dots, are currently under study by Raman and micro-Raman measurements.
3. The electronic properties of Ge/SiGe multiple quantum wells are studied by transmission and photoluminescence measurements in a wide temperature range.
4. Electron spin sensitive measurements on Ge/SiGe structures are performed; the photoluminescence with light polarization control is studied.

QUANTUM STRUCTURES BASED ON III-V SEMICONDUCTORS

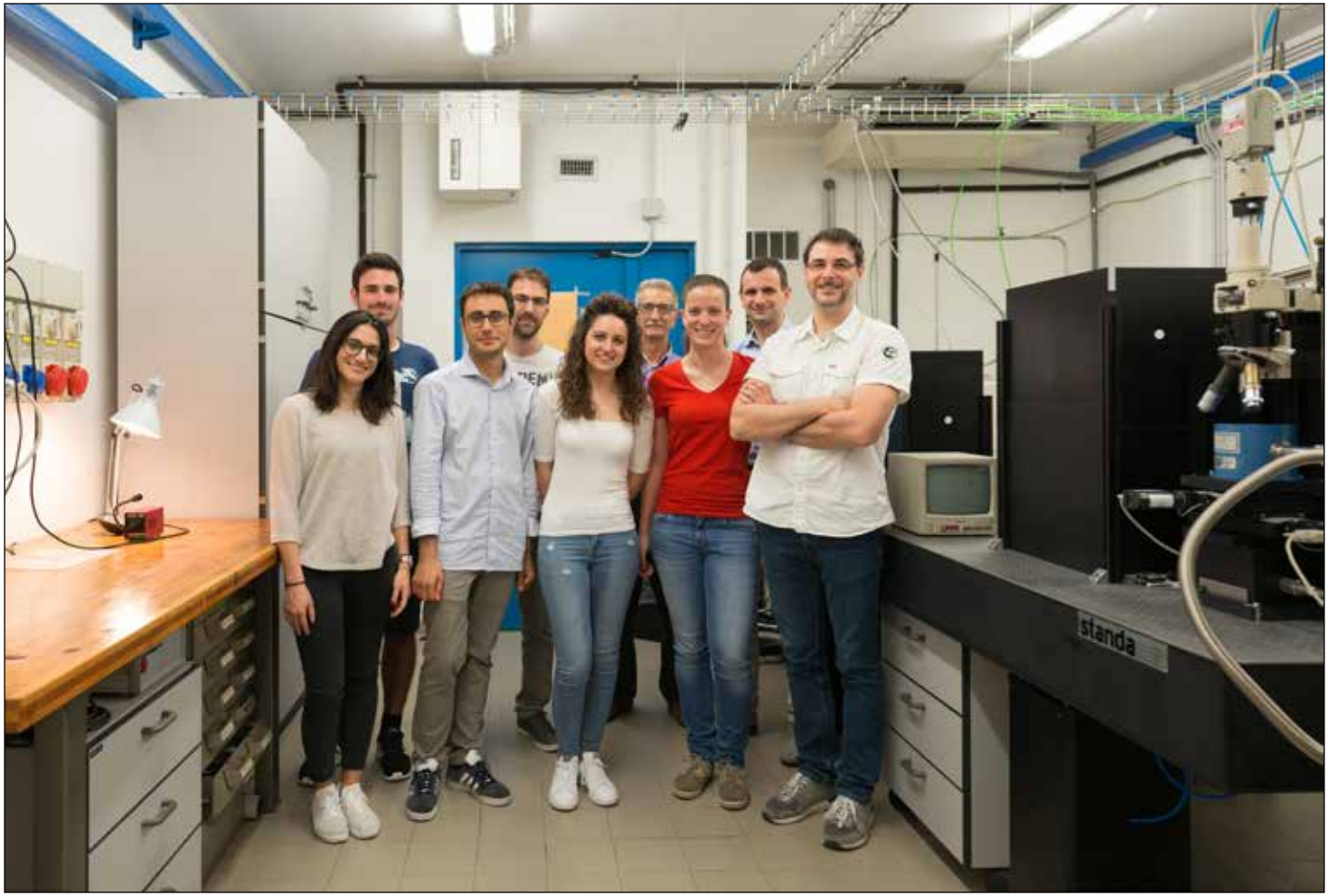
Amongst the nanoscience advancements, relevant place is taken by quantum confinement effects that take place in semiconductor quantum dots (QDs). Like the natural atoms QDs show discrete energy levels. Laser, infrared photodetectors, as well as third generation photovoltaic cells show can be improved by the use of QDs in the active layer. The study of QD-based devices has provided new ways for the understanding of strongly correlated few electrons/excitons systems and their possible applications, such as single-electron devices and single photon emitters for quantum cryptography and computation.

1. We develop innovative growth procedures for the fabrication quantum nanostructures with ad-hoc designed electronic properties;
2. We study the nanostructure properties via spectroscopic measurements addressing electronic structure and carrier relaxation mechanisms;
3. We study the transfer of the III-As QD devices on Si for integration with standard electronics.

FACILITIES

Spectroscopic apparatuses based on dispersive and FT spectrometers are used for photoluminescence, photoluminescence excitation, transmission and Raman measurements in the 0.4 - 5.0 eV

spectral range. Raman spectroscopy can be operated down to 5 cm-1. Working temperatures: 2 K to 450 K. Sources: He-Ne, Ar, doubled-Ar, Ti-Sapphire, DPSS and Diode lasers, incandescent and high pressure lamps. A low temperature (4 K – 300 K) micro-photoluminescence and micro-Raman apparatus working in the 0.75 – 3.4 eV spectral range is available. Time resolved photoluminescence and photoluminescence decay down to 10-8 s can be measured with DPSS-QS lasers. Molecular-beam epitaxy for III-V semiconductors and AFM characterization.



Photophysics of Molecular Materials and Semiconductor Nanostructures

SERGIO **B**ROVELLI, **F**RANCO **M**EINARDI, **A**NGELO **M**ONGUZZI

SEMICONDUCTUR NANOSTRUCTURES

Using colloidal semiconductor nanocrystals (NCs) one can produce extremely strong spatial confinement of electronic excitations not accessible with other type of nanostructures. Because of spatial constraints imposed on electronic wave functions, energy levels in NCs are directly dependent on their dimensions, a phenomenon known as quantum confinement. This effect is a powerful tool for controlling spectral responses of NCs, enabling potential applications such as multicolor labeling for biomedical diagnostics, lasing, solid-state lighting, photovoltaics and photon managing through a cost-effective bench-top chemistry approach. In addition to spectral tunability, strong spatial confinement alters Coulombic and magnetic interactions involving quantum confined carriers, leading to: large splitting of electronic states due to electron-hole exchange, ultrafast decay via Auger recombination and multiexciton generation by single photons via carrier multiplication. Furthermore, confinement induced mixing between the conduction and valence band can lead to interesting peculiarities in magnetic interactions such as recently observed persistent photo-magnetism, where the UV/blue light triggers photochemical reactions and the IR emission stimulates the cell activity. The potential of interfacial engineered nanostructures is further amplified by the remarkable achievements in active doping, which provide an additional degree of freedom for tuning the functionality colloidal NCs.

NON COHERENT PHOTON UP-CONVERSION

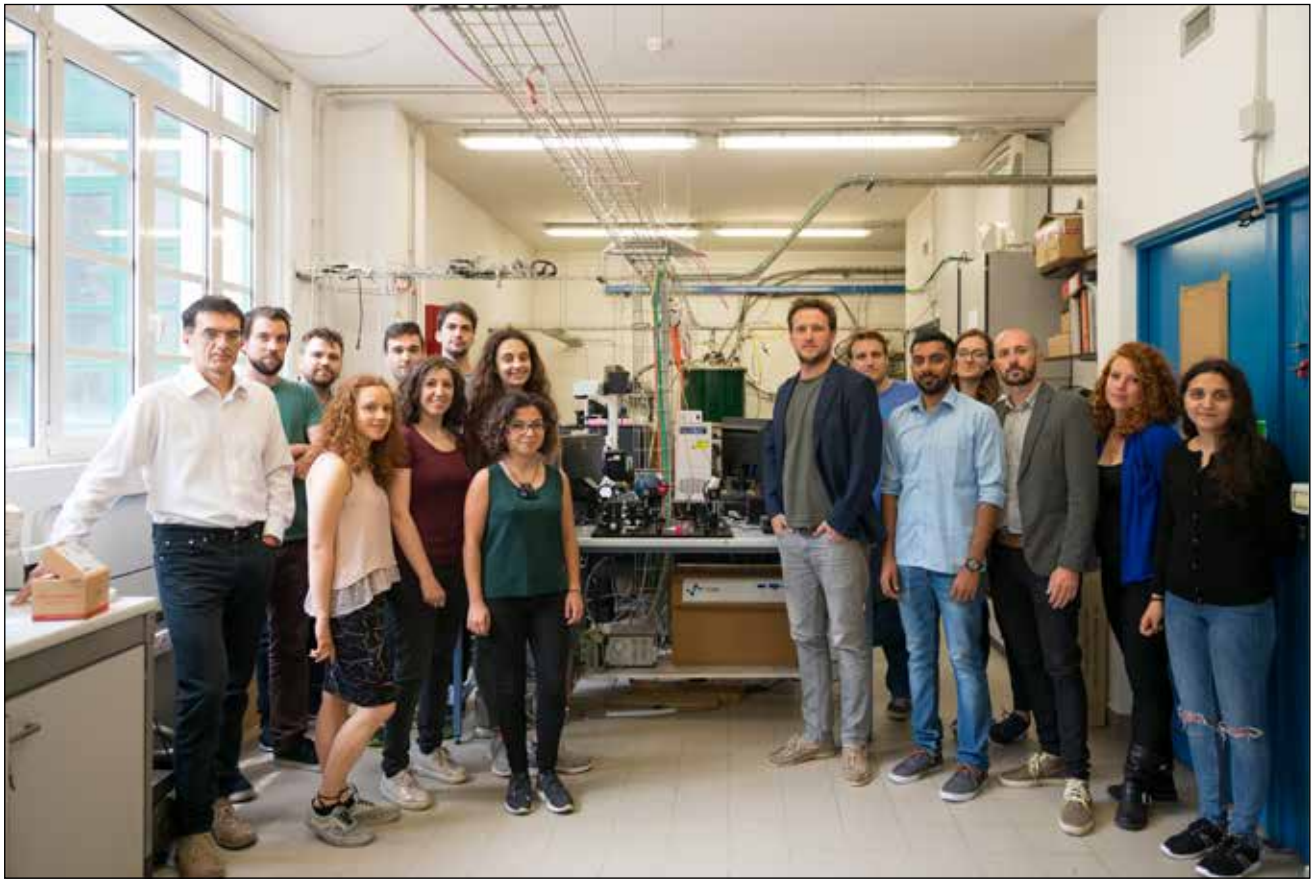
The generation of photons at higher energy in respect to the excitation, namely the up-conversion, through non-linear optical response of materials is useful to reach spectral region not easily accessible. Anyway, traditional techniques are appreciably efficient only by employing coherent light sources with intensity of the order of MW/cm^2. Our research is focused on the development of multicomponent organic and hybrid supramolecular systems (MOF) able to convert non-coherent harvested photons with intensity down to μW/cm2, where up-conversion is achieved by annihilation of metastable states indirectly excited by resonant energy transfer. Excitation light blue-shift could have important application in the photovoltaic technologies to recovers the low energy tail of sub-bandgap photon of the solar spectrum, as well as a potential new approach to build blue and UV light sources exploitable for lightning technologies such as WOLED and color displays.

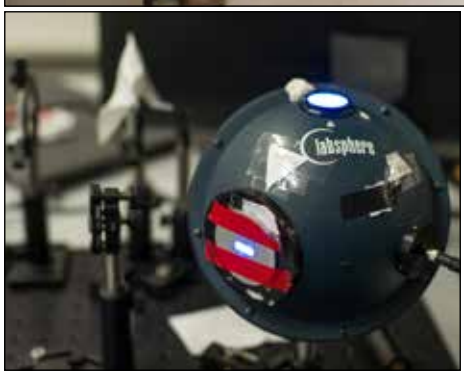
OPTICAL PROPERTIES OF METAL QUANTUM CLUSTERS

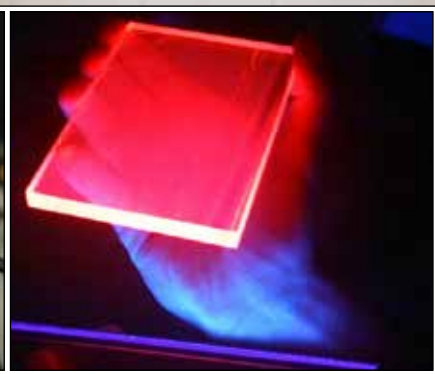
Metal quantum clusters are functional nanomaterials with potential for use in sensing, bio imaging, optoelectronics, and nanomedicine. These few-atom structures bridge the gap between atoms and colloidal nanoparticles combining a molecule-like electronic structure with quantum effects. We exploited this feature to fabricate permanent excimer-like colloidal superstructures made of ground-state non-interacting gold cores connected by a network of hydrogen bonds. This previously unknown aggregation state of matter conveys the photophysics of excimers into stable nanoparticles, which overcome the intrinsic limitation of excimers in single-particle applications. In vitro experiments demonstrate their potential as non-resonant intracellular probes and reveal their ability as anticytotoxic agents.

FACILITIES

Optical spectroscopy laboratory with setups for steady state and time-resolved photoluminescence measurements in the visible-near UV and IR regions, optical absorption measurements, confocal fluorescence and Raman micropy, spectro-electrochemistry. A superconducting crio-magnet (up to 5 T) with variable temperature insert (1.5-300 K) for optical experiments in high magnetic fields and cryogenic temperature, and a photoinduced absorption setup in the ns time regime.







Oxide nanostructures and silica-based materials for optical technology

MAURO **F**ASOLI, **A**LBERTO **P**ALEARI, **A**NNA **V**EDDA

Our research is focused on the physical properties of silica-based glass and glass-ceramics for applications in photonics and optolectronics. Bulk and film materials are synthesized and investigated looking at the particular optical properties one can obtain and control by doping with active ions and crystalline nano-phases. Doped silica glass and glass-ceramics are technologically interesting for their signal amplification properties in the telecom windows, nonlinear and light-emission properties induced by dopants and crystalline nano-phases, and good optical transmission and compatibility with existent glassy-silica based devices. Fundamental aspects of the study regard the spectroscopy of rare earth ions, point defects, and wide-energy-gap nanostructures in optical hosts. Synthesis techniques have also been optimized to obtain good dispersion of active ions and crystalline nano-clusters in glass-based materials.

RESEARCH LINES

Optical properties of rare earth ions such as Ce, Gd, Tb, Eu in bulk silica and in Hf-based oxide nanoparticles, studying the interaction with the host matrix, to obtain materials suitable to be used as scintillators in the detection of low-energy ionizing radiations for industrial and medical applications. The role of point defects in crystalline scintillators is also investigated.
Light-emission and non-linear optical properties of wide-band-gap oxide nanostructures in glasses, such as Ga_2O_3 and SnO_2 nanocrystals in silicates, analyzing the applicability as light-emitting systems, photo-sensitive optical materials, cubic non-linear components, and transparent conductors.

FACILITIES

SPECTROSCOPY LABORATORY: optical absorption, photo- thermo- and radio-luminescence spectroscopy, micro-Raman scattering, refractive index and film thickness measurements, thermostimulated currents and complex impedance spectroscopy. Micro-ATR-FTIR analysis, micro-profilometryr, pulsed luminescence spectroscopy and SHG by Nd-YAG laser with second and fourth harmonics.
SYNTHESIS LABORATORY: inorganic chemistry laboratory for sol-gel preparations in controlled conditions, comprising hoods and dry-boxes for the synthesis of bulk samples and films. Film deposition by spin-coating. Samples from aerogel can also be obtained by hypercritical drying process. Furnaces for densification processes in controlled temperature and atmosphere, as well as instrumentation for optical finishing.

Materials and spectroscopies for nanoelectronics and spintronics (MSNS Laboratory)

MARCO **F**ANCIULLI

Our research is mainly devoted to the experimental investigation of semiconductors, oxides, semiconductor/oxide interfaces, silicon and germanium nanostructures, MoS_2 growth, for advanced and innovative nanoelectronic, spintronic, and neuroelectronic devices. The research activity is carried out in strong collaboration with the CNR-IMM, MDM Laboratory and leading semiconductor industries, Micron and STMicroelectronics

POINT DEFECTS IN SEMICONDUCTORS AND OXIDES

Study of the electronic properties of point defects in semiconductors (Si, Ge) and in high dielectric constant materials (transition metal oxides) using electron spin resonance techniques and inelastic electron tunneling spectroscopy.

SEMICONDUCTOR/OXIDE INTERFACES

Investigation of silicon/oxide, germanium/oxide interfaces using electrically detected magnetic resonance (EDMR) and inelastic electron tunneling spectroscopy (IETS).
In-situ investigation by EDMR of the early stages of oxidation and interface formation at the Si/oxide and Ge/oxide interfaces.

Si AND Ge NANOSTRUCTURES

The electronic and spintronic properties of the following nanostructures
- Silicon nanowires produced by e-beam lithography and oxidation.
- Silicon nanowires produced by metal-assisted chemical etching (MACE)

Silicon and germanium nanowires and nanoclusters produced by CVD and MBE are investigated using mainly spin dependent transport techniques aiming at the characterization of shallow donors, electrostatically confined electrons, Coulomb blockade.

GROWTH AND CHARACTERIZATION OF TMDC (MoS_2, WS_2)

TMDC are grown with a novel method and their properties characterized with Raman spectroscopy (Collaboration with E. Bonera) and electrical measurements.

EXPERIMENTAL FACILITIES

Growth and processing
Atomic Layer Deposition (ALD) mini-chamber with O_3 line for in-situ characterization.
Horizontal and vertical furnaces for annealing and diffusion
Q-switched Ruby laser for laser annealing
Characterization

Two CW X-band systems for electron spin resonance (ESR) spectroscopy, electrically detected spin resonance spectroscopy (EDMR) and electron nuclear double resonance spectroscopy (ENDOR).
Variable temperature measurements (4-600 K).
Multi-frequency (0.1-40 GHz) EDMR
Set-up for inelastic electron tunnelling spectroscopy (IETS) working in the temperature range 4-300 K

Modeling and simulations of epitaxial semiconductor depositions and nanostructures

LEO **M**IGLIO, **F**RANCESCO **M**ONTALENTI

Deposition of Ge (or SiGe alloys) on Si leads to a wealth of different phenomena, mostly caused by the elastic energy unavoidably accumulated when trying to epitaxially grow one material (Ge) on a substrate (Si) with a different lattice parameter. In our group, we investigate such phenomena by formulating interpretative models based on computer simulations.

For example, we are interested in understanding strain-release triggered formation, stability, morphological evolution, and ordering of Ge nanostructures (islands), including the effect of Si/Ge intermixing. A combination of different methods is needed to achieve this goal. If atomistic Kinetic Monte Carlo and/or continuum models are needed to describe growth kinetics, thermodynamic aspects can be tackled by a synergic use of Density Functional Theory, providing surface energies, and classical molecular dynamics simulations or elasticity theory (numerically solved by Finite Element Methods), used to establish the volumetric elastic energy.

Particular attention is also dedicated to understanding the onset of plastic relaxation (injection of misfit dislocations) both in flat SiGe/Si films and in SiGe 3D islands, and its competition with elastic relaxation. To this goal, we developed a suitable methodology to treat extended defects within a continuum approach.
Lately most of our attention has been focused on exploiting suitable patterning of a Si(001) substrate to obtain ordered arrays of islands and/or to influence dislocation nucleation, confining defects in desired positions. We have discovered that on a suitably pit-patterned substrate, very peculiar processes take place, leading to an extra-relaxation (with respect to the flat substrate case) of nanoislands, with important consequences also on the onset of plastic relaxation.

Our connection with experiments is extremely tight: we work in very close collaboration with several international groups, and most of our representative works are jointly published with them, offering at the same time both experimental evidence and theoretical interpretation of a given phenomenon.

Fabrication and study of semiconductor quantum nanostructures (EpiLab)

STEFANO **S**ANGUINETTI

The research activity is aimed at the development of epitaxial semiconductor quantum nanostructures for applications in quantum photonics, quantum optoelectronics and electrochemistry
EpiLab is part of L-NESS Inter-University Laboratory (Epitaxial Nanostructures Laboratory of Semiconductors and Spintronics) in collaboration with the Politecnico di Milano and Joint QUCAT Laboratory (Quantum Nanostructure Photo-Catalysis) with the South China Normal University (SCNU) in Guanzhou (China)

QUANTUM DOT EMITTERS FOR QUANTUM PHOTONICS APPLICATIONS

Fabrication of semiconductor and semiconductor quantum dots with shape and strain control for quantum photonics applications (quantum teleportation, quantum cryptography etc.)

NANOSTRUCTURED SEMICONDUCTORS FOR OPTOELECTRONICS

Development of monolithic integration processes of compound semiconductor materials on silicon substrates using non-equilibrium growth techniques for imaging and optoelectronics applications. Development of devices, through electronic design, band engineering and quantum design for thermal infrared imaging (Quantum Dot Infrared Photodetectors) for space applications (Earth Observation).

QUANTUM FUNCTIONAL MATERIALS FOR PHOTO-ELECTRO-CHEMICAL APPLICATIONS

Growth and characterization of nanostructured InN/InGaN materials for photocatalytic electrodes for applications in biochemical sensors and hydrogen solar generation.

FUNDAMENTAL STUDY OF EPITAXIAL GROWTH OF SEMICONDUCTORS

Study of the theoretical-experimental fundamentals of epitaxial growth of semiconductors: kinetic growth control, nanostructuring, droplet epitaxy.

FACILITIES

Two Molecular Beam Epitaxy deposition chambers (MBE) for Arsenic and Nitrogen based semiconductors
Atomic Force Microscope (AFM)
Clean Room equipped for the fabrication of electronic devices

Organic molecular films and heterostructures

ADELE **S**ASSELLA

Thin film growth. Films of organic molecular semiconductors are grown by organic molecular beam epitaxy (OMBE) under different conditions, such as pressure, substrate type and temperature, absence or presence of external fields. The study of the OMBE growth process itself is carried out by detecting in situ and in real time the properties of the growing samples. The main interest rests in the intrinsic properties of the molecular materials in the solid state and, in particular, in the form of thin layers of high crystalline quality, suitable for device applications. Several molecules, such as oligothiophenes, oligocenes, acridines, and porphyrines are studied. The main technique applied in-situ is reflectance anisotropy spectroscopy (RAS), which gives insight on the evolution of the electronic properties of the films during growth. The morphology and structural properties of the samples, closely related to the growth mode, are then studied ex-situ, mainly by atomic force microscopy; finally, the optical properties of the molecular films are studied in comparison with the single crystal properties. In the frame of well established collaborations, the structure of the thin films is checked by X-ray diffraction and, for some materials, the transport properties determined

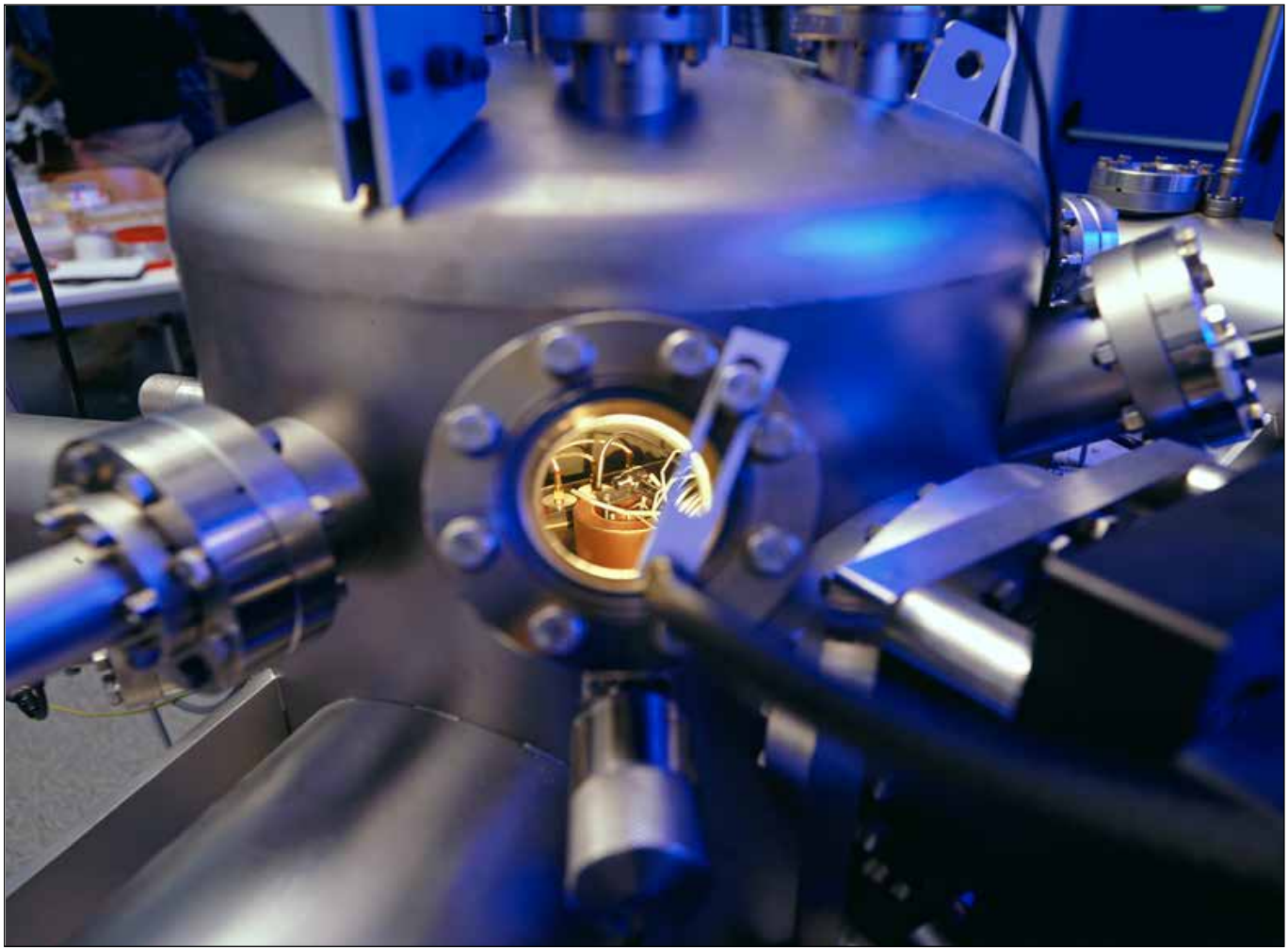
Heterostructures. Films of different molecules are grown on high quality single crystals of the same or similar molecular organic compounds, to reach the conditions for epitaxy, therefore preparing artificial structures with high quality interfaces and controlled properties. Few nm-thick films are also stacked in multilayers on different inorganic and organic substrates. The morphology and structure of each layer, the interface quality, and the electronic states of the whole structure are studied by scanning probe microscopies and by optical techniques

Single crystals. Single crystals of the same molecular compounds are grown from solution, from the vapour phase, and from floating drop, a technique developed in order to obtain crystals of higher quality in terms of structure and surface control, with shape and size suitable for their use as substrates for OMBE and for the structural and optical studies. In addition, also different molecules are considered to grow single crystals to be used as OMBE substrates: the selection favors materials which can promote epitaxial growth and those which can be easily removed after film growth, to permit the film transfer on different, technologically relevant substrates. Recently, some aminoacids have demonstrated to offer both these characteristics.

FACILITIES

The OMBE apparatus consists of several ultra-high vacuum chambers where up to six sources can be installed for depositing different compounds; during OMBE growth, the film thickness is monitored in-situ by a quartz microbalance and its optical behavior by RAS. Optical spectroscopies, such as absorption, reflection, photoluminescence and ellipsometry, are used for the study of thin films and multilayers ex-situ, also in comparison with the properties detected in-situ by RAS. Optical measurements can be

carried out as a function of temperature, down to few K, under polarized light and at different incidence angles. Atomic force microscopy is used ex-situ for the morphology characterization of all the samples and for the study of the film growth process; morphology is usually checked over sereval μm2 wide regions, while on crystalline samples molecular resolution is also achievable.



Materials science and cultural heritage. Dating and characterization of ancient materials.

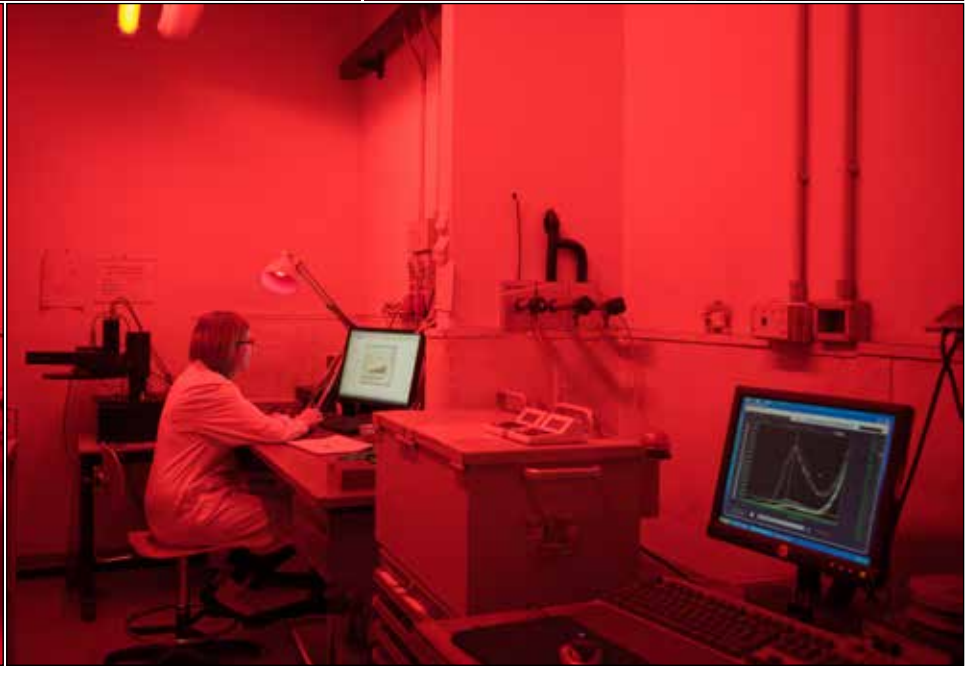
ANNA **G**ALLI, **M**ARCO **M**ARTINI, **E**MANUELA **S**IBILIA

THE ARCHAEOMETRY LAB

Since 1980 our activity focused on the application of scientific techniques to archaeology, geology and cultural heritage, in particular in the field of absolute dating and characterization of archaeological materials.
Thermoluminescence (TL) and optically stimulated luminescence (OSL) are used to determine the event of ceramics firing and sediment deposition respectively. Other available techniques are dendrochronology and radiocarbon. Recently, we started investigating the new Rehydroxylation (RHX) dating technique, based on the water gain of pottery after firing in kiln.
Our research also deals with non-invasive spectroscopic methods, mainly performed using portable instruments, to study polychrome artefacts of various kind (paintings on boards, enamels, decorated ceramics, metal artifacts ...).
The laboratory is member of CUDaM (Centro Universitario Datazioni Università di Milano Bicocca amd of BIPAC, Centro Ricerche per il Patrimonio Storico, Artistico e Culturale.
The laboratory is associate member of EURADOS (European Radiation Dosimetry Group, Working Group 10), of MODIS (Mortar Dating Intercomparison Study) and of the RHX International Research group to validate and study the rehydroxylation dating technique.
Since 2012 the laboratory is a first level hub in the CH_NET E-RIHS Italian cultural heritage network.

RESEARCH LINES

Fundamental studies of the low temperature TL peak in quartz and of the Pre-dose effect
Optical properties of mosaic glasses
Charge transfer phenomena in quartz and feldspars luminescence.
New procedures for the extraction of collagen for 14C dating
New procedures for identifying and selecting the anthropogenic calcite in archaeological mortars.
TL and OSL dating of mortars, Surface dating
Study and characterization of natural materials for accident dosimetry
Rehydroxylation (RHX) dating of archaeological pottery
Joined use of non-invasive methods (EDXRF, FORS, Raman) for the characterization of Renaissance pigments.
Development of portable systems for in situ XRF analysis



Organic and hybrid materials and devices for photovoltaics, artificial photosynthesis and optoelectronics (MIB-SOLAR)

ALESSANDRO **A**BBOTTO

Present energy needs are classified into two main sectors: a) production of electricity; b) production of reactant and fuels for heat and transportation. We focus our interest on the use of clean sources like sunlight and water to provide these energy sources, that is photovoltaics and artificial photosynthesis. In the MIB-SOLAR lab, containing an ISO7 clean room and state-of-the-art facilities, we investigate materials and devices for photovoltaics and artificial photosynthesis.

ARTIFICIAL PHOTOSYNTHESIS: CLEAN AND RENEWABLE SOLAR FUELS

We study dyes and catalysts to produce hydrogen and oxygen, also in combination with bio-inspired and bio-mimic materials. Two main approaches are used: a) photocatalysis; b) phoelectrochemical cells (PEC). In particular, we focus our attention on solar induced water splitting in PCE, investigating materials for photoanodes (oxidation of water), photocathodes (reduction of water), and tandem PEC devices (artificial leaf). Focus is on metal-free, low cost molecular antennas based on earth-abundant materials in order to provide enhanced light harvesting, solar-to-fuel conversion efficiency, and long-term stability.

ORGANIC AND HYBRID 3RD GENERATION PHOTOVOLTAICS

We investigate last generation organic and hybrid photovoltaics, namely:
-dye-sensitized solar cells (DSSC)
-perovskite solar cells (PSC)
-tandem multijunction cells.
Focus is on last generation devices such as graphene-based sensitizers and eco-friendly drinkable media.We also investigate tandem multijunction cells in combination with silicon and thin film inorganic technologies, in order to access higher performances. A large variety of materials (organic and organo-metallic dyes, electron and hole transporting materials, electrolytes, semiconductor oxides, electrodes) are investigated as well as lab-scale and pre-industrial photovoltaic panels.


CodecBot

Functional dyes and pigments for photonics, electronics and optoelectronics

LUCA **B**EVERINA

Organic-conjugated compounds have experienced over the last decades a tremendous interest as versatile and highly performing active components in a large variety of devices and applications including, among the others, OLEDs, OFETs, solar cells, sensors, photodetectors, electrochromic devices, anti static coatings and actuators. The vast majority of the above mentioned applications rely on the peculiar nature of the charged states in organic semicondutors, namely: a strong electron-phonon coupling and a major dependence of optical properties on the doping process.We are currently exploring the ability of carefully designed organic materials to:
-change colour upon multiple oxidation and reduction processes (electrochromic devices);
-convert incident Vis-NIR light in electric power (solar cells);
-show efficient photoconductivity in NIR window (photodetectors);
-absorb light all over the visible spectrum and convert it to efficient and concentrated NIR emission (luminescent solar concentrators).

LUMINESCENT SOLAR CONCENTRATORS

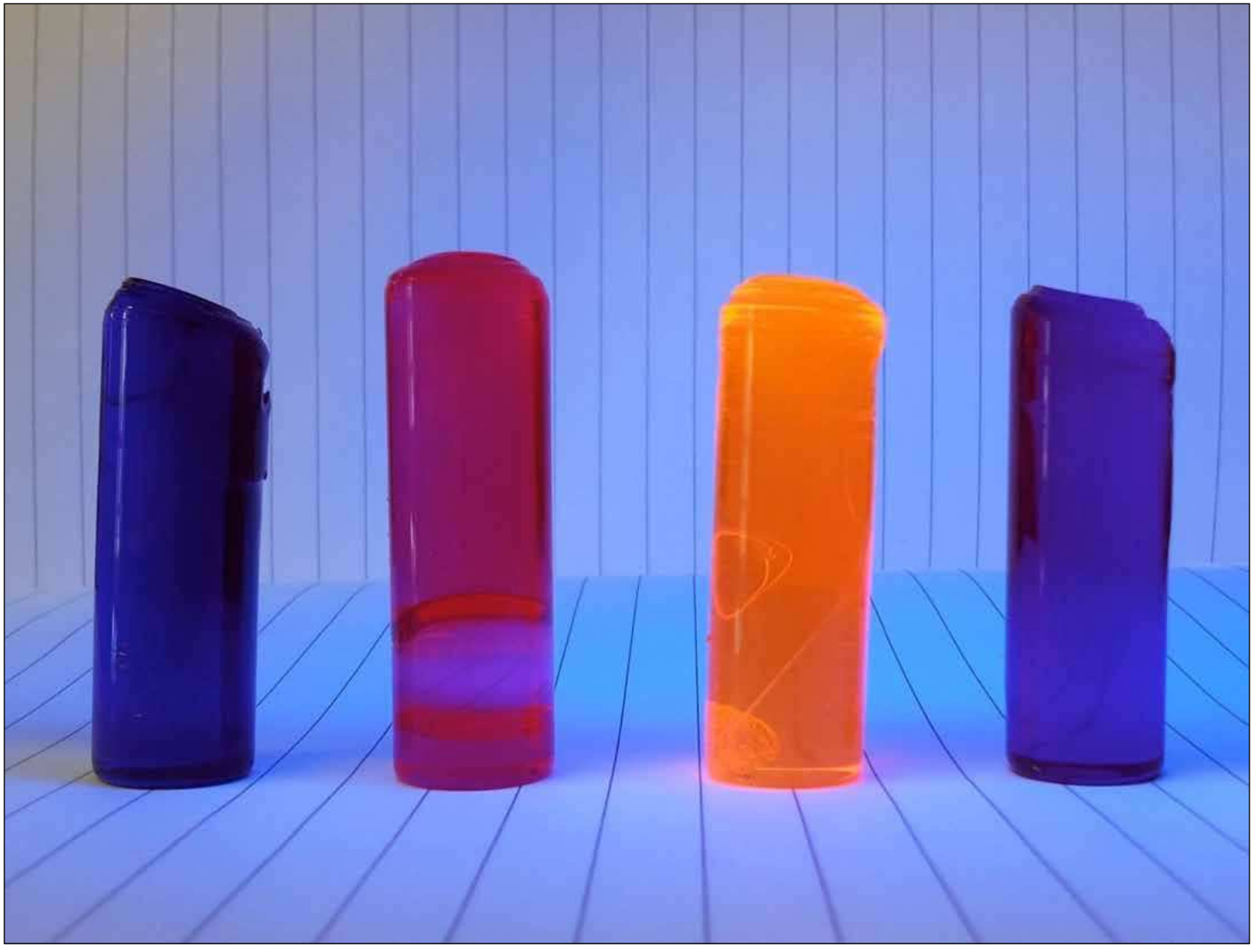
The potential of solar power is enormous, yet still largely unexploited because of the high cost of efficient silicon-based solar cells. Moreover, the efficiency of standard photovoltaic devices strongly depends on the light incidence angle and intensity. Luminescent Solar Concentrators (LSCs) could provide cost reduction, while ensuring operational capabilities under diffuse illumination conditions. LSCs are slabs of transparent, high optical quality materials doped with luminescent molecules. The molecules absorb sunlight and emit inside the slab. Since the refractive index of the slab is higher than that of air, most of emitted light is guided to edges and there collected by small area solar cells.

CONJUGATED ORGANIC MATERILAS FOR OPTELECTRONIC-SUMINESCENT SOLAR CONCENTRATORS

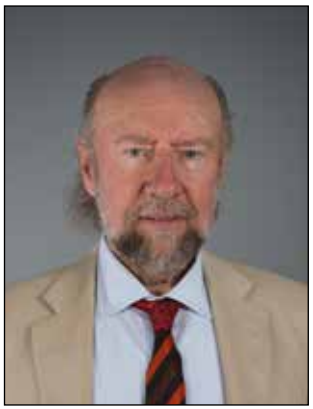
The development of efficient structure-properties relationships in pi-conjugated materials in particular is boosting the emerging field of the molecular electronics, along with other interesting applications in research areas normally associated with standard inorganic semiconductors such as high-speed telecommunication. We have a strong experience in the synthesis and supramolecular ordering on highly performing organic materials for electro-optic modulators.

OTHER ACTIVITIES

Photoresist, Organic secondary batteries, Singlet oxygen sensitizer, Lantanide chelates



Nanostructured materials and magic angle spinning NMR



SILVIA **B**RACCO, **P**IERO **S**OZZANI

The preparation and characterization of novel composite and nanocomposite materials is the target of our research group. Reinforcing agents for polymers and polymers as binders for reactive inorganic materials are mainly addressed. The effort for optimizing the interfaces lead to the preparation of highly porous and shape controlled silica-based materials and nanostructures which confine a second component. In the latter case the nanocomposites show unusual mechanical and optical properties. Electro-optical properties can be also modulated in the composite and compared to the bulk. The link between structure and properties is provided by a detailed characterization by magic angle spinning nuclear magnetic resonance (MAS NMR), wide-line NMR and by other solid-state techniques (atomic force microscopy, DSC and dynamic-mechanical analyzer). An NMR laboratory dedicated to solids is available.

CURRENT RESEARCH PROJECTS

Composite materials based on ceramics and polymers and characterization of heterogeneous interfaces (elastomeric materials reinforced with silica, in-situ formation of silica by gelification in polymer matrices). Confinement of molecules and macromolecules to cylindrical nano- and mesotubes (cross section of 0.5, 1 and over 30 nm). Some matrices, showing extended interactive areas (>1200 m^2/g), form supramolecular adducts endowed with unusual properties (liquid-crystalline behaviour, anomalous glass-transition, conformational solitons propagating along the polymer-chains even at very low temperature). The study of reactivity and interactions among included species in molecular vessels is also addressed (gamma ray initiated polymerization). Preparation of end-functionalized polymers to be reactive onto heterogeneous materials. Crystal morphology, defects and mesomorphysm of polymeric materials (ethylene-propylene copolymers). Diffusion processes of gases into materials and exploitation of spin-active gases (^{129}Xe) diffusing into solids, for microphases determination and nanoporosity by NMR.

FACILITIES

NMR Bruker Avance with wide bore 7.05 Tesla superconduction magnets fully equipped for high power output, 7kHz and 15kHz magic angle spinning probes and several heads for wide-line spectroscopy, including deuterium. High vacuum (10^{-9} torr) pump and equipment for hyperpolarized Xenon spectroscopy -laser excited NMR). Dynamic Mechanical Analyzer, Differential Scanning Calorimetry Gel Permeation Cromatography and access to large NMR facilities.

Organic molecular systems for II order non-linear materials, low energy emitters and organic semiconductors

ANTONIO **P**APAGNI

The current research interests are essentially focused on the development of organic materials for applications in photonics and optoelectronics; the main topic is the design and synthesis of semiconducting materials for alternative energy applications.

Organic solar cells (both bulk heterojunction solar cells and crystalline organic solar cells) are the main target and the research activity involves two different kinds of applications.

Bulk heterojunction solar cells (BHJSCs) are experiencing an impressive growth, both for the continuous increase of photoconversion efficiency (PCE) and for the increasing numbers of research groups and industrial players involved in this subject. The still increasing values of PCE are the result of a careful design of the active materials composing the core of BHJSC. The third generation of semiconducting materials for BHJSC is give by internal donor-acceptor conjugated polymers. The design of new electron-acceptors and the correct synthesis of donor-acceptor polymers based on them are currently undertaken exploiting the know-how in the field of fluorinated materials and also exploring alternative synthons. The fabrication of solar cells and their analysis is carried out in collaboration with Italian and European research centres and companies.

Crystalline organic solar cells are a less studied alternative to BHJSC, to overcome some of their intrinsic limits. Crystalline organic materials, based on substituted acenes, are a viable solution to get materials with higher mobility and with a lower density of defects. Acting on the dimension and electronic properties of the peripheral substituents groups it is possible to tune the semiconducting properties, absorption and emission energies and to act on crystal packing. For the fabrication of crystalline organic solar cells Organic Beam Molecular Deposition (OMBD) is the most suitable approach, allowing the controlled growth of crystalline organic multilayers and nanostructures. This activity is carried out with other researchers of this Department and with the ISMAC centre of CNR.

A significant effort is also devoted to the analysis of degradation in organic solar cells, to investigate the phenomena responsible for their thermal and photodegradation and to develop strategies to increase their durability.

Synthesis and characterization of novel polymeric nanostructures

ROBERTO **S**IMONUTTI

Nanostructured polymer materials have attracted growing interest due to their applicability in many different areas: from microelectronics to photonics, from catalysis to water purification, from biomedical to military applications. Among many different strategies used for preparing polymeric nanostructures, we focus our research on self-organization of block copolymers and dispersion of inorganic nanoparticles in polymer matrices.

NEW MATERIALS BASED ON BLOCK COPOLYMERS

Block copolymers are constituted by two or three different types of polymer chains connected at the ends with a covalent bond. They display self-organization on the nanometre scale modulated by the external environment. For example, the interaction between block copolymer and solvent produces a diversity of self assembled shapes, including vescicles, spheres, cylinders, that can be tuned by concentration, solvent polarity, temperature and other external stimuli. The morphology in the solid state can also be very complex and is finely tuned by the conditions and the method of solid formation (melt cooling, casting from solvent).

Recently, by implementing advanced polymerization techniques like RAFT (Reversible Addition-Fragmentation chain Transfer polymerization) we synthesized several samples of highly controlled amphiphilic block copolymers. Our interest is currently focused on innovative techniques for their characterization in liquid and solid state, as well as the almost unexplored intermediate soft matter states: highly concentrated solutions, gels and sponge-like materials.

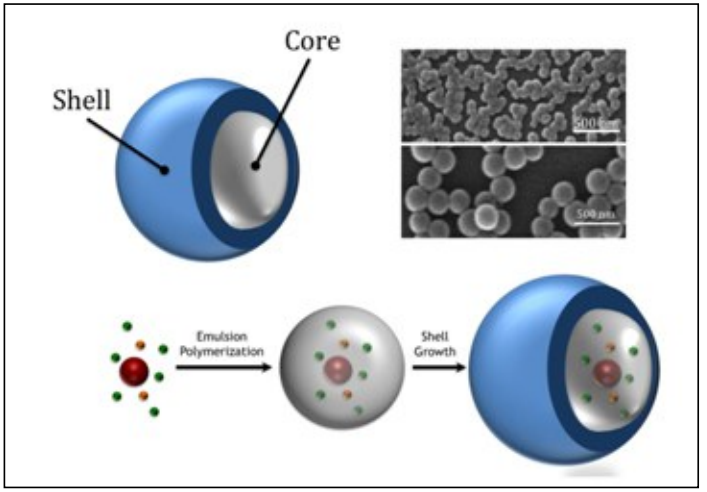
NANOPARTICLE POLYMER NANOCOMPOSITES

The mixing of polymers and inorganic nanoparticles, like oxides, semiconductors (usually defined as quantum dots) or noble metals, is opening pathways for engineering flexible composites that exhibit advantageous electrical, optical, or mechanical properties. In particular, the nanocomposite optical characteristics, as the refractive index, absorption of UV light, birefringence or scattering properties, can be modulated by carefully choosing the particle size and electronic structure of the nanoparticle used for its preparation.

Our research is now directed to the use of oxide nanoparticles with all the dimensions less than 100 nm. A key point of the experimental activity is the surface modification of the nanoparticles by a capping agent in order to increase the stability of the colloidal dispersion.

Nanocomposite molecular structure, morphology and mechanical properties are characterized by a comprehensive suite of advanced techniques, (among others: FTIR, TGA, NMR, DLS, AFM). The measurement of optical properties (absorption, transmission, angular scattering) of nanocomposite monolithic objects is done in collaboration with the University of Insubria.

Another possible application of these nanocomposites is in the conservation of cultural heritage, as protective layer that can protect the painting surface from UV radiation, preserving the aesthetics.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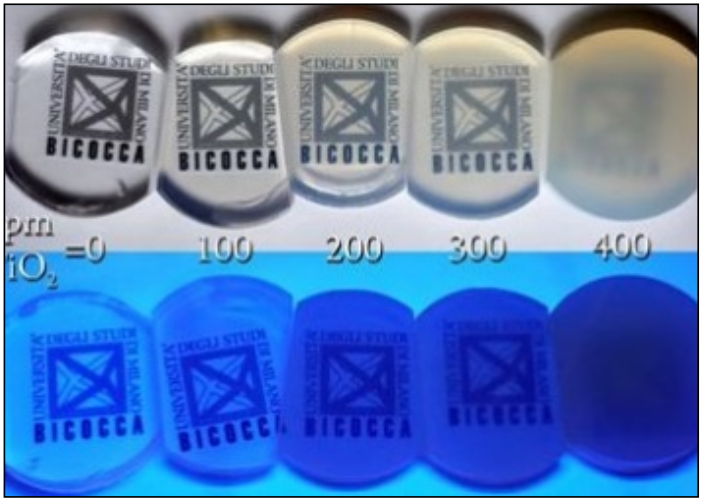
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Singular elliptic equations: asymptotic analysis, unique continuation, spectral stability for singularly perturbed problems

VERONICA **F**ELLI

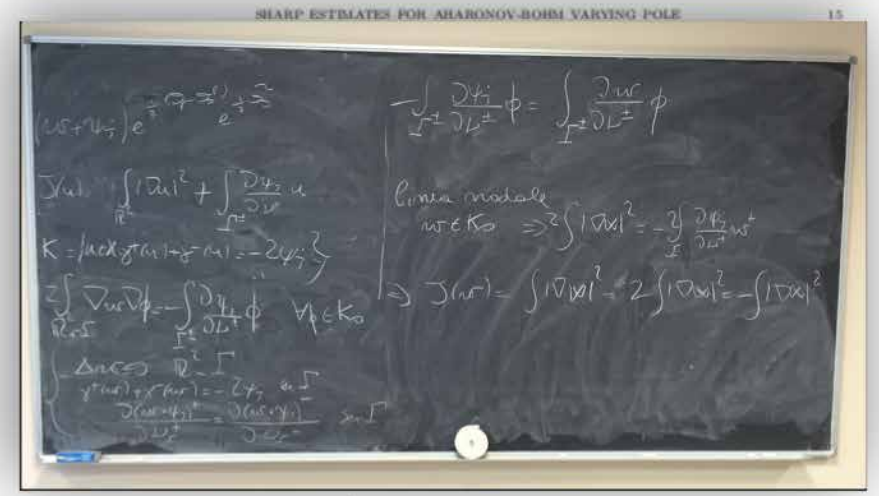
The following problem are investigated:

Spectral stability for singularly perturbed problems.
We study elliptic stability for elliptic operators, looking for sharp eigenvalue estimates for the following singularly perturbed problems:

-elliptic problems in perturbed domains obtained by attaching a thin handle to a fixed region;
-elliptic problems with mixed boundary conditions of Dirichlet-Neumann type;
-Aharonov-Bohm operators with (one or more) moving poles.

In these problems the sharp asymptotic behaviour of eigenvalues with respect to the perturbation parameter is expected to depend strongly on the vanishing order of the limit eigenfunction. The problem of the evaluation of the exact rate of convergence of eigenvalues of the perturbed problem to the eigenvalues of the limit problem is performed by using an Almgren type monotonicity formula combined with a fine blow-up analysis: indeed an Almgren type monotonicity argument allows obtaining quite precise energetic estimates near the singularity, which can be applied to the blow-up analysis of scaled eigenfunctions.

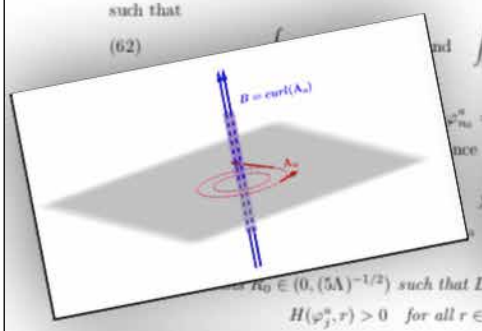
Asymptotic behavior and unique continuation properties for elliptic equations. We study the local asymptotic behavior of solutions to linear or nonlinear elliptic equations with applications to unique continuation principles. In particular we are interested in fraction elliptic equations (also the higher order case is considered): exploiting the Caffarelli-Silvestre characterization of fractional laplacian as the Dirichlet-to-Neumann operator, a monotonicity formula for fractional elliptic equations is developed.

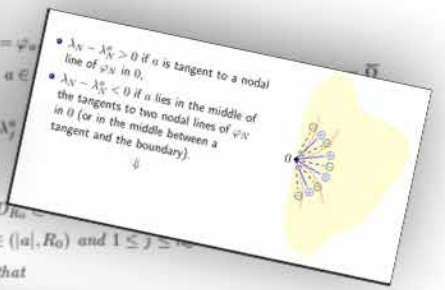


(61) $$\begin{cases} (i\nabla + A_a)^2 \varphi_j^a = \lambda_j^a \varphi_j^a, & \text{in } \Omega, \\ \varphi_j^a = 0, & \text{on } \partial\Omega, \end{cases}$$

such that

(62) $\int_\Omega \varphi_j^a(x)\overline{\varphi_\ell^a(x)}\,dx = 0$ if $j \neq \ell$.





$H(\varphi_j^a, r) > 0$ *for all* $r \in (|a|, R_0)$ *and* $1 \le j \le$

(ii) *There exist* $C_0 > 0$ *and* $\alpha_0 \in (0, R_0)$ *such that*

$H(\varphi_j^a, R_0) \ge C_0$ *for all* a *with* $|a| < \alpha_0$ *and* $1 \le j \le n_0$.

$$A_a(x_1, x_2) = \gamma\left(\frac{-(x_2 - a_2)}{(x_1 - a_1)^2 + (x_2 - a_2)^2}, \frac{x_1 - a_1}{(x_1 - a_1)^2 + (x_2 - a_2)^2}\right)$$

and assume that, for all n sufficiently large, there
such that $H(\varphi_{j_n}^{a_n}, r_n) = 0$, i.e.
we obtain

$0 = \int_{D_{r_n}}$

Since $r_n \to 0$, for n sufficiently large $1 - \Lambda r_n^2 > 0$ and
$\int_{D_{r_n}} |(i\nabla + A_{a_n})\varphi_{j_n}^{a_n}|^2\,dx = 0$. Lemma 3.1 then implies that $\|\varphi_{j_n}^{a_n}\|_{H^1(D_{r_n})}$
$\varphi_{j_n}^{a_n} \equiv 0$ in D_{r_n}. From the unique continuation principle (see [12, Corollary 1.4]) we conclude that
$\varphi_{j_n}^{a_n} \equiv 0$ in Ω, a contradiction.

Optics and Optometry

SILVIA **T**AVAZZI

The research activities concern materials science, optics, and spectroscopy applied to systems of interest for optometry and/or ophthalmology. Few examples are (i) the development and characterization of polymers for contact lenses and also for drug release by contact lenses, (ii) the material characterization before and after wear (surface morphology, roughness, rheology, geometry, etc.), (iii) the characterization of the preservative solutions for contact lenses and also of tears for diagnostic purposes, (iv) the development of specific instrumentation, and (v) the study of the mechanisms of vision, also in collaboration with specialists of this field.

MATERIALS FOR CONTACT LENSES

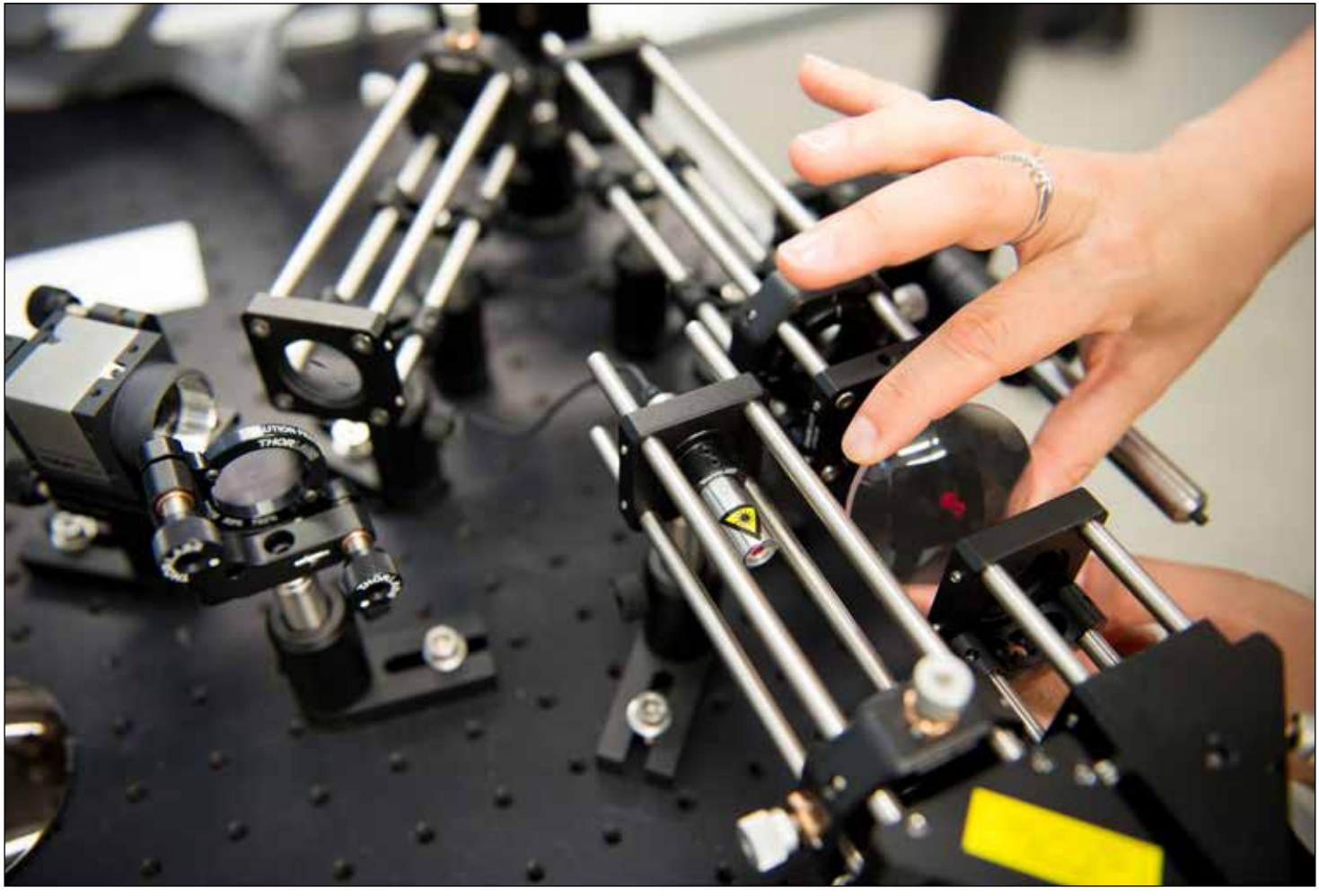
Recent studies were focused on the properties of materials for soft contact lenses in terms of microscopic structure and uptake/release of hyaluronan, lactoferrin, and drugs. Different materials were investigated. The uptake was studied in terms of loading capability, penetration depth in the lens, release profile as a function of time. The properties of the lenses were also characterized after wear. In some cases, a completely different scenario was observed compared to the unworn lenses, with the appearance of regions of swelling, depending on the type of material, attributable to the progressive relaxation of the polymeric network. Since the eyelid pressure is expected to be one of the factors causing material modifications, a study was focused on the pressure effects on the lenses. In siloxane-hydrogel materials, the mechano-synthesis of hydrogen peroxide was observed and attributed to the cleavage of siloxane bonds at the water/polymer interfaec.

OPTICAL SYSTEMS

A method was recently developed, which allows the acquisition under a slit-lamp bio-microscope of images of the corneal endothelium cells, which can be automatically recognized by a new procedure of morphometric analysis. The method provides data of the investigated endothelium area, the cell density, the frequency distribution histograms of cell area and shape. Cell density and morphology are clinical information of interest before and after corneal refractive surgery or implantation of intraocular lenses, for quality evaluation of donor corneal tissue in eye banks, before and after cornea transplantation, etc.

FACILITIES

The main facilities are UV-visible-NIR spectrophotometry, refractometry, spectroscopic ellipsometry, instrumentation for photoluminescence and illuminance analyses, fluorescence and polarized optical microscopy, instrumentation for visual analyses, such as phoropters, slit lamps, non-mydriatic retinal camera with fundus autofluorescence, non-contact tonometer/pachymeter, corneal topographer, ocular aberrometer, keratometers, ophthalmoscopes, retinoscopes, etc..



FUNDED PROJECTS

	Project	Funded by	PI
1	Costruzione e fornitura di dispositivi fotovoltaici basati su materiali fotoattivi perovskitici	ENI	ALESSANDRO ABBOTTO
2	Nuovi materiali coniugati per celle solari organiche	ENI	LUCA BEVERINA
3	Ab Initio Simulations of Chalcogenide Materials	Micron Semiconductor Italia	MARCO BERNASCONI
4	CHEETAH-Cost-reduction through material optimisation and Highert EnErgy outpuT of solAr pHotovoltaic modules-joining Europe's research and development efforts in support of its PV industry	EU	SIMONA BINETTI
5	Caratterizzazione di silicio multicristallino cresciuto in condizione di microgravità, a partire da silicio metallurgico	AGENZIA SPAZIALE ITALIANA (ASI)	
6	PLS - PN - SCIENZA DEI MATERIALI	MIUR	
7	Sviluppo di strati buffer per celle a base di CZTS	ENEA	
8	Caratterizzazione e analisi di celle solari ad alta efficienza tramite misure di risposta spettrale	CESI	
9	Crescita e caratterizzazione di film sottili di calcogenuri per applicazioni FV	RSE	
10	Misure di spettroscopia Raman per la caratterizzazione dello stress indotto nel silicio	CNR	EMILIANO BONERA
11	THINFACE-Thin-film Hybrid Interfaces: a training initiative for the design of next-generation energy devices	EU	GIANPAOLO BRIVIO
12	Electronic doped colloidal nanocrystal heterostructures for transformational breakthrought in solid-state lighting	FONDAZIONE CARIPLO	SERGIO BROVELLI

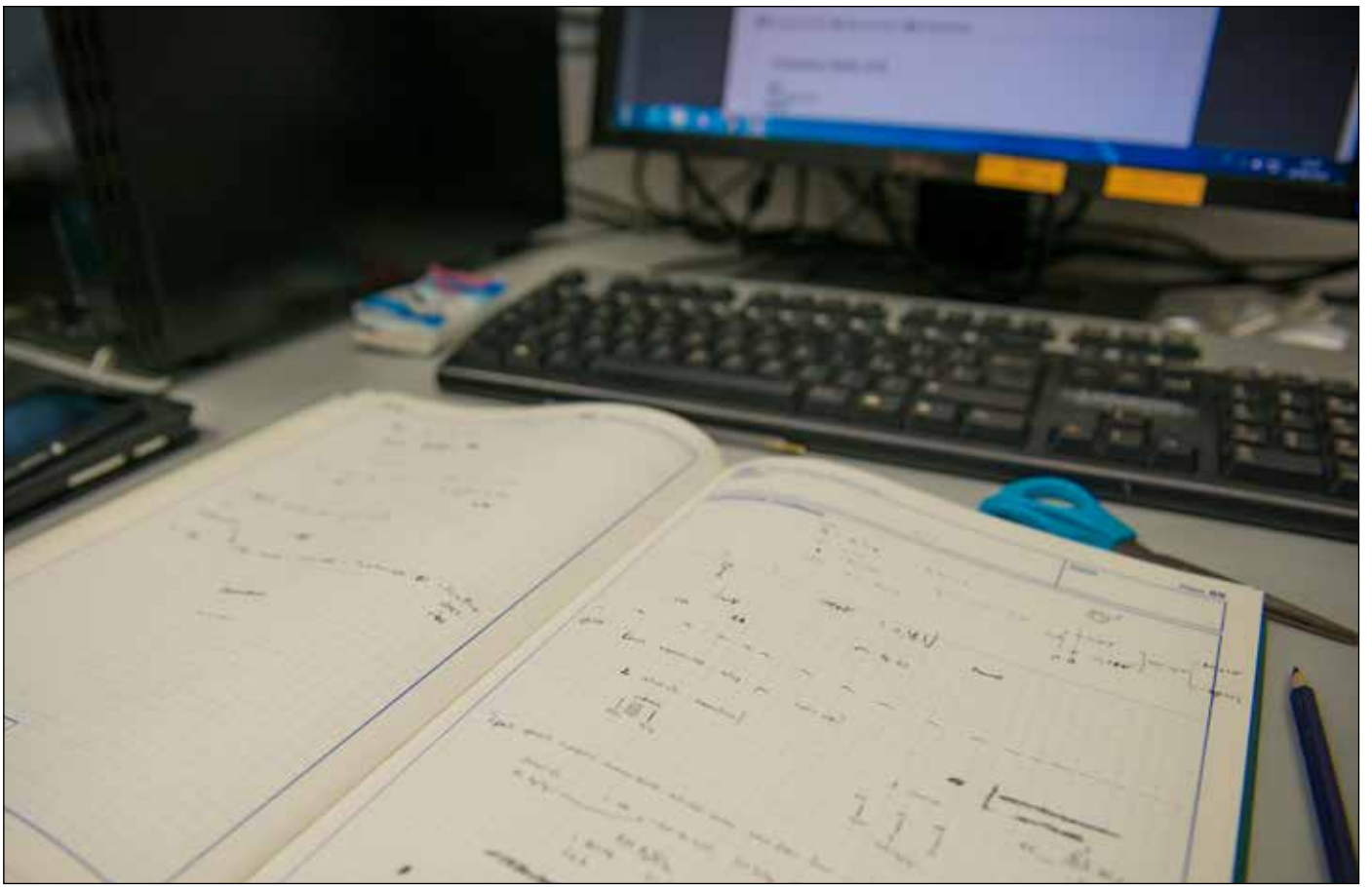
13	Realizzazione di preforme e caratterizzazione di fibre scintillanti da impiegare come elementi di sensori di radiazione ionizzante	Prysmian	NORBERTO CHIODINI ANNA VEDDA
14	Nanoporous materials with tailored structure for high performance methane storage and purification	MIUR	ANGIOLINA COMOTTI
15	Biomethane low impact production and carbon dioxide bio-capture for circular economy balance	FONDAZIONE CARIPLO	
16	KiC- LIGHTBODY- Infrastructure and expertise network for Lightweight mobility: body and chassis	EIT RAW MATERIALS GMBH	
17	Meccanismi di attivazione della CO2 per la progettazione di nuovi materiali per l'efficienza dell'energia e delle risorse	MIUR	
18	BIOINOHYB-Smart bioinorganic hybrids for nanomedicine	EU	CRISTIANA DI VALENTIN
19	DECORE-Direct ElectroChemical Oxidation Reaction of Ethanol: optimization of the catalyst/support assembly for high temperature operation	EU	
20	Nuovi materiali fotocatalitici per la conversione di energia solare basati su eterogiunzioni	FONDAZIONE CARIPLO	
21	Oltre il grafene: strati di carbonio nanostrutturati disegnati su misura per ottenere nuovi materiali per la catalisi e la chimica sostenibile	MIUR	
22	A new course on the physics and technology of semiconductor devices with hand-on activity in a characterization and simulation lab	MICRON TECHNOLOGY FOUNDATION INC	MARCO FANCIULLI
23	Variational methods, with applications to problems in mathematical physics and geometry	MIUR	VERONICA FELLI

24	Nanostructured oxide-in-oxide glasses for solar-blind UV-monitoring of work-safety and energy-saving in electric power distribution	FONDAZIONE CARIPLO	ROBERTO LORENZI
25	Studio e sviluppo applicativo di ossicarbonati e ossidi misti contenenti ioni lantanidi con proprietà luminescenti per applicazioni nel bio-imaging e nell'optoelettronica	MIUR	MARCO MARTINI
26	Luini in nuova luce	FONDAZIONE CARIPLO	
27	MOBARTECH: una piattaforma mobile tecnologica, interattiva e partecipata per lo studio, la conservazione e la valorizzazione di beni storico-artistici	REGIONE LOMBARDIA	
28	Nuove nanostrutture colloidali con molteplici funzionalità ottiche e magnetiche per applicazioni avanzate in elettronica, fotonica e diagnostica biomedica. II annualità	FONDAZIONE CASSA DI RISPARMIO DI TORTONA	FRANCESCO MEINARDI
29	Electronic doped colloidal nanocrystal heterostructures with designed interfacial composition: towards the development of new nano-device concepts for lighting and energy technologies	EU	
30	Nuove nanostrutture colloidali con molteplici funzionalità ottiche e magnetiche per applicazioni avanzate in elettronica, fotonica e diagnostica biomedica	FONDAZIONE CASSA DI RISPARMIO DI TORTONA	
31	CHALLENGE 3C-SiC Hetero-epitaxiALLy grown on silicon compliancE substrates and new 3C-SiC substrates for sustaiNable wide-band-Gap powEr devices	EU	LEO MIGLIO
32	Materiali per Up-conversion a bassa potenza con applicazione nel solare e nella bio-teranostica multimodale	REGIONE LOMBARDIA	ANGELO MONGUZZI
33	Theoretical analysis of the dislocation distribution in siltronic SiGe/Si(001) graded layers	SILTRONIC AG	FRANCESCO MONTALENTI

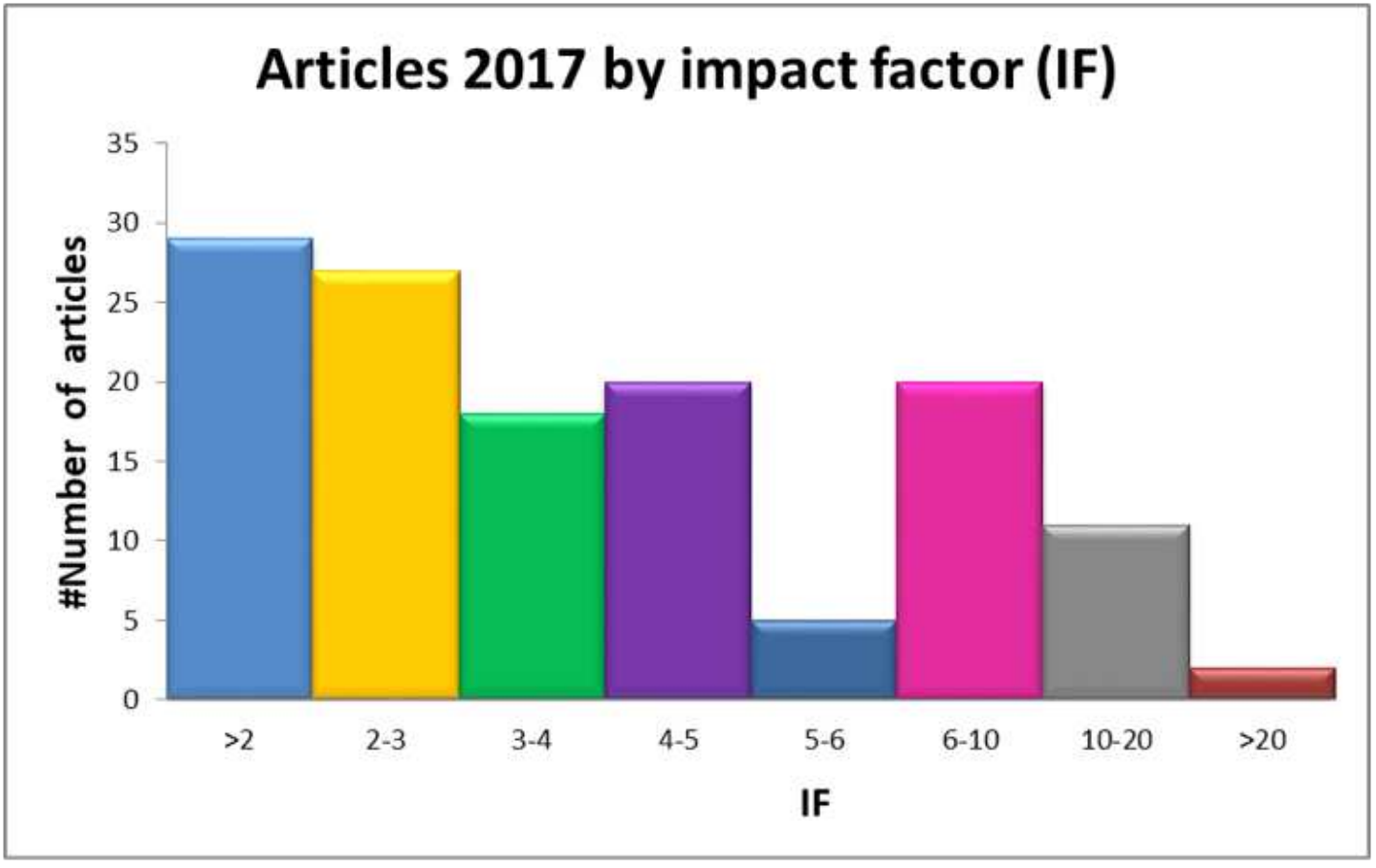
34	Advanced simulation design of nanostructured thermoelectric materials with enhanced power factors	EU	DARIO NARDUCCI
35	Novel hybrid thermoelectric photovoltaic devices: modeling, development, and characterization - HTEPV	EU - Marie Sklodowska-Curie Global Fellowship	DARIO NARDUCCI BRUNO LORENZI
36	Solar driven chemistry: new materials for photo- and electro-catalysis (SMARTNESS)	MIUR	GIANFRANCO PACCHIONI
37	Cascade deoxygenation process using tailored nanocatalysts for the production of biofuels from lignocellulosic biomass	EU	
38	CATSENSE	EU	
39	Ossidi nanostrutturati: multi-funzionalità e applicazioni	MIUR	
40	KiC- IMAGINE- Development and implementation of EIT KIC raw materials master program(s) in sustainable materials	EU	ALBERTO PALEARI
41	Spin optoElectronics ARCHitectures based on group IV compounds – SEARCH IV	FONDAZIONE CARIPLO	FABIO PEZZOLI
42	Sviluppo di materiali elettrodici per batterie ricaricabili a sodio ione	MINISTERO DEGLI ESTERI	RICCARDO RUFFO
43	Preparazione e caratterizzazione elettrochimica di materiali elettrodi per batterie a ioni sodio (NIB)	RSE S.p.A	

44	4PHOTON-Novel Quantum Emitters monolithically grown on Si, Ge and III-V substrates	EU	STEFANO SANGUINETTI
45	COSMITO - COmpressive Sampling Multispectral Imaging camera for remoTe Observation	REGIONE LOMBARDIA	
46	COSMOS	FONDAZIONE CARIPLO	
47	FemToTera- Plasmon-enhanced Tera-Hertz emission by femtosecond laser pulses of nanostructured semiconductor/metal surfaces	EU	
48	TEcnologie INnovative per i VEicoli Intelligenti	REGIONE LOMBARDIA/EU	
49	Micro-crystals single photon infrared detectors – μSPIRE – Horizon 2020 FET project	EU	
50	La sapienza è figliola della sperienza. La fisica degli sperimentali da Pavia a Milano-Bicocca	MIUR	ADELE SASSELLA
51	Rational design of hybrid organic-inorganic interfaces: the next step towards advanced functional materials – Action MP1202	EU	ROBERTO SCOTTI
52	CHNET_LILLIPUT	INFN	EMANUELA SIBILIA
53	Comparison of standard and professional versions of spectacle lens for driving in single vision and progressive additional designs	Hoya Holding	SILVIA TAVAZZI
54	Augmented environment for control in amyotrophic lateral sclerosis	ARISLA - AGENZIA DI RICERCA PER LA SCLEROSI LATERALE AMIOTROFICA	SILVIA TAVAZZI
55	Multifocal masterfitter	CooperVision	
56	Contratto di licenza per la distribuzione e la vendita dell'apparato Endoker	Frastema Ophthalmics	

57	AIDA 2020. Advanced european infrastructures for detectors at accelerators	EU	ANNA VEDDA
58	INTELUM-International and intersectoral mobility to develop advanced scintillating fibres and Cerenkov fibres for new hadron and jet calorimeters for future colliders	EU	
59	KiC-Otnewopt. Materials substitution in optoelectronic devices	EU	
60	KiC- IDS Fun Mat Inno. International doctoral school in functional materials and innovation	EU	
61	ASCIMAT- Increasing the scientific excellence and innovation capacity in advanced scintillation materials of the Institute of Physics from the Czech Academy of Sciences	EU	
62	KiC-RAMSES- Advanced school on critical raw materials substitution for energetics and photonics	EU	



PUBLICATIONS
PHD THESIS



INTERNATIONAL JOURNALS

#	Citation (by first author's name)	IF
1	Abatangelo, L; Felli, V; Léna, C, *On Aharonov-Bohm Operators with Two Colliding Poles*, ADVANCED NONLINEAR STUDIES 17, 283	1,072
2	Abatangelo, L; Felli, V; Noris, B; Nys, M, *Sharp boundary behavior of eigenvalues for Aharonov-Bohm operators with varying poles,* JOURNAL OF FUNCTIONAL ANALYSIS 273, 2428	1,254
3	Albanese, E; Di Valentin, C; Pacchioni, G, *H_2O Adsorption on WO3and WO3-x(001) Surfaces*, ACS APPLIED MATERIALS & INTERFACES 9, 23212	7,504
4	Albanese, E; Pacchioni, G, *Ferromagnetism in nitrogen-doped BaO: A self-interaction corrected DFT study*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS 19, 3279	4,123
5	Asnaghi, D; Corso, R; Larpent, P; Bassanetti, I; Jouaiti, A; Kyritsakas, N; Comotti, A; Sozzani, P; Hosseini, M, *Molecular tectonics: Gas adsorption and chiral uptake of (L)- and (D)-tryptophan by homochiral porous coordination polymers*, CHEMICAL COMMUNICATIONS 53, 5740	6,319
6	Baby, A; Gruenewald, M; Zwick, C; Otto, F; Forker, R; van Straaten, G; Franke, M; Stadtmüller, B; Kumpf, C; Brivio, G; Fratesi, G; Fritz, T; Zojer, E, *Fully Atomistic Understanding of the Electronic and Optical Properties of a Prototypical Doped Charge-Transfer Interface,* ACS NANO 11, 10495	13,942
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13	Bosoni, E; Sosso, G; Bernasconi, M, G*rueneisen parameters and thermal conductivity in the phase change compound GeTe*, JOURNAL OF COMPUTATIONAL ELECTRONICS 16, 997	1,526
14	Bracco, S; Asnaghi, D; Negroni, M; Sozzani, P; Comotti, A, Porous dipeptide crystals as volatile-drug vessels, CHEMICAL COMMUNICATIONS 54, 148	6,319
15	Bracco, S; Castiglioni, F; Comotti, A; Galli, S; Negroni, M; Maspero, A; Sozzani, P, *Ultrafast Molecular Rotors and Their CO_2 Tuning in MOFs with Rod-Like Ligands*, CHEMISTRY-A EUROPEAN JOURNAL 23, 11210	5,317
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18	Brooks, N; Castiglione, F; Doherty, C; Dolan, A; Hill, A; Hunt, P; Matthews, R; Mauri, M; Mele, A; Simonutti, R; Villar-Garcia, I; Weber, C; Welton, T, *Linking the structures, free volumes, and properties of ionic liquid mixtures*, CHEMICAL SCIENCE 8, 6359	8,668
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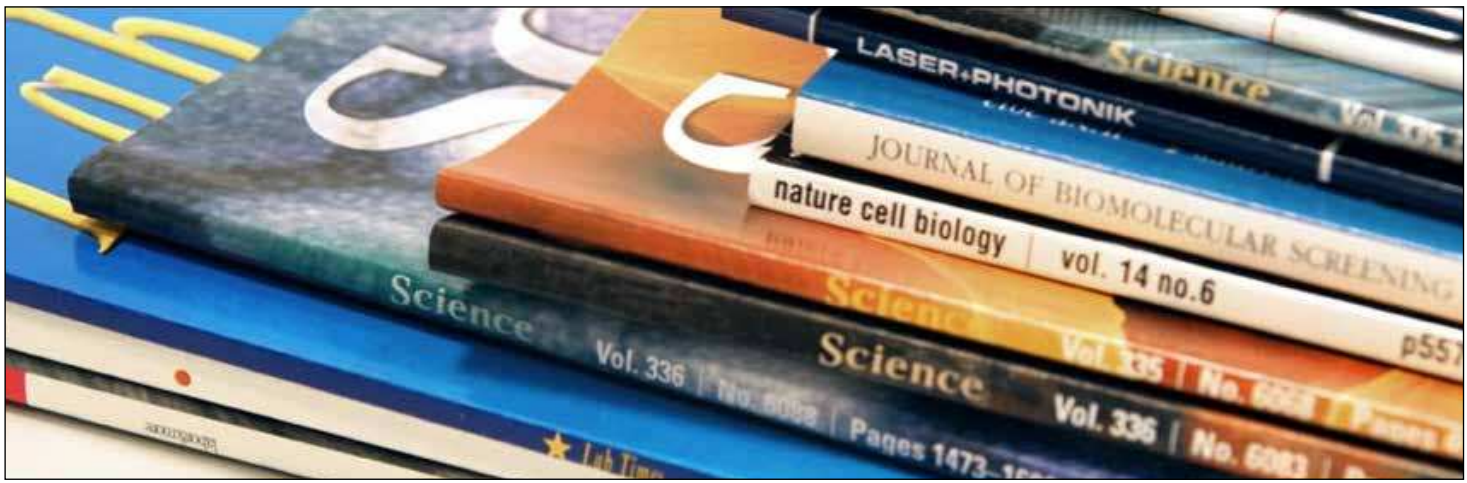


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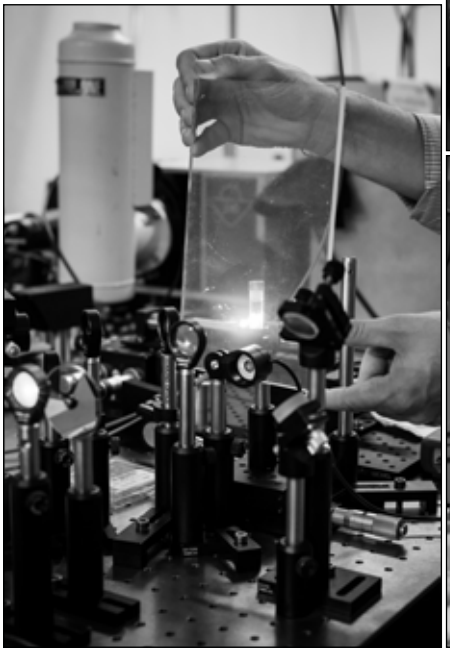

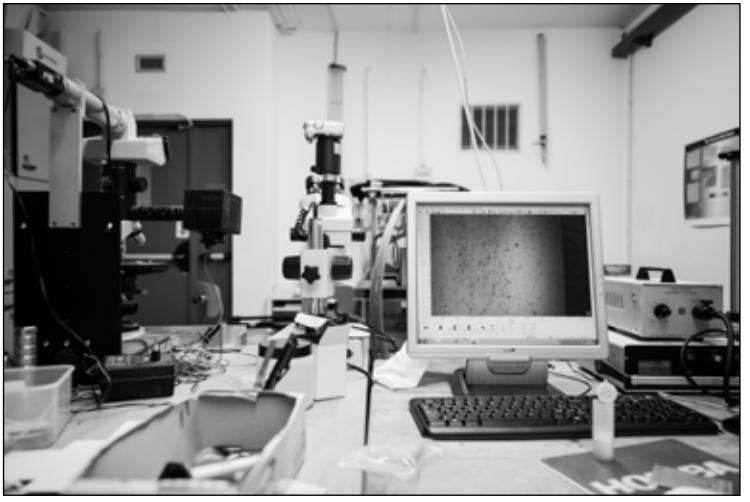

CONFERENCES AND SEMINARS

#	Authors and Title (by first author's name)	Conference/Workshop
1	Albani, M; Bergamaschini, R; Gagliano, L; Assali, S; Verheijen, M; Bakkers, E; Miglio, L *Strain relaxation in semiconductor core/shell nanowires*	ICG2017 Italian Crystal Growth 2017. University of Milano Bicocca, MIlan, Italy
2	Albani, M; Bergamaschini, R; Rovaris, F; Miglio, L; Montalenti, F; *Modeling semiconductor heteroepitaxy: a continuum approach*	ICG2017 Italian Crystal Growth 2017. University of Milano Bicocca, MIlan, Italy
3	Anu Baby, Christian Zwick, Marco Gruenewald, Elisabeth Verwüster, Oliver T. Hofmann, Gian Paolo Brivio, Guido Fratesi, Torsten Fritz, Egbert Zojer; *Electronic and optical properties of K doped PTCDA monolayer on Ag(111)*	2017 PCAM / Thinface Summer School on Surfaces and Interfaces. San Sebastian, Spain
4	Asnaghi, D; Sozzani, P; Comotti, A; Bassanetti, I; Corso, R; Larpent, P; Abdelaziz Jouaiti, A; Mir Wais Hosseini, N; *Homo-chiral porous coordination polymers: gas adsorption properties and enantiomeric separation of (L)- and (D)-tryptophan*	International Symposium on Macrocyclic and Supramolecular Chemistry (ISMSC) in conjunction with ISACS, University of Cambridge. Cambridge, UK
5	Baby, A; Gruenewald, M; Zwick, C; Otto, F; Forker, R; Van Straaten, G; Franke, M; Stadtmu¨ller, B; Kumpf, C; Brivio, GP; Fratesi, G; Fritz, T; Zojer, E; *Electronic and Structural properties of K doped PTCDA monolayer on Ag(111)*	Italian National Conference on the Physics of Matter - FisMat 2017. Trieste, Italy
6	Bergamaschini, R; *Continuum modeling of the heteroepitaxial growth of semiconductor nanostructures (invited)*	Internationa Conference Nanomeeting 2017. Minsk
7	Bergamaschini, R; Albani, M; Montalenti, F; Miglio, L; *Understanding the kinetics segregation in core-shell nanowires: a phase-field approach (invited)*	Semicon Nano 2017: 6th International Workshop Epitaxial Growth and Fundamental Properties of Semiconductor Nanostructures. Como
8	Bernasconi, M; *Atomistic Simulations of Crystallization of GeTe Nanowires (invited)*	European Phase Change and Ovonics Symposium, E/PCOS 2017. Aachen (D)

9	Bietti, S; *Quantum nanostructures by droplet epitaxy for advanced devices (invited)*	19th European Workshop on Molecular Beam Epitaxy EuroMBE. Korobytsino, St. Petersburg (Russia)
10	Binetti, S; *Chalcogenide thin film solar cells: research activity at UNIMIB-MIBSOLAR center (invited)*	Italian-Kazak bilateral workshop “Our Common Future: Energy, Environment & Develop-ment” EXPO2017, Italian Pavilion, 30-31 August 2017 Astana . Kazakistan. Astana (Kazakistan)
11	Binetti, S; *Defects and Impurities in Silicon for Solar Cell (invited)*	The 7th International Symposium on Advanced Science and Technology of Silicon Materials (JSPS Si Symposium). Kona, Hawaii, USA
12	Binetti, S;. *Photoluminescence and infrared spectroscopy for impurities identification in silicon for pho-tovoltaic applications (invited)*	Workshop on: Crystalline Silicon for Low Cost Photovoltaics. Paris (France)
13	Binetti, S; Le Donne, A; Acciarri, M; Marchionna, S *Earth-abundant thin film solar cells based on Cu_2MnSnS_4*	XXVI Congresso Nazionale della Società Chimica Italiana 11-14 settembre 2017. Paestum, Italia
14	Bracco, S; *Molecular Rotors in Porous Supramolecular Architectures and Dynamics Modulation (invited)*	3rd ICSU/IUPAC Workshop On Crystal Engineering. Milano
15	Bracco, S; Comotti, A; Castiglioni, F; Negroni, M; Sozzani, P *Molecular Rotor Dynamics in Nanoporous Architectures (invited)*	ISNSC-9, 9th International Symposium on Nano & Supramolecular Chemistry (4-7 Settembre 2017). Napoli, Italy
16	Bracco, S; Negroni, M; Castiglioni, F; Perego, J; Piga, D; Comotti, A; Sozzani, P *Metal-organic and organic frameworks: porosity, gas adsorption and fast dynamics*	Italian Crystal Growth 2017 - Materials and Methods in Crystal growth Conference (20-21 November 2017). Milano
17	C. Lubritto1, P. Ricci, D.Angelici, F. Fantino, E. Sibilia, M.F. Alberghina, S. Schiavone, C. Grifa, M. Mercurio, C. Germinario, F. Izzo, C. Grimaldi, A. Langella, E. Massa, S. Bracci, D. Magrini, R. Costa, M.E. Oddo; *Difendi il bello, combatti il falso. results of diagnostic campaign promoted by AIAR in the deposit of the archaeological museum of Paestum*	Convegno AIAR, Beni Culturali: grandi facilities, reti e networks di laboratori. Firenze, 8 – 10 Marzo 2017
18	Caglio, S, Maspero F; *b-sites: il lato “nascosto” dell’archeologia*	Convegno AIAR, Beni Culturali: grandi facilities, reti e networks di laboratori. Firenze, 8 – 10 Marzo 2017

19	Comotti, A; *Nanoporous Architectures: Gas Uptake and Molecular Rotors Dynamics (invited)*	NanomeetsBio@NanoMat. Salerno, Italy
20	Comotti, A; Bracco, S; Castiglioni, F; Negroni, M; Sozzani, *P Molecular Rotors in Porous Supramolecular Architectures (invited)*	ICCOSS XXIII, 23rd International Conference on the Chemistry of the Organic Solid State (2-7 April 2017). Stellenbosch, South Africa
21	Cova, F; Fasoli, M; Moretti, F; Chiodini, N; Pauwels, K; Auffray, E; Lucchini, M; Bizarri, G; Bourret, E; Baccaro, S; Cemmi, A; Vedda, A; *Radiation hardness of Rare Earth doped sol-gel silica fibers*	SCINT 2017 - 14th International Conference on Scintillating Materials and their Applications. Chamonix, France
22	Di Valentin, C; *A Quantum Chemical Simulation of Stimuli-Responsive Nanomaterials for Biomedical Applications (invited)*	ERC10th Italian CHEM Day. Pavia
23	Di Valentin, C; *Simulazione quantistica di nanomateriali foto- e magneto-sensibili per applicazioni biomediche (invited)*	IERC10th Italian CHEM Day. Pavia
24	Di Valentin, C; Fazio, G; Ferrighi, L; Selli, D; *Photoexcited carriers recombination and trapping in spherical vs faceted TiO_2 nanoparticles (invited)*	ACS National Meeting Spring 2017. S. Francisco, CA
25	Di Valentin, C; Ferrighi, L; Datteo, M; Fazio, G; Selli, D; *Quantum chemical simulation of nanostructured materials: 2D sheets and 0D nanoparticles (invited)*	Chemistry for the Future 2017. Pisa
26	Di Valentin, C; Ferrighi, L; Datteo, M; Fazio, G; Selli, D ;Quantum chemical simulation of nanostructured materials: 2D sheets and 0D nanoparticles(invited)	Swedish Theoretical Chemistry 2017 Bridging gaps. Goteborg, Sweden
29	Facchinetti, I; Ruffo, R; *Structure properties relationship in organic semiconductor: the case of poly(dispiro[1,3-dioxalane-2,4'(5'h)-benzo[2,1-b:3,4-b'] ditiophene)*	ECHEMS 2017. Milano Marittima/Cervia
27	Fanciulli, M; *Investigation of the Si/SiO2 interface in silicon nanowires and its role in donor deactivation and charge transport (invited)*	Progress in Applied Surface, Interface and Thin Film Science 2017. SURFINT-SREN V. Firenze
28	Felli, V; *On spectral stability of Aharonov-Bohm operators with moving poles (invited)*	Nonlinear Days in Turin, Politecnico di Torino, 22 settembre 2017.
30	Felli, V; Spectral stability under removal of small capacity sets and applications to Aharonov-Bohm operators	Roma CAput PDE, Roma, 24 gennaio 2017
31	Felli, V; *Unique continuation properties and essential self-adjointness for relativistic Schrödinger operators with singular potentials (invited)*	International Conference on Elliptic and Parabolic Problems, Gaeta, 23 maggio 2017 .

32	Fiore, M; Ruffo, R; Maria Mari, C; Pantò, F; Frontera, F; Stellitato, S; Santangelo, S; *An investigation on electrospun Fe_2O_3 nanofibers ad anodo material for sodium-ion rechargeable batteries*	21st international conference Solid Date Ionics. Padova
33	Galli A., Alberti R., Aresi N., Bonizzoni L., Caccia M., Castiglioni I., Gargano M., Interlenghi M., Ludwig N., Salvatore C., Martini M; *L'officina di Giotto nel XXI secolo: investigando la cuspide "Padreterno con gli Angeli"*	Convegno AIAR, Beni Culturali: grandi facilities, reti e networks di laboratori. Firenze, 8 – 10 Marzo 2017
34	Galli A., Caccia M., Martini M., Panzeri L., Maspero F., Fiorentino S., Vandini M., Sibilia E; *Applying the "pre-bleached with blue LEDs" protocol to date Umayyad mosaic tesserae by thermoluminescence*	LED 2017, Cape Town, SA
35	Galliani, D; Piro, A; Battiston, S; Narducci, D; *Partially conjugated copolymers: a novel tool to tune organic material thermoelectric properties*	Giornate della Termoelettricità (GiTe) 2017 22-23 febbraio. Torino, Italia
36	Le Donne, A; Marchionna, S; Acciarri, M; Binetti, S; *Emerging Cu_2MnSnS_4 thin film solar cells grown by sulfurization of evaporated precursors*	Italian Crystal Growth 2107 (ICG 2017), Materials and Methods in Crystal Growth. Milano (Italy)
37	Maspero, F., Panzeri L., Sibilia, E., Martini M; *Reidrossilazione: una sfida verso una tecnica di datazione autocalibrata per le ceramiche*	Convegno AIAR, Beni Culturali: grandi facilities, reti e networks di laboratori. Firenze, 8 – 10 Marzo 201.
38	Meinardi, F; *Luminescent Solar Concentrators: The Next Generation Of Transparent PV Devices (invited)*	World's First Conference on Energy Independent Electric Vehicles: Land, Water & Air. Delft, Netherlands
39	Miglio, L; Albani, M; Bergamaschini, R; Gagliano, L; Assali, S; Verheijen, M; Bakkers, E; *Strain and strain-driven effects in coaxial nanowires (invited)*	Semicon Nano 2017 - 6th International Workshop Epitaxial Growth and Fundamental Properties of Semiconductor Nanostructures. Como, Italy
40	Mostoni, S; D'Arienzo, M; Di Credico, B; Morazzoni, F; Susanna, A; Scotti, R; *ZnO nanoparticles anchored to silica as reinforcing filler and curing accelerator for rubber nanocomposites*	Italian-Nordic Polymer Future. Pisa
41	Mostoni, S; Trifiletti, V; Binetti, S; Scotti, R; *High quality Cu_2ZnSnS_4 thin films for photovoltaic applications*	Italian Crystal Growth 2017, ICG2017. Università Milano Bicocca, Milano, Italy
	Narducci, D; *Empowering communication by powering electronics. Thermoelectrics for heat microharvesting (invited)*	MIDEM 2017. Ljubljana (Slovenia)

42	Narducci, D; Lorenzi, B; *Enhanced solar energy conversion by hybrid photovoltaic–thermoelectric generators (invited)*	EUROMAT 2017. Thessaloniki (Greece)
43	Pacchioni, G; *Oxide doping for photocatalysis: pros and cons (invited)*	2nd International Conference of New Photocatalytic Materials for Environment, Energy and Sustainability. Lubiana
44	Pacchioni, G; *Oxide reducibility in catalysis: from biomass conversion to CO oxidation (invited)*	7th Bonn Humboldt Award Winners' Forum "Fundamental Concepts and Principles of Chemical Energy Conversion. Bonn
45	Pacchioni, G; O*xide surfaces in catalysis: clusters, defects, and 2D oxides (invited)*	IDS-FunMat and EDJ-FunMat Joint Training School. Aveiro
46	Pacchioni, G; Role of oxide reducibility in catalysis: from biomass conversion to CO oxidation (invited)	13th European Congress on Catalysis (EUROPACAT). Firenze
47	Pacchioni, G; *Solid state quantum chemistry: towards the rational design of nano- and photo-catalysts (invited)*	XXVI Congresso Nazionale della Società Chimica Italiana. Paestum
48	Pacchioni, G; T*iO_2 and ZrO_2 in biomass conversion: why catalyst reduction helps (invited)*	Discussion Meeting Providing sustainable catalytic solutions for a rapidly changing world, Royal Society. Londra
49	Panzeri L., Cantù M., Martini M., Sibilia E; *Datazione di malte di terra con OSL: effetto dell'applicazione di diversi protocolli di misura e di differenti modelli statistici*.	Convegno AIAR, Beni Culturali: grandi facilities, reti e networks di laboratori. Firenze, 8 – 10 Marzo 2017
50	Panzeri L., Maspero F., Martini M., Sibilia E; *Rehydro-xylation (RHX): a new technique for ceramics dating*.	EMAC (European Meeting on Ancient Ceramic). Bordeaux, 6-9 September 20177
52	Panzeri, L., Maspero, F., Martini, M., Sibilia, E; *MoDIS-Mortar dating Inter-Comparison Study: datazione delle malte mediante ^{14}C e OSL.*	Convegno AIAR, Beni Culturali: grandi facilities, reti e networks di laboratori. Firenze, 8 – 10 Marzo 2017
51	Panzeri, L; Caroselli, M; Lugli, S; Matini, M; Sibilia, E; *Mortar OSL and brick TL dating: the case study of the UNESCO world heritage site of Modena*	LED 2017 Cape Town
53	Potkins, D; Braccini, S; Nesteruk, K; Carzaniga, T; Vedda, A; Chiodini, N; Timmermans, J; Melanson, S; Dehnel, M; *A Low-cost Beam Profiler Based on Cerium-doped Silica Fibers*	Conference on the Application of Accelerators in Research and Industry, CAARI 2016. Fort Worth, USA
54	Raimondo, L; Trabattoni, S; Sassella, *A Growth and selection of metalloporphyrin nanostructures: organic epitaxy vs post-growth processes*	Italian Crystal Growth 2017 - materials and methods in crystal growth. Milano

55	Rappoldi, A; Cattaneo, P; Adriani, O; Agnesi, A; Albergo, S; Auditore, L; Basti, A; Berti, E; Bigongiari, G; Bonechi, L; Bonechi, S; Bongi, M; Bonvicini, V; Bottai, S; Brogi, P; Cappello, G; Carotenuto, G; Castellini, G; D'Alessandro, R; Detti, S; Fasoli, M; Finetti, N; Italiano, A; Lenzi, P; Maestro, P; Marrocchesi, P; Miritello, M; Mori, N; Olmi, M; Orzan, G; Pacini, L; Papini, P; Pellegriti, M; Pirzio, F; Ricciarini, S; Spillantini, P; Starodubtsev, O; Stolzi, F; Suh, J; Sulaj, A; Tiberio, A; Tricomi, A; Trifirò, A; Trimarchi, M; Vannuccini, E; Vedda, A; Zampa, G; Zampa, N; *CaloCube: a novel calorimeter for high-energy cosmic rays in space*	International Conference on Astroparticle Physics, RICAP 2016. Roma, Italy
56	Remondina, J; Acciarri, M; Azarbod, A; Golubev, N; Ignat'Eva, E; Mereu, R; Paleari, A; Sigaev, V; Lorenzi, R; *AC and DC characterization of γ-Ga_2O_3-containing glassceramic thin films*	IWGO 2017 - 2nd International Workshop on Gallium Oxide and Related Materials. Parma, Italy
57	Remondina, J; Acciarri, M; Azarbod, A; Golubev, N; Ignat'Eva, E; Paleari, A; Sassella, A; Sigaev, V; Trabattoni, S; Lorenzi, R; *Investigation of nanostructured glass-ceramic MOS devices*	ICG 2017 - Italian Crystal Growth, Materials and Methods in Crystal growth. Milano (Italy)
58	Rovaris F; Bergamaschini R; Montalenti F; *Modeling the competition between elastic and plastic relaxation in semiconductor heteroepitaxy: From cyclic growth to flat films*	GDRi Mecano General Meeting May 10-12. Toulouse (France)
59	Ruffo, R; Negative *Electrode Materials for Sodium Ion Batteries (invited)*	XXVI Congresso Nazionale della Società Chimica Italiana. Paestum (SA)
60	Ruffo, R; *Reaction mechanisms and structure properties correlations in carbonaceous anode materials for sodium ion batteries (invited)*	EEWS 2017 Next generation Technology for Advanced Ebergy Storage Systems. Dajeon (Corea del Sud)
61	Ruffo, R; Fiore, M; Santangelo, S; Patanè, S; Lee, H; *Reaction mechanisms and structure properties correlations in carbonaceous anode materials for sodium ion batteries (invited)*	ICAE 2017 The 4th International Conference on Advanced electromaterials. Jeju (Corea del Sud)
62	Sassella, A; Raimondo, L; Trabattoni, S; Moret, M; Masciocchi, N; Masino, *M Oxidation of rubrene crystalline thin films and properties of the rubrene/oxide interface*	ECME 2017 - 14th European Conference on Molecular Electronics, August 29-September 2, 2017. Dresden (Germany)
63	Scotti, R; D'Arienzo, M; Di Credico, B; Morazzoni, F; Mostoni, S; Susanna, A; *ZnO nanoparticles anchored to silica filler as curing accelerator for rubber composites*	XIV AIMAT National Congress. Ischia

64	Sozzani, P; Bracco, S; Perego, J; Piga, D; Bassanetti, I; Comotti, A; *In situ polymerization in 3D porous materials (invited)*	MIPOL2017 Milan Polymer Days February 15-16. Milano, Italia
65	Sozzani, P; Perego, J; Piga, D; Asnaghi, D; Bassanetti, I; Bracco, S; *Absorptive Organic and Hybrid Materials for Gases and Polymers (invited)*	ICCOSS XXIII, International Conference on the Chemistry of the Organic Solid State. Stellenbosch, South Africa
66	Tavazzi, S; *Photon correlation spectroscopy on tears (Invited)*	Congresso Nazionale della Società italiana di Fisica. Trento
67	Trabattoni, S; Raimondo, L; Moret, M; Masciocchi, N; Masino, M; Sassella, A; *Oxidation of Crystalline Rubrene Films: Evidence of an Epitaxial Native Oxide*	Italian Crystal Growth 2017 - materials and methods in crystal growth. Milano
68	Trifiletti, V; Manfredi, N; Listorti, A; Altamura, D; Giannini, C; Colella, S; Gigli, G; Rizzo, A; *Engineering Titania based Planar Heterojunction for Hysteresis-Less Perovskite Solar Cells*	International Conference on Hybrid and Organic Photovoltaics (HOPV 17). Lausanne
69	Trifiletti, V; Mostoni, S; Butrichi, F; Scotti, R; Binetti, S; *Monolithic gel formation of high quality Cu2ZnSnS4 thin films*	8th European Kesterite Workshop. Barcelona, Spain
70	Ugolotti, A; Harivyasi, S; Baby, A; Dominguez, M; Pinardi, A; López, M; Martín-gago, J; Fratesi, G; Floreano, L; Brivio, GP; *Chemisorption of Pentacene on Pt(111) with a Little Molecular Distortion*	FisMat 2017, the Italian National Conference on the Physics of Matter (including Optics, Photonics, Liquids, Soft Matter). Ictp, Trieste, IT
71	Ugolotti, A; Harivyasi, SS; Baby, A; Dominguez-Rivera, M; Pinardi, A; Lopez, MF; Martin-Gago, JA; Fratesi, G; Floreano, L; Brivio, GP; *Chemisorption of Pentacene on the Pt(111) with little molecular distortion*	2017 PCAM / Thinface Summer School on Surfaces and Interfaces. San Sebastiàn (Spagna)
72	Ugolotti, A; Ravikumar, A; Fratesi, G; Brivio, GP; *Tuning the electronic properties of Silicene through half-hydrogenation or Graphene support*	International Meeting on Silicene. SOLEIL synchrotron, France
73	Vedda, *A Substitution and recycling towards sustainable materials life cycles (invited)*	Towards a Bio-Based Economy: Science, Innovation, Economics, Education. UNIMIB, Milan, Italy
74	Veronese, I; Chiodini, N; Cialdi, S; D'Ippolito, E; Fasoli, M; Gallo, S; Mones, E; Vedda, A; Loi, G; *Characterization of Yb-doped silica optical fiber as real-Time dosimeter*	Hard X-Ray, Gamma-Ray, and Neutron Detector Physics XIX 2017. San Diego; USA
75	Villa, I; Lauria, A; Moretti, F; Fasoli, M; Dujardin, C; Niederberger, M; Vedda, A; *Spectroscopic Properties of Scintillating Hafnium Dioxide Nanocrystals*	SCINT 2017 - International Conference on Scintillating Materials and their Applications. Chamonix (Francia)

76	Vitiello, E; Giorgioni, A; Paleari, S; Cecchi, S; Grilli, E; Isella, G; Jantsch, W; Fanciulli, M; Pezzoli F; *Long-lived conduction electron spins in Ge quantum wells*	International Conference on Silicon Epitaxy and Heterostructures - ICSI-10. Warwick, UK

BOOKS AND CONTRIBUTIONS

Abatangelo, L; Felli, V; *Rate of convergence for eigenfunctions of Aharonov-Bohm operators with a moving pole*. In: Solvability, Regularity, and Optimal Control of Boundary Value Problems for PDEs (pp. 1-30). Springer International Publishing.
Comotti, A; Bracco, S; Sozzani, P; *Solid-State NMR of Supramolecular Materials*. In: Comprehensive Supramolecular Chemistry II, (pp. 75-99). Elsevier.
D'Arienzo, M; Scotti, R; Di Credico, B; Redaelli, M; *Synthesis and Characterization of Morphology-Controlled TiO_2 Nanocrystals Opportunities and Challenges for their Application in Photocatalytic Materials*. In: Studies in Surface Science and Catalysis (pp. 477-540). Elsevier.
Morazzoni, F; D'Arienzo, M; Di Credico, B; Scotti, R; Cangiotti, M; Fattori, A; et al.; *The Use of EPR Spectroscopy for the Study of Hybrid Materials and Interphases*. In: Hybrid Organic-Inorganic Interfaces: Towards Advanced Functional Materials (pp. 879-924). Wiley.
Pacchioni, G; *Scienza, quo vadis?* Società Editrice Il Mulino.
Scotti, R; D'Arienzo, M: Di Credico, B; Giannini, L; Morazzoni, F; *Silica-Polymer Interface and Mechanical Reinforcement in Rubber Nanocomposites*. In: Hybrid Organic-Inorganic Interfaces: Towards Advanced Functional Materials (pp. 151-198). Wiley.
Vedda, A; Villa, I; *Medical applications of nanomaterials*. In: NATO Science for Peace and Security Series B: Physics and Biophysics (pp. 369-386). Springer Verlag.

PHD THESIS

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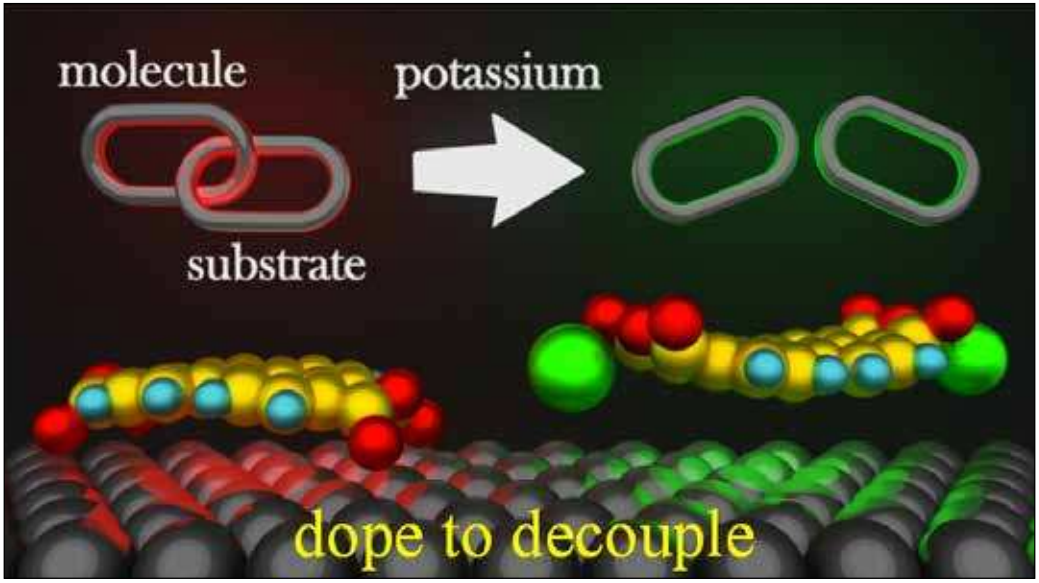
Davide BARANA, Lignin-based elastomeric composites for sustainable tyre technology
Michael BARGET, Optimization steps of germanium as light emitter: strain and n-type doping
Francesco BRUNI, Novel material design and manipulation strategies for advanced optoelectronic applications
Veronica COLLICO, Development of plga hybrid nanoparticles for biomedical application
Sebastiano DE CESARI, Spin properties of germanium-based heterostructures
Daniela MANZONE, Autoassemblaggio di copolimeri a blocchi anfifilici da buoni solventi: verso una mappa morfologica predittiva per la scelta del sistema di trasporto dei farmaci
Jacopo PEDRINI, Advanced strategies for light management in photonics, imaging, and sensing
Abhilash RAVIKUMAr, Electronic, spin dependent conductive properties of modified graphene
Matteo REDAELLI, Polysilsesquioxane as advanced “molecular” filler for rubber reinforcement
Matteo SALAMONE, Organic materials for energy
Benedetta SANTINI, Studies of different administration routes of engineered colloidal nanoparticles
Philomena SCHLEXER, Nanostructures in catalysis - support effects on metal clusters and oxide thin films
Simone SELMO, functional analysis of in-based nanowires for low power phase change memory applications

Highlights

Brivio, G.P., Baby, A; Fratesi, G; Gruenewald, M; Zwick, C; Otto, F; Forker, R; van Straaten, G; Franke, M; Stadtmüller, B; Kumpf, C; Fritz, T; and Zojer, E; *Fully Atomistic Understanding of the Electronic and Optical Properties of a Prototypical Doped Charge-Transfer Interface*, ACS Nano 11, 10495-10508 (2017).

The alkali-metal doping-induced changes of the structural, electronic, and optical properties of the prototypical PTCDA/Ag(111) interface is presented in this work. For doping K atoms are used, as KxPTCDA/Ag(111) has the distinct advantage of forming well-defined stoichiometric phases. K atoms are observed to both structurally and electronically reduce the organic molecule-metal bonding. To arrive at a conclusive, unambiguous, and fully atomistic understanding of the interface properties, we combined the state-of-the-art density-functional theory calculations using VASP, Quantum Espresso and Yambo with the various experimental techniques. In combination with the full structural characterization with low-energy electron diffraction of the KxPTCDA/Ag(111) interface, where for the first time the dopant atoms were visualized by scanning tunneling microscopy experiments (ACS Nano 2016, 10, 2365–2374), the present comprehensive study provides access to a fully characterized reference system for a well-defined metal-organic interface in the presence of dopant atoms, which can serve as an ideal benchmark for future research and applications.

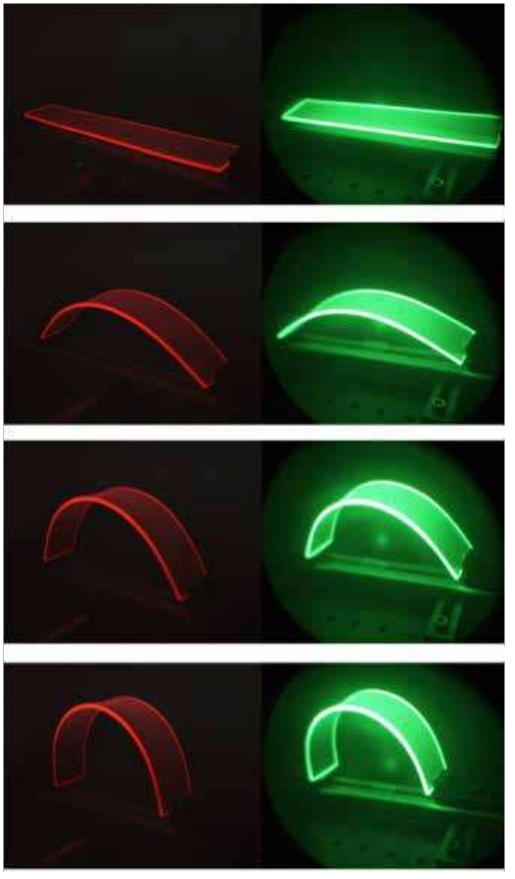


In the figure: Structural and electronic decoupling of PTCDA from the Ag(111) surface by K doping.

Highlights

Meinardi, F; Ehrenberg, S; **Dhamo, L; Carulli, F; Mauri, M; Bruni, F; Simonutti, R**; Kortshagen, U; **Brovelli, S**; *Highly efficient luminescent solar concentrators based on earth-abundant indirect-bandgap silicon quantum dots*. NATURE PHOTONICS, 11, 177 (2017).

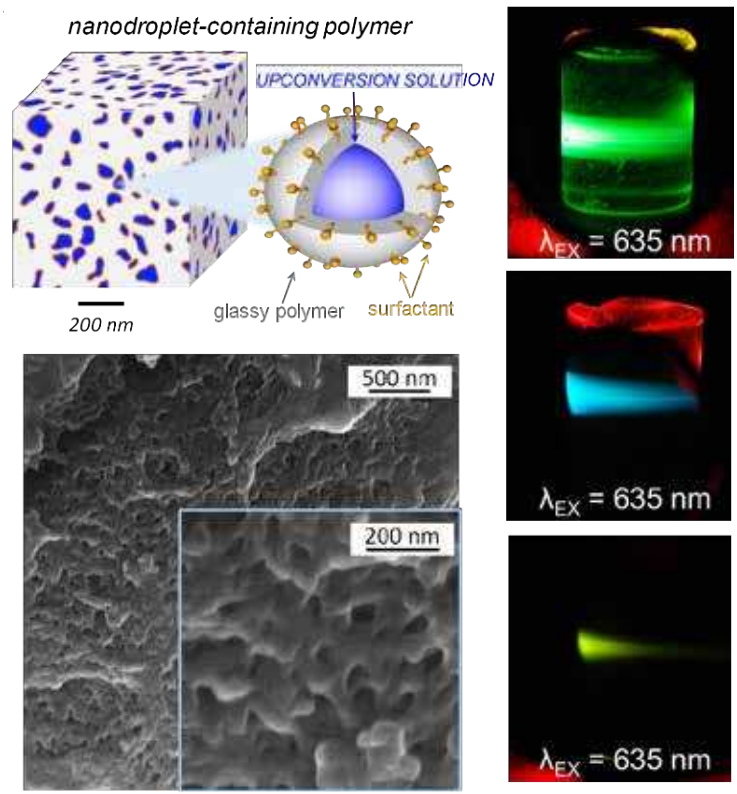
Building-integrated photovoltaics is gaining consensus as a renewable energy technology for producing electricity at the point of use. Luminescent solar concentrators (LSCs) could extend architectural integration to the urban environment by realizing electrode-less photovoltaic windows. Crucial for large-area LSCs is the suppression of reabsorption losses, which requires emitters with negligible overlap between their absorption and emission spectra. This work demonstrates the use of indirect-bandgap semiconductor nanostructures such as highly emissive silicon quantum dots. Silicon is non-toxic, low-cost and ultraearth-abundant, which avoids the limitations to the industrial scaling of quantum dots composed of low-abundance elements.
Suppressed reabsorption and scattering losses lead to nearly ideal LSCs with an optical efficiency of η=2.85%, matchingstate-of-the-art semi-transparent LSCs. Monte Carlo simulations indicate that optimized silicon quantum dot LSCs have aclear path to η > 5% for 1m2 devices. We are finally able to realize flexible LSCs with performances comparable to those of flat concentrators, which opens the way to a new design freedom for building-integrated photovoltaic elements.



In the figure: Visible and NIR picture of a flexible Si-based LSC under UV illumination for curved building integrated photovoltaic elements.

Highlights

Vadrucci R; **Monguzzi, A**; Saenz, F; Wilts, BD; Simon, YC; Weder C.; *Nanodroplet-Containing Polymers for Efficient Low-Power Light Upconversion* ADVANCED MATERIALS 29, 1702992 (2017).



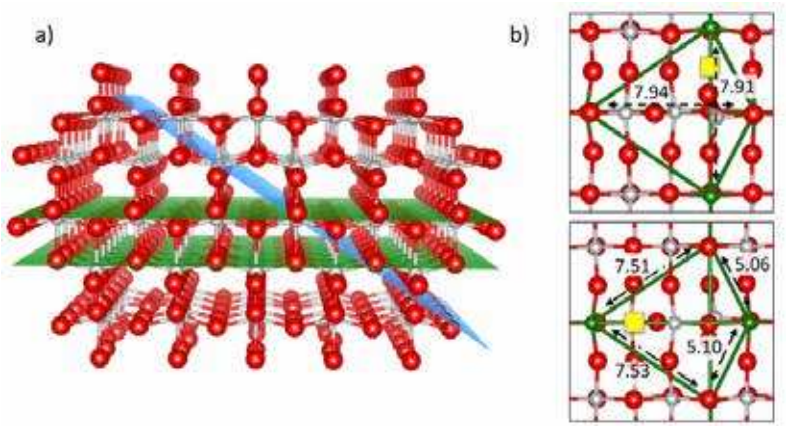
Sensitized triplet–triplet-annihilation-based photon upconversion (TTA-UC) permits the conversion of light into radiation of higher energy at low intensity light, which makes it particularly suitable for solar-energy harvesting technologies. High upconversion yields can be observed for low viscosity solutions of dyes; but, in solid materials, which are better suited for integration in devices, the process is usually less efficient. We show that this problem can be solved by using transparent nanodroplet-containing poly-mers that consist of a continuous polymer matrix and a dispersed liquid phase containing the upconverting dyes. These materials can be accessed by a simple one-step procedure that involves the free-radical polymerization of a micro-emulsion of hydrophilic monomers, a lipophilic solvent, the upconverting dyes, and a surfactant. Several glassy and rubbery materials are explored and ranges of dyes that enable TTA-UC in different spectral regions are utilized. The materials display UC efficiencies approaching the performance of optimized reference solutions and grants good protection against the atmospheric oxygen.

In the figure: Sketch of the material morphology and scanning electron microscopy images of a nanodroplet-containing glassy polymer. Pictures of dye-doped nanodroplet-containing polymer glasses under laser excitation for red-to-green, red-to-blue and red-to-yellow photon upconversion.

Highlights

Chiesa, M; Livraghi, S; Giamello, E; **Albanese, E; Pacchioni, G;** *Novel High Spin (S=2) States in TiO_2 Anatase* ANGEWANDTE CHEMIE INTERNATIONAL EDITION 56, 2604 (2017).

Turning titanium dioxide (TiO_2), a well-known white pigment, into a colorful solid, is one of the current strategies to shift the TiO_2 absorption edge into the visible-light region, for the development of new advanced materials with emphasis on energetic and photochemical applications. The insertion in diamagnetic matrices of defect centers, mutually interacting by virtue of well-defined and controlled magnetic interactions, has become a highly important topic in the quest for new materials. In this work we describe the synthesis, characterization, and DFT modeling of TiO_2 anatase nanoparticles featuring unprecedented magnetically active centers characterized by an *S*=2 spin state, originating from four ferromagnetically interacting Ti^{3+} centers. The observation of high spin states in TiO_2 provides an interesting platform for the exploration of new spin-bearing multifunctional oxide based materials.

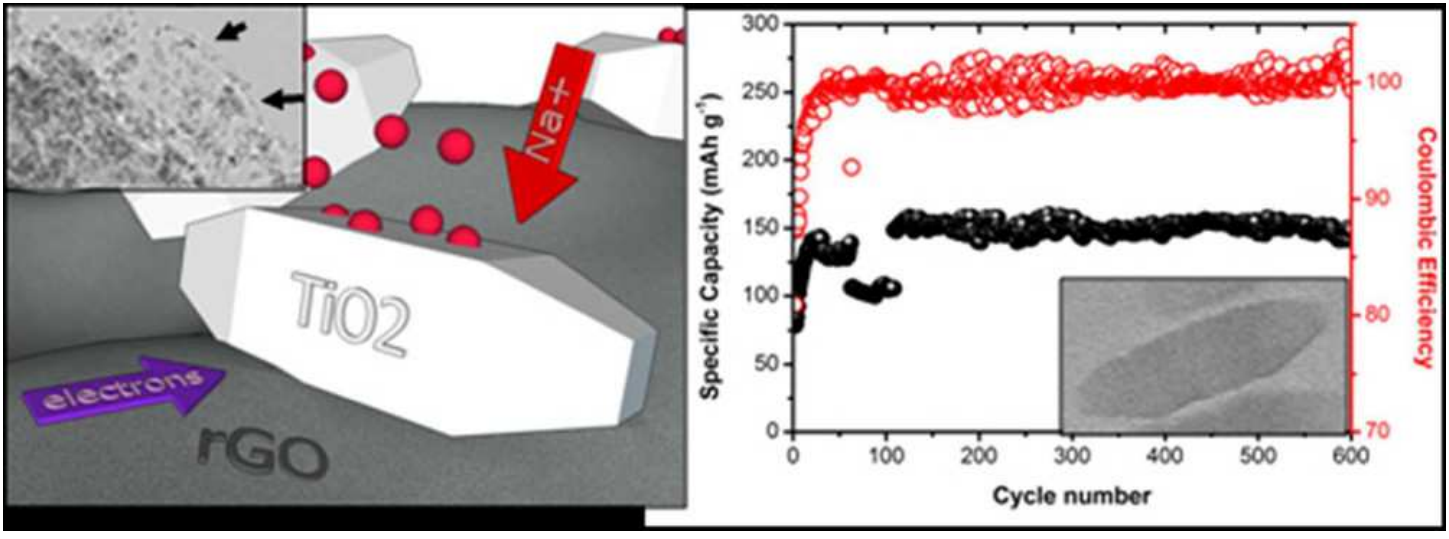


In the figure: (a) Side view of the supercell adopted. The light blue plane contains the four Ti3+ ions; the green planes contain the reduced Ti centers that form the more stable tetrahedral cluster. (b) Top and bottom view of the main features of the relaxed tetrahedral cluster with S=2. Distances between Ti3+ are in Å.

Highlights

Longoni, G; Pena Cabrera, R. L; Polizzi, S; **D'Arienzo, M; Mari, C.M**; Cui, Y; **Ruffo, R;** *Shape-Controlled TiO_2 Nanocrystals for Na-Ion Battery Electrodes: The Role of Different Exposed Crystal Facets on the Electrochemical Properties*. NANO LETTERS 17, 992. (2017).

Rechargeable sodium-ion batteries are becoming a viable alternative to lithium-based technology in energy storage strategies, due to the wide abundance of sodium raw material. Notwithstanding the large number of research papers concerning sodium-ion battery electrodes, the development of a low-cost, well-performing anode material remains the largest obstacle to overcome. The well-known anatase, one of the allotropic forms of natural TiO_2, suffers from reduced cyclability and limited power, due to kinetic drawbacks and to its poor charge transport properties. A systematic approach in the morphological tuning of the anatase nanocrystals is needed, to optimize its structural features toward the electrochemical properties. Aiming to face with these issues, we were able to obtain a fine tuning of the nanoparticle morphology and to expose the most favorable nanocrystal facets to the electrolyte and to the conductive wrapping agent (graphene), thus overcoming the intrinsic limits of anatase transport properties. The result is a TiO_2-based composite electrode able to deliver an outstandingly stability over cycles (150 mA h g^{-1} for more than 600 cycles in the 1.5–0.1 V potential range) never achieved with such a low content of carbonaceous substrate (5%). Moreover, it has been demonstrated for the first time than these outstanding performances are not simply related to the overall surface area of the different morphologies but is directly related to the peculiar surface characteristics of the crystals.

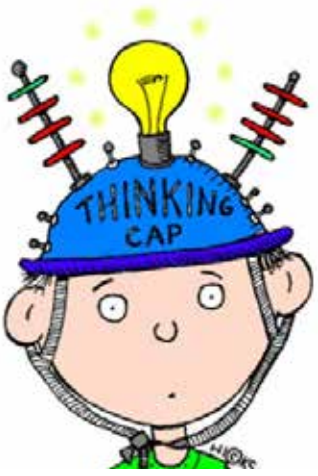


PATENTS

Pub No. WO2018078500A1, International application number PCT/IB2017/056540, L. Giannini, L. Tadiello, T. Hanel, E. Cobani, M. D'Arienzo, F. Morazzoni, R. Scotti, B. Di Credico: MATERIALI ELASTOMERICI PER COMPONENTI DI PNEUMATICI E PNEUMATICI COMPRENDENTI FIBRE DI SILICATI MODIFICATE

Pub. No. WO2018078480A1, International Application No PCT/IB2017/056345, L. Tadiello, L. Giannini, T. Hanel, M. Redaelli, B. Di Credico, M. D'Arienzo, F. Morazzoni, R. Scotti: NUOVI MATERIALI DI RINFORZO, COMPOSIZIONI ELASTOMERICHE E PNEUMATICI PER RUOTE DI VEICOLI CHE LI COMPRENDONO

Italian Patent n. 102016000130904, 23-12-2016, L. Tadiello, L. Giannini, T. Hanel, R. Scotti, B. Di Credico, M. D'Arienzo, F. Morazzoni, I. Tagliaro: COMPOSIZIONI ELASTOMERICHE COMPRENDENTI FIBRE DI SILICATI A MORFOLOGIA AGHIFORME DI DIMENSIONI NANOMETRICHE E PNEUMATICI PER VEICOLI CHE LE COMPRENDONO.



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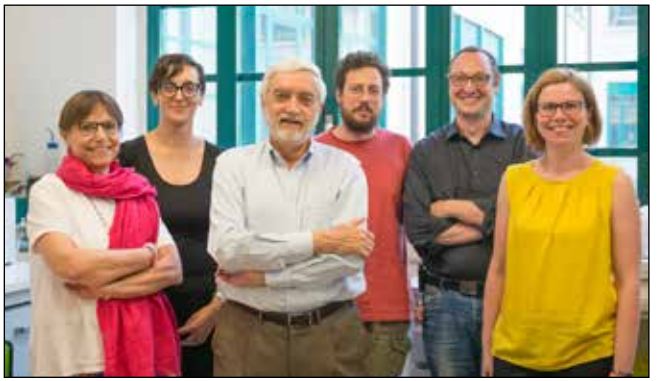

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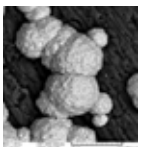
http://lness.como.polimi.it/index.php

L-NESS (Laboratory for Epitaxial Nanostructures on Silicon and Spintronics)
This is a joint research center of University of Milano Bicocca and Politecnico di Milano, established in 2002 by Prof. Leo Miglio of the Department of Materials Science, with Politecnico colleagues of the Department of Physics and the Department of Electronics, and Prof. Hans von Känel from the Department of Physics of ETH Zürich. The main laboratories are located at the Politecnico site in Como, equipped by MBE and CVD deposition systems, clean room, optical lithography, XRD, AFM, electrical station, e-beam lithography. Partners laboratories of PL and Raman spectroscopy, materials modeling, and PV cells material characterization are located at the Department of Materials Science of the University of Milano Bicocca.

Running research activities are mainly focused on group IV and III-V semiconductors and graphene for micro-electronic, optoelectronic and energy-saving/production applications. L-NESS gives a unique opportunity to work in one international environment, fully equipped with high-tech deposition and micro-fabrication tools.



Laboratory of Scanning Electron Microscopy and Microanalysis

www.mater.unimib.it/utenti/sem/SEMWEB/

The Scanning Electron Microscope (SEM) allows to obtain three-dimensional images at high resolution (~ 5 nm) by scanning an electron beam in a small area of the test sample. All the effects that are produced in the point of impact of the beam can be used, with appropriate detectors, to produce a contrast, and then the image. Furthermore, the analysis of the producedX-rays allows to perform compositional analysis with high spatial resolution (microanalysis). The sample to be examined must be conductive.
In case the sample is not conductive it is possible to deposit a thin gold film in order to make possible the vision. The microscope available in our laboratory allows the viewing of non-conductive samples even in the absence the gold film. Our SEM offers the opportunity to work in conditions of variable pressure of argon using an exclusive detector for low vacuum LVSTD.

Instrument
VEGA TS 5136XM variable pressure (5x10-3- 500 Pa).
Beam Acceleration 1-30 kV
Chamber dimensions: 300 mm x 250 mm x 280 mm.
Backscattered detector
EBIC detector for electrical mapping
EDS detector for composition analysis

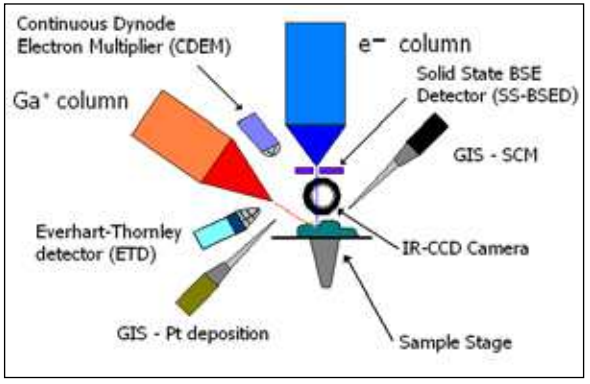
FIB/SEM BOMBAY LABORATORY. SOFT AND BIOLOGICAL MATERIALS MICROMANIPULATION AND MICROSCOPY

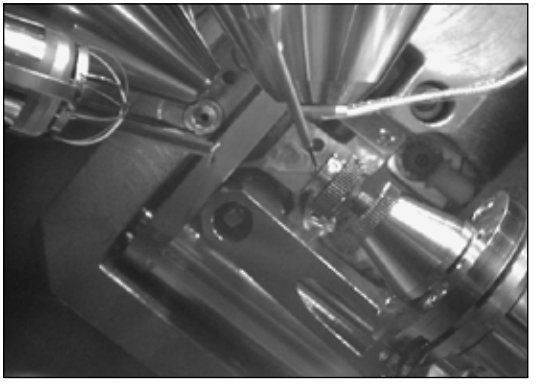
Following a joint application of the Department of Materials Science and Department of Physics, a FEI Quanta 3-D DualBeam™ system was installed at Milano-Bicocca University in the mid of 2006.

This important system (hosted by the Center of Excellence Plasma Prometeo) is devoted to studies on soft materials and biological specimens, that hopefully could invade the field of nanomedicine. Actually nanotechnology has led to a remarkable convergence of disparate fields including biology, applied physics, optics, computational analysis, modeling, and materials science.

The DualBeam system combines a Scanning Electron Microscope (SEM) with a Focused Ion Beam (FIB). The SEM is based on a tungsten electron column, able to operate as a conventional, high vacuum SEM or as an Environmental SEM, which allows working pressures up to 3000 Pa during electron microscopy by means of special gaseous detectors.
The Focused ion beam (FIB) is a tool that performs basically three functions: ion imaging (from secondary electrons or ions), milling (precision down to 10 nm) and deposition (with the insertion of a small needle delivering special gases).

The FIB/SEM Quanta 3-D provides further options, e.g.:
• electron imaging of the sample during navigation without erosion or gallium implantation produced by the ion beam;
• on-line operations in which the SEM is used 'to film' the cross-section face while FIB mills normal to the surface;
• the electron imaging of charging specimen in absence of metallization can take place before or after the FIB operations in the same chamber;
• Charge neutralization of the sample with electron beam during FIB milling;
• Two gas injector systems (GIS) for selective carbon milling (SCM) and Pt deposition;
• Alternative use of the electron beam induce deposition instead of the ion beam induced deposition in order to deposit films and growth nanostructures in a milder way.





MIB-SOLAR SOLAR ENERGY RESEARCH CENTER

www.mibsolar.mater.unimib.it

MIB-SOLAR was constituted in July 2010 with the goal to assemble and organize the diverse experiences of research in the field of materials and devices for solar energy applications at the University of Milano-Bicocca.

Through MIB-SOLAR the department of Material Science supports the national business community in research and development of new materials and technologies for solar energy application, mainly photovoltaics and solar fuels (artificial photosynthesis and water splitting). The Centre presently counts about 25 members. MIB-SOLAR has been included amongst the top players in the power industry 'made in Italy' (“100 italian energy stories” by Enel and Symbola)

Main objectives of MIB-SOLAR are:
- Study and research of new materials and devices related to solar energy in its various forms;
- The aggregation and coordination of researchers in the field of solar energy;
- Training of young researchers in the field of materials science and technology for solar energy;
- The development of intellectual property of the University of Milano-Bicocca in the field of solar energy;
- Cooperation with institutions, public and private research centers, and Fondazioni in the field of solar energy;
- Support and technology transfer to companies operating in the field of solar energy;
- Promotion of seminars, conferences, meetings and discussions for the study and exchange of information and knowledge in the field of solar energy.

MIB-SOLAR facilities include fully equipped laboratories for computational investigation, synthesis and characterization of inorganic and organic materials, and state-of-the-art instrumentation for lab scale and pre-industrial preparation of solar small and medium devices with full investigation of solar production of energy (electricity, fuels) and stability properties.

a) preparation and full characterization of materials and devices for photovoltaics, from silicon, to inorganic and organic thin films;
b) preparation and full characterization of materials and devices for solar fuels (artificial photosynthesis);
c) fully equipped laboratories for organic and organometallic synthesis and characterization;
d) fully equipped laboratories for optical and electrochemical investigation;
e) main facilities for the preparation of devices (sputtering system, nitrogen and argon filled glove boxes, laser scribing machine, titanium hotplates, screen printers, UV-ozone cleaners, etc.)
f) main facilities for the full characterization of solar devices (solar simulators up to 6 x 6 inches, I/V characterization, internal and external quantum efficiency, light soaking chamber for cell ageing, stability studies, electrochemical impedance spectrometer, mesurements of hydrogen and oxygen via water splitting under irradiation).

CNISM - Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia

www.cnism.it

The University of Milano-Bicocca is member of the Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia (CNISM). The activities of the CNISM Research Unit at the Department of Materials Science are devoted to the

- Growth and optical spectroscopy of semiconductor quantum dots and heretostructures
- Optical and dielectric properties of oxide nanostructures for optical technology
- Thin films for applications in photonics and optoelectronics
- Simulation and modeling of the epitaxial growth of semiconductor nanostructures
- Growth, optical properties and photophysics of organic molecular semiconductors
- Chemical physics of the surface of semiconductors for gas sensing and photovoltaic applications
- Theory of low dimensional materials
- Ab-initio simulations of materials for data storage

INSTM - Consorzio Interuniversitario Nazionale per la Scienza e la Tecnologia dei Materiali

www.instm.it

Our University participates in INSTM, the National Interuniversity Consortium of Materials Science and Technology; its local Research Units is hosted by the Materials Science Department. The INSTM Consortium was founded in order to provide organisational, technical and financial support to disseminate knowledge in the field of materials science and technology within its affiliate universities. Its efficiency in bringing together and managing their considerable talents creates an effective critical mass that renders them highly competitive in taking on innovative research projects.
General Fields of Research are: Advanced mechanics, construction and transport, Energy and environment, Systems for the preparation, transmission and storage of information, Health and Nutrition.
The success of INSTM is underlined by the sheer number and quality of the domestic and international projects involving INSTM's research groups that have been financed to date.

CORIMAV - CONSORZIO PER LA RICERCA SUI MATERIALI AVANZATI

Since 2001, thanks to an agreement between the University of Milano-Bicocca and Pirelli Company, the Corimav Consortium for research on materials funds three scholarships per year for the industrial curriculum of the doctorate in Materials Science. Such Ph.D. positions often foster research activities related to tyres, but also more general topics such as nanotechnology and simulations of materials. Pirelli Company's experts lecture on management and intellectual properties at the Ph.D. school of Science and present seminars on specialized topics.

ETSF-European Theoretical Spectroscopy Facility

www.etsf.eu

The University of MIlano Bicocca is member of the European Theoretical Spectroscopy Facility, a research network and e-infrastructure dedicated to providing support and services for ongoing research in academic, government and industrial laboratories. Comprised of 68 research teams across Europe and the United States, the ETSF carries out state-of-the-art research on theoretical and computational methods for studying electronic and optical properties of materials. All fields in need of knowledge about electronic excitations, transport and spectroscopy will benefit from the ETSF, such as condensed matter physics and chemistry, biology, materials and nano science. The ETSF gathers the experience and know-how of more than 200 researchers in Europe and the United States, facilitating innovation and rapid knowledge transfer. The ETSF is headquartered in Louvain-la-Neuve, Belgium.

DeltaTi Research

http://www.universita.it/brevetto-universita-bicocca-ricupero-energia/

DeltaTi Research was founded in 2011 as a joint spin-off between the University of Milano-Bicocca and ERG SpA. The consortium, fully financially supported by ERG, has aimed at the development of nanostructured silicon-based thermoelectric generators. Thermal harvesting is actually a key enabling technology to power the so-called Internet of Things, further to be a way to recover waste heat released at low temperatures by industrial plants, cars, and buildings.

Over the last five years DeltaTi Research has empowered a novel technological approach developed at the Department of Materials Science and protected now by eleven international patents. Low-cost, high-efficiency generators based upon silicon nanocomposites have now reached full technological maturity. Technology was pre-industralised in 2014 and has then been transferred to LFoundry srl, which has joined the Consortium in 2015.

Over its five years of activity the Consortium R&D has signed research contacts for more than four million euros with a number of external institutions, including CNR, the Universities of Modena, Naples, and Vienna, the Fondazione Bruno Kessler, the Demokritos Research Center, and Altran SpA.

PILEGROWTH TECH S.R.L.

http://www.pilegrowth.com

The company, established in September 2012 and spin-off of the University of Milano Bicocca, originates from one technological breakthrough for semiconductor integration in silicon obtained by Prof. Leo Miglio (CEO) and Prof. Hans von Känel (ETH Zürich, CTO), within the L-NESS inter-university center. It aims at developing, licensing, or selling innovative technologies manufacturing semiconductor structures and devices, with specific application to thick-film systems, such as high-efficiency photovoltaic cells, imaging detectors and power electronics devices. The company received Seed Money financing from Italian venture capital investors and one industrial partner.

The targets of the first year are to provide one demonstrator of Ge/GaAs-, or Ge/GaAs/InGaP-based PV cells for satellite applications, and the proof of concept that SiC-based power devices can be integrated in silicon. PileGrowth Tech is characterized by a strong link to international semiconductor laboratories, both in academia and in the industry. Contracts with the University of Milano Bicocca, Politecnico of Milano, the IMM-CNR Institutes of Catania and Bologna, PV cell manufacturers, such as CESI in Milano and ENE in Brussels, and ETC srl, SiC process developer in Catania, are already running. A strong scientific collaborations with Swiss federal institutions, such as ETH Zürich, CSEM SA (Swiss Center for Electronics and Micromachining) Neuchatel, and EMPA (Federal Institute of Materials Certification) are particularly active, within a collaboration for developing a new Ge-based X-ray imaging detector, integrated on a Si CMOS chip.

GALATEA BIOTECH- THE WHITE BIOTECH COMPANY

www.galateabiotech.com

Galatea Biotech is a White Bio Tech and Green Chemistry Spin-off of Milano-Bicocca University . The core business of Galatea is the R&D of technologies and processes for the production of fine and bulk chemicals by bio fermentation, as well as the production and marketing of these products and their derivatives.
Galatea biotech is specialized in the production of bio plastics, enzymes, bi-functional molecules, organic acids and microbial strains suitable for the production of many different bio molecules. Our strength is the University Knowledge in biotechnology and materials science we can provide. In particular, our ability in using the DNA recombinant technique makes it possible for us to engineer selected microorganisms aiming to obtain a large number of molecules and materials that can be used in many different applications; a thorough material characterization permits a deep knowledge of our products in view of their applciations.
The technological processes developed by Galatea biotech build molecules with a low carbon footprint, which is typical of products of plant origin and which contributes to the reduction of greenhouse gas emissions, achieving thus Kyoto's Protocol targets.

GRAFTONICA. TECNOLOGIE D'INNESTO, INNESTO DI TECNOLOGIE

www.graftonica.it

Graftonica produces and brings to market nanotech additives to meet the evolving needs of the rubber and plastics industry. Additives produced by Graftonica are easily dispersed in polymers can be provided as masterbatches. They improve the performance of polymer products, making them suitable for applications currently reserved to other classes of materials providing smart solutions: high dielectric constant materials for electronics, water and gas barrier for food packaging, high refraction index transparent materials for optics and photonics, modulated scattering materials for lighting, UV coatings for conservation and restoration of cultural heritage and biocompatible and biomimetic materials for implants, prosthetics, phantoms. The methodology developed at Graftonica for compatibilizing and dispersing inorganic nanofillers is inspired by state of the art scientific concepts («lab on a particle») and combines the functional properties of nanoparticles with the structural properties of the polymer. The compatibilization technology can be applied on a wide range of commercial products, as well as on custom made nanoparticles and on metal surfaces. As part of an integrated approach to develop and prototype innovative materials, Graftonica can also provide: analysis and deformulation of existing materials, including failure analysis; scale up of processes and reactions from literature.

GLASS TO POWER
www.glasstopower.com

Glass to Power is a spin-off of the University of Milan-Bicocca that was established in September 2016 with the goal of developing semi-transparent photovoltaic windows that can be integrated into the architecture of building façades. Interest in Building Integration Photovoltaics (BIPV), where the photovoltaic elements become an integral part of the building body, is growing worldwide. Photovoltaic specialists and innovative designers in Europe, Japan, and the U.S. are now exploring creative ways of incorporating solar electricity into buildings. The BIPV market is forecasted to significantly grow to over $6 billion by 2022 at a yearly rate of ~30%. Europe will account for about 40% of the total market. Specifically, the nearly-Zero Energy Buildings (nZEB) sector is expected to be the fastest growing segment.

Glass to Power was founded under the guidance of Professor Francesco Meinardi (present chairman of the spin-off) and ProfessorSergio Brovelli (chairman of the scientific committee) with an initial capital of 300,000 Euro. The main share holders are: Industrie De Nora, Karma Srl, TEC Srl, University of Milan-Bicocca, and Management Innovations Srl.

Glass to Power's project is aimed at the industrialization and successive commercialization of Luminescent Solar Concentrators (LSCs) consisting of a semi-transparent panel of plastic material doped with chromophores that absorb the solar radiationand re-emit infrared photons. These latter are guided to the panel edges and here converted into electricity by conventional PV cells. Patents by Professors Brovelli and Meinardi have dramatically improved the LSC technology using as chromophores colloidal Quantum Dots (QDs) that can effectively decouple the processes of absorptionandemission of light. This makes it possible to obtain colorless poly acrylate panels, with an electrical generation efficiency close to 5%, made of non-toxicmaterials that can be easily integrated into building walls and windows. Glass to Power currently enrolls two young researchers, Dr. Graziella Gariano and Dr Francesco Bruni, who were recently recruited for the realization of the first industrial-grade LSCs whose installation in beta-test environments is scheduled within the end of 2017.

TEACHING

Teacher	Course	Where
A. Abbotto	Materiali e dispositivi per l'energia	SdM
	Chimica organica	SdM
	Chimica organica II e laboratorio	STC
	Chimica organica per l'energetica sostenibile	STC
M. Acciarri	Fisica	BIO
	Esperimentazioni di fisica dei solidi	FIS
	Storia della fisica moderna e degli strumenti ottici	O&O
M. Bernasconi	Struttura della materia	FIS
	Complementi di struttura della materia	SdM
L. Beverina	Chemistry of molecular materials	MATSC
	Chimica organica II e laboratorio	STC
	Chimica organica III e laboratorio	STC
	Chimica organica superiore	STC
S. Binetti	Materiali e dispositivi per l'energia	SdM
	Physical chemistry of solid state and surfaces	MATSC
	Chimica fisica dei materiali	SdM
	Chimica fisica III e laboratorio	STC
E. Bonera	Esperimentazioni di fisica dei solidi	FIS
	Fisica dei materiali con laboratorio	SdM
	Sistemi ottici e oftalmici con laboratorio	O&O
A. Borghesi	Fisica II	O&O
G. Brivio	Teoria della materia condensata i	FIS
	Teoria della materia condensata II	FIS
	Complementi di struttura della materia	SdM
S. Brovelli	Nanotecnologie	SdM
	Physical characterization of materials with laboratory	MATSC
	Laboratorio di fisica II	SdM
M. Catti	Thermodynamics and kinetics of materials	MATSC

A. Comotti	Chemistry and technology of polymers and industrial applications	MATSC
	Laboratorio di chimica analitica strumentale	SdM
	Laboratorio di tecnologia dei materiali II	SdM
M. D'arienzo	Chimica generale e inorganica con laboratorio	SdM
C. Di Valentin	Chimica generale e laboratorio	STC
	Spettroscopia e sintesi di composti inorganici	STC
M. Fanciulli	Physical characterization of materials with laboratory	MATSC
	Physics of semiconductors	MATSC
	Laboratorio di tecnologia dei materiali I	SdM
E. Grilli	Spettroscopia ottica dello stato solido	FIS
	Laboratorio di stato solido ed elettronica I	FIS
M. Martini	Radiation matter interaction	MATSC
	Laboratorio di fisica I	SdM
F. Meinardi	Physical characterization of materials with laboratory	MATSC
	molecular electronics and photonics	MATSC
	Interazione luce materia	O&O
L. Miglio	Solid state physics	MATSC
	Surfaces and interfaces	MATSC
	Laboratorio di Tecnologia dei Materiali i	SdM
F. Montalenti	Termodinamica statistica computazionale dei solidi	FIS
	Physical characterization of materials with laboratory	MATSC
	Struttura della materia II	SdM
F. Morazzoni	Chimica di coordinazione e metallorganica	STC
M. Moret	Chimica	FIS
	Chemistry of inorganic materials	MATSC
	Chimica inorganica II e laboratorio	STC
D. Narducci	Chimica fisica	SdM
	Chimica fisica dei sistemi complessi	STC
	Chimica fisica superiore	STC
G. Pacchioni	Chimica dei materiali ceramici	SdM
	Chimica inorganica II e laboratorio	STC
	Chimica per le nanotecnologie	STC

A. Paleari	Physics of homogeneous and nanostructured dielectrics	MATSC
	Fisica II	SdM
A. Papagni	Laboratorio di chimica organica	SdM
	Chimica	O&O
	Sintesi e tecniche speciali organiche dei materiali	STC
	Chimica organica per l'energetica sostenibile	STC
R. Ruffo	Applied physical chemistry with laboratory	MATSC
	Chimica fisica dei materiali	SdM
	Chimica fisica applicata	STC
S. Sanguinetti	Fisica dello stato solido	FIS
	Laboratorio di stato solido ed elettronica II	FIS
	Fisica dei materiali con laboratorio	SdM
A. Sassella	Struttura della materia i	SdM
	Fisica I	O&O
R. Scotti	Chimica generale e inOrganica con Laboratorio	SdM
	Chimica inorganica I e laboratorio	STC
R. Simonutti	Physical characterization of materials with laboratory	MATSC
	Chimica dei materiali polimerici	SdM
	Chimica analitica strumentale e laboratorio	STC
P. Sozzani	Chimica macromolecolare con laboratorio	SdM
	Chimica macromolecolare	STC
S. Tavazzi	Ottica geometrica e oftalmica con laboratorio	O&O
	Storia della fisica moderna e degli strumenti ottici	O&O
A. Vedda	Physical characterization of materials with laboratory	MATSC
	Fisica I	SdM

Legend:
BIO Biologia
MATSC Materials Science
O&O Ottica e Optometria
FIS Physics
SdM Scienza dei Materiali
STC Scienze e Tecnologie Chimiche

GRADUATE STUDENTS 2017

Materials Science

Bachelor's Degree

Omar ABOU EL KHEIR, Leonardo BATTAGLIA, Antonio Luca BERARDINO, Dario BERTUZZI, Roberto BISCOTELLI, Cristina BOMBELLI, Gabriele Alvin BOTTA, Andrea FILIPPI, Simone FIORINI GRANIERI, Giorgio Luigi GRAVINA, Davide LAMBARDI, Daniele LANZONI, Giorgio MAGGI, Marco MELZI D'ERIL, Andrea OLIVATI, Matteo ORFANO, Irene OSTROMAN, Francesca PALLINI, Laila RODARI, Malithi RUPASINGHE ARACHCHIGE, Federico SCARPIONI, Pietro SCAUSO, Pietro STEINER, Pierre Luca STIGLIANO, Andrea TAMIAZZO, Pietro TREMOLADA, Valeria VANOLI, Michael VITARI

Post graduate Master's degree

Tommaso ANTONELLI, Francesco ARCADI, Silvia BANDELLONI, Alessandro BARZANI, Denise BESGHINI, Luca BETTAMIN, Gabriele BIANCA, Valentina BONERA, Giorgio BORZINI, Chiara CAPITANI, Simone CIMÒ, Alessandro DANEI, Laura DEI CAS, Marianna DITERLIZZI, Luigi FRIONI, Andrea Maurizio MONTI, Massimo PALERMO, Davide PARINI, Giorgia PARODI, Andrea ROLFI, Cristina SANDIONIGI, Ivonne Andrea SANTILLAN ORELLANA, Michele TOSI

Optics and Optometry

Bachelor's Degree

Riccardo ACCARDI, Giulia ACQUATI, Chiara Nives ARRARA, Kriseilda BEGOLLI, Silvia BERARDI, Nadia BONASSI, Chiara BORTOLOTTI, Elena BOSI, Giulia BRIANZA, Cristina CAPRA, Alessio CERRI, Matteo CICERI, Federica CORLAZZOLI, Annalisa CORTAZZO, Valentina DEL FORNO, Serena DELBONO, Carmela DELLA MONICA, Riccardo DELL'ORO, Alex DI DIO PALERMO, Simone DI MURO, Vanessa GALLO, Federica GARLATI, Ramona GERVASONI, Nicole GHIRARDI, Alessandro GIRMENIA, Luana GIUDICE, Elisa GOZZINI, Marisa INDELICATO, Manuel INNOCENTE, Ambra MANNELLA, Arianna MARELLI, Giulia Paola MARINI, Adriana MORO, Filippo PEREGO, Chiara POGGIANI, Michela PORRO, Margherita POZZI, Marianna RADAELLI, Nicola RIZZIERI, Luca ROSSIN, Jessica SACCANI, Giacomo SAIZ, Davide Sean SALA, Roberta SIVIERO, Jessica Francesca TOMINETTI, Sorina Ruth TRAISTARU, Marianna VALLI, Mirko VERDERIO, Daniele VERRENTI, Eleonora VIGANÒ, Valentina VIZZUTTI

Chemistry

Bachelor's Degree

Ludovico Andrea ALBERTA, Veronica BENUZZI, Enrico BIANCHETTI, William BONVINI, Raissa BRAMBILLA, Gabriele BRUGNETTI, Giacomo BUSALACCHI, Fabio BUTRICHI, Stefano CADEDDU, Gloria CARINI, Silvia CHIAPPA, Ambra CHIODINI, Catalina CIOBANU, Marco COLOMBO, Eleonora Maria CORACI, Giulia CORADELLO, Mattia DELLEGRAZIE, Samantha Veronica FACCHETTI, Luca FANTONI, Andrea FRIGERIO, Giulia Maria GARAVAGLIA, Erika GHIGLIETTI, Elena GIANETTI, Alessia GRITTINI, Davide LOCATELLI, Alessio MACORANO, Andrea MANZO, Pietro MARONI, Paola MATOZZO, Anna MAURI, Gaetan MINKOUMBA SONFACK, Andrea MOLIN, Alberto MOTTA, Simone MURGANTI, Monica NAVA, Michela NEGRI, Jessica NEGRINI, Mattia PAGNONCELLI, Federico PARENTI, Martina PICCIOLI, Edoardo PICHEO, Anna RANAUDO, RENIS Dario, Alessio ROMERIO, Lorenzo ROSSI, Alessia ROTASPERTI, Sabrina SARTORI, Giulia SILVESTRI, Elisa SORTI, Rebecca STARA, Matteo TIRONI, Dario TORRICELLI, Asia TRABUCCHI, Chiara TRETTENE, Michele TRIBBIA, Mirko TRONCIA, Jael Novuyo TSHUMA, Marina VECCHIERELLI, Marco VIMERCATI, Paolo VISCONTI, Martina VOLPI

MATERIALS SCIENCE GOES TO TOWN

MEETmeTONIGHT, the Researchers' Night in Lombardy, is an annual event that aims to spread scientific culture and knowledge of the research professions among citizens of all ages through events and fun and challenging initiatives.

In the 2017 edition, we were present with the stand SOLAR LAST FRONTIER. Toward the energy of the future, counteracting the greenhouse effect and limiting the global warming. Alessandro Abbotto, Maurizio Acciarri and Simona Binetti explained how to produce renewable energies and lower the CO_2 immission in atmosphere: last generation fotovoltaic cells, "clean" hydrogen from water and sun, biogas from waste.

In an evening talk titled *L'archeometria* svela i segreti dell'arte (Archaeometry reveals the secrets of art), Marco Martini presented the current state of the art of Archaeometry.

CREDITS

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