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THE MATERIALS SCIENCE DEPARTMENT

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

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Mail	Secretariat: lucia.rodolfi@unimib.it
Director	Prof. Marco Martini
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:

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

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

DIRECTOR Marco Martini

DEPUTY DIRECTOR Alessandro Abbotto

Angiolina Comotti Massimilano D'Arienzo Alberto Paleari Luisa Raimondo Adele Sassella Anna Vedda





TEACHING

Alessandro Abbotto Chemical Science Courses, Chairman

> Marco Bernasconi Students career commission

> > **Gianpaolo Brivio** Doctorate Coordinator

Angiolina Comotti Study advisory

Dario Narducci Library Board, Chairman

Alberto Paleari Materials Science Courses, Chairman

Antonio Papagni Optics and Optometry Course, Coordinator

> Piero Sozzani Erasmus

Anna Vedda Thesis commission

NUMBERS

PERSONNEL	#
Emeritus	2
Researchers	43
Administration	4
Technical personnel	9
Post doc	81
Total	139

FUNDINGS		
TOTAL	4.800.000 €	
EU	48%	
Cariplo	24%	
Regione Lombardia	13%	
MIUR	9%	
Other	6%	

RESEARCH

Organic and polymeric materials



Alessandro Abbotto

Organic and Hybrid Materials and Devices for Photovoltaic, Artificial Photosynthesis and Optoelectronics (MIB-SOLAR Solar Energy Research Centre)

Luca Beverina

Functional dyes and pigments for photonics, electronics and optoelectronics

Massimo Moret

Crystal growth and characterization of organic and inorganic crystals: surface chemical reactions and sorption processes

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 nanostructures

Silvia Bracco, Piero Sozzani

Nanostructured materials and magic angle spinning NMR

Materials for microelectronics and photonics



Marco Bernasconi

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

Emiliano Bonera, Emanuele Grilli, Fabio Pezzoli, Stefano Sanguinetti

Optical spectroscopy and fabrication of semiconductors and semiconductor quantum structures

Silvia Tavazzi Optics and optometry

Adele Sassella Organic molecular films and heterostructures

Sergio Brovelli, Francesco Meinardi, Angelo Monguzzi **Photophysics of molecular semiconductors**

Mauro Fasoli, Alberto Paleari, Anna Vedda

Oxide nanostructures and silica-based materials for optical technology

Marco Fanciulli

Materials and Spectroscopies for Nanoelectronics and Spintronics – MSNS Laboratory

Leo Miglio, Francesco Montalenti

Simulation and modelling of the epitaxial growth of semiconductor nanostructures and thin films

9

Materials for energy and environment

Maurizio Acciarri, Simona Binetti, Dario Narducci

Chemical physics of surface modifications, gas sensing and materials for photovoltaic applications

Gian Paolo Brivio

Theory and computations of adsorbate interfaces

Angiolina Comotti

Materials for gas storage and energy production: X-ray, neutron diffraction and physico-chemical properties

Cristiana Di Valentin, Livia Giordano, Gianfranco Pacchioni, Sergio Tosoni **Theory of oxide surfaces, interfaces, and supported clusters**

Claudio Maria Mari, Riccardo Ruffo Electrochemical activities

Massimiliano D'Arienzo, Barbara Di Credico, Roberto Scotti Chemistry of inorganic and organometallic materials

Materials for cultural heritage

Anna Galli, Marco Martini, Emanuela Sibilia

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





Organic and Hybrid Materials and Devices for Photovoltaics, Artificial Photosynthesis and Optoelectronics





ALESSANDRO ABBOTTO

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 (sun light; water) to provide these energy sources, that is a) photovoltaics; b) 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.

ORGANIC AND HYBRID 3RD GENERATION PHOTOVOLTAICS

We investigate last generation organic and hybrid photovoltaics, namely:

- a) dye-sensitized solar cells
- b) organic solar cells
- c) perovskite solar cells

Furthermore we study 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 organometallic dyes, electron and hole transporting materials, electrolytes, semiconductor oxides, electrodes) are investigated as well as lab-scale and pre-industrial photovoltaic panels.

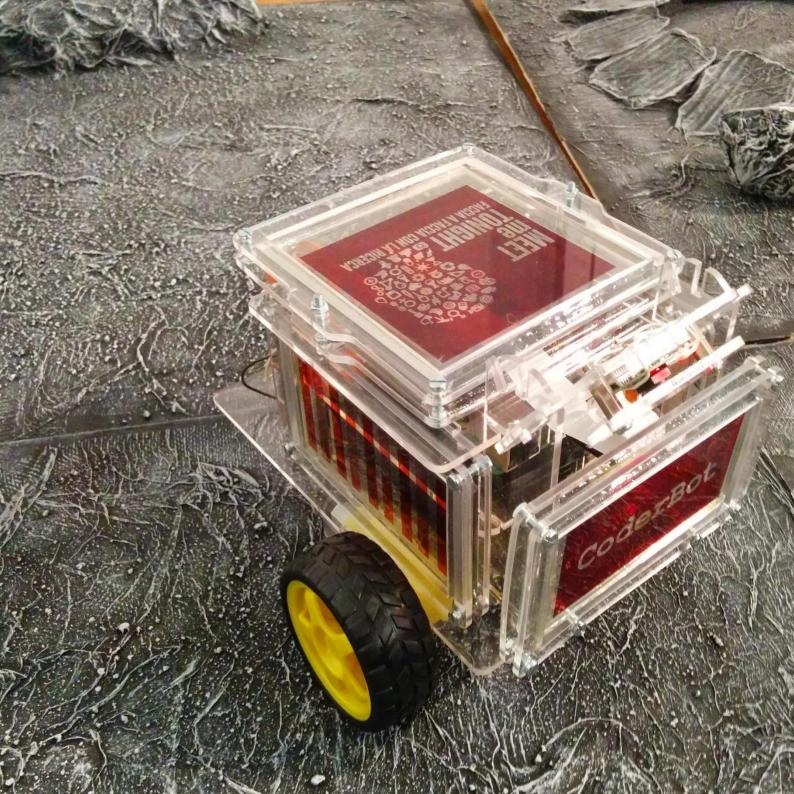
ARTIFICIAL PHOTOSYNTHESIS: CLEAN AND RENEWABLE SOLAR FUELS

We study dyes and catalysts for the photocatalytic production of hydrogen and oxygen (water splitting), also in combination with bio-inspired and bio-mimic materials. Focus is on the use of molecular antennas in order to provide enhanced light harvesting and solar-to-fuel conversion efficiency.

MAIN FACILITIES

Fully equipped organic synthesis and characterization laboratory.Spectroscopic (absorption, emission, NMR) characterization.Glove box.

Clean room for preparation and characterization of photovoltaic cells and modules. **F**acilities for the measurement of photocatalytic hydrogen production



Functional dyes and pigments for photonics, electronics and optoelectronics





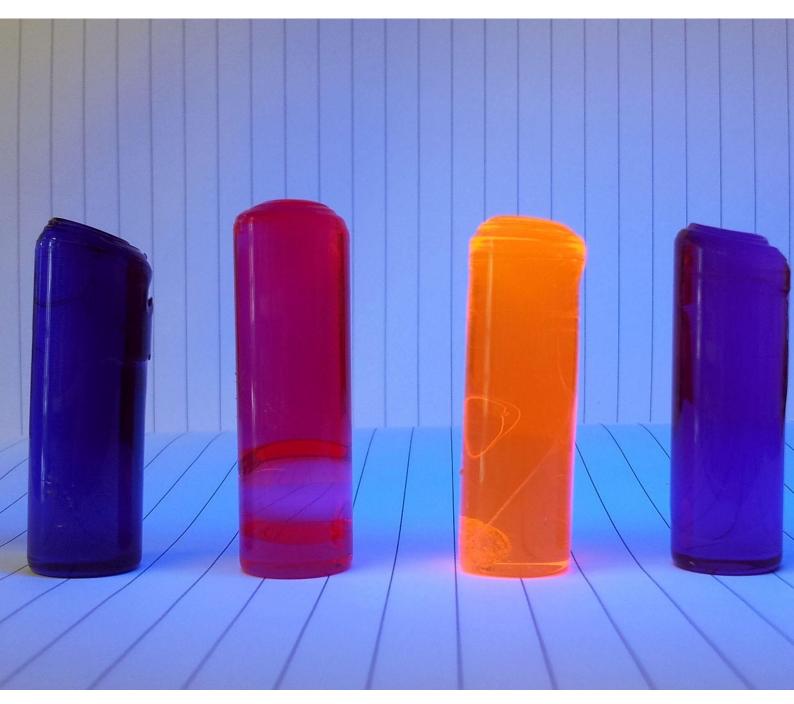
LUCA BEVERINA

Organic conjugated molecular and macromolecular materials have experienced a tremendous interest due to their potentially low cost manufacturing, tailor made properties and compatibility with a variety of rigid and flexible substrates. Decades of research efforts made it possible to establish detailed structure-properties relationships linking a precise function (light emission, charge transport, light shading, sensing capabilities, charge storage,...) to general structural motifs identifying most performing materials. Early guidelines were mostly focused on single molecule properties, whilst today's approach is more focused on solid state, interphases and interfaces. Nonetheless, the implementation of such general rules in the design of one particular structure still remains a rather difficult task due to the extreme variety of the possible organic residues and connection motifs that are in principle possible (even though perhaps unpractical from the point of view of synthetic feasibility).

The purpose of our research is the exploitation of the electronic characteristics of the fundamental conjugated building blocks (double and triple bonds, benzene rings, heteroaromatics) and the way such units can be joined together in order to build up a particular electronic structure leading to a specific function. Special emphasis is given to the electronic features and chemical behavior of those eteroaromatic rings more frequently employed as building blocs of molecular and polymeric performing semiconductors. We are also interested in the influence of such organic moieties on solid-state morphology, particularly regarding to thin films, interphases and interfaces.

Amongst the main classes of functional materials we are interested in are:

Active molecules and polymers for photovoltaics and photodetectors; Electrochromic organic materials and devices; Molecular materials for organic filed effect transistors; Thermochromic molecules for Time/Temperature Integrators (smart labels); Organic rechargeable batteries; Colloidal organic nanoparticles for biological imaging; Luminescent Solar Concentrators; Hybrid Transparent Conductive Materials; Singlet Oxygen Sensitizers (Photodynamic Therapy); Photoresists; Photocrosslinkable organic semiconductors; Squaraines (for all purposes).



Crystal growth and characterization of organic and inorganic crystals





MASSIMO MORET

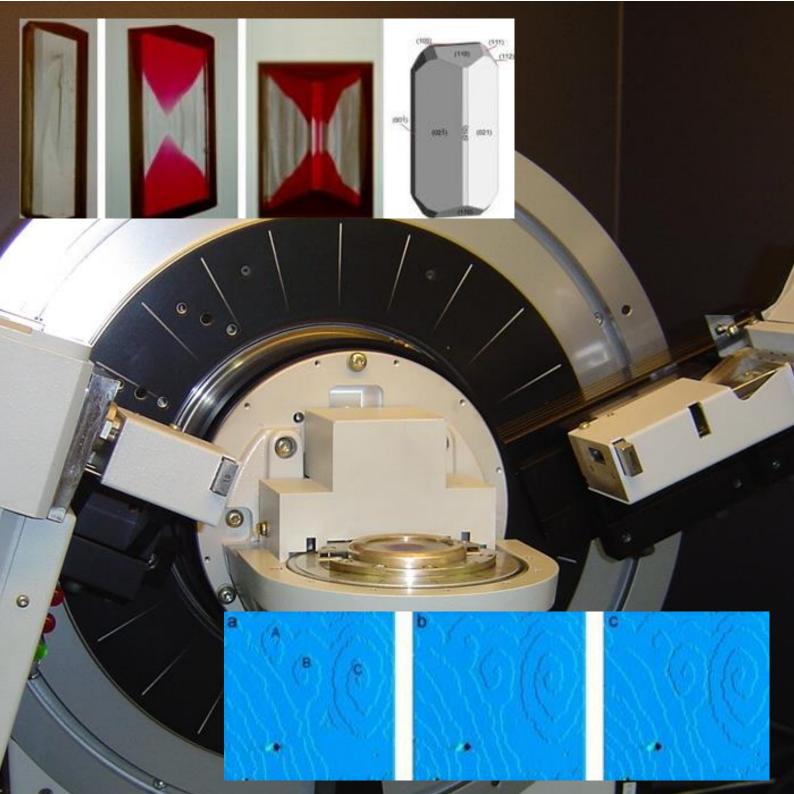
Growth and characterization of crystals is a mandatory step in many fields of science and technology. Growth of crystals involves several surface chemical processes where surface reactivity is a key point to understand and optimize crystal growth as well as the interactions of crystals with natural or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

Major areas of interest are: crystal growth from solution (amino acids, organic semiconductors and coordination polymers), study of sorption processes at the crystal/solution interface in natural environments and in laboratory processes (e.g. doping of crystals or setting of cements/plasters in the presence of organic additives).

In situ characterization of reacting crystal surfaces is mainly based on scanning probe microscopy (SPM) with a dedicated fluid cell and a controlled environment. In situ SPM allows recording of time evolution of surface topography and the study of surface reaction kinetics.

Growth of organic semiconductor crystals (with solution, sublimation, physical vapour transport, or organothermal methods) is complemented with ex-situ SPM, 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.

Simulations of organic-organic heteroepitaxial layers are also performed by docking methods using empirical force fields and classical molecular dynamics simulations. Aim of these studies is analysis and prediction of epitaxial relationships between organic thin films deposited in ultra high vacuum onto organic crystal substrates.



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





ANTONIO PAPAGNI

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 synthess. 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 SIMONUTTI

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).

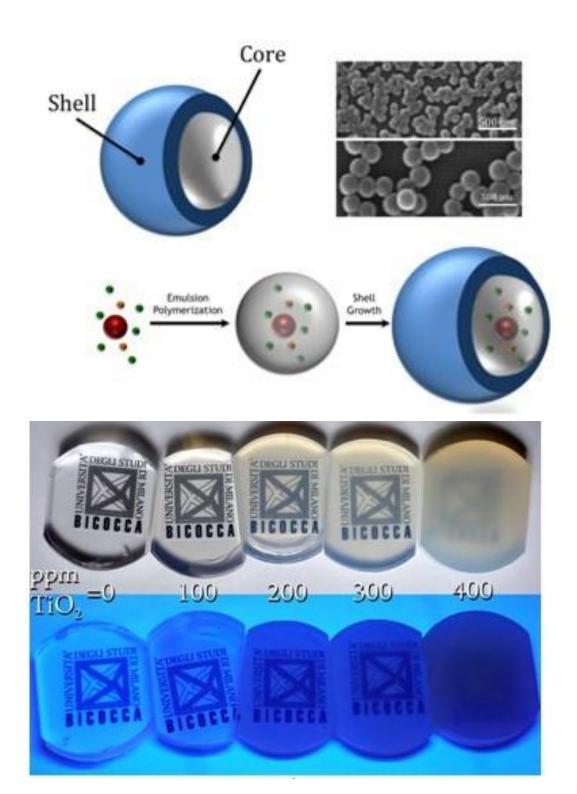
Recently, by implementing advanced polymerization techniques like RAFT (Reversible Addition-Fragmentation chain Transfer polymerization) we synthesized several samples of highly controlled amphiphilic block copolymers. Our interest is currently focused on innovative techniques for their characterization 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. **N**anocomposite 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.



Nanostructured materials and magic angle spinning NMR







SILVIA BRACCO, PIERO SOZZANI

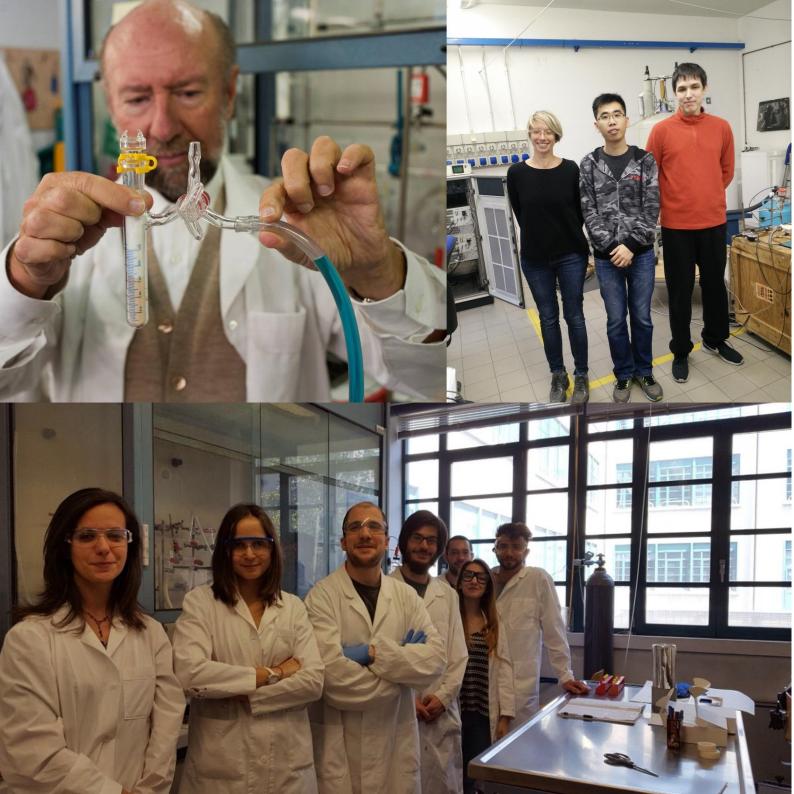
The preparation and characterization of novel composite and nanocomposite materials is the target of our research group. Reinforcing agents for polymers and polymers as binders for reactive inorganic materials are mainly addressed. The effort for optimizing the interfaces lead to the preparation of highly 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 m²/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 (¹²⁹Xe) 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 wideline 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.



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





MARCO BERNASCONI

PHASE CHANGE MATERIALS FOR DATA STORAGE

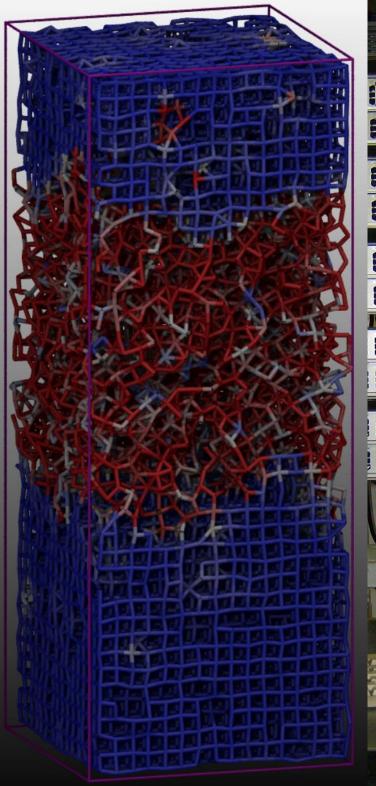
Phase change materials ($Ge_2Sb_2Te_5$ and related telluride alloys) are attracting an increasing interest worldwide for applications in optical disks (DVDs) and in a novel non volatile electronic memory, the phase change memory cell. Both applications rely on a fast (10-100 ns) and reversible transformation 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.

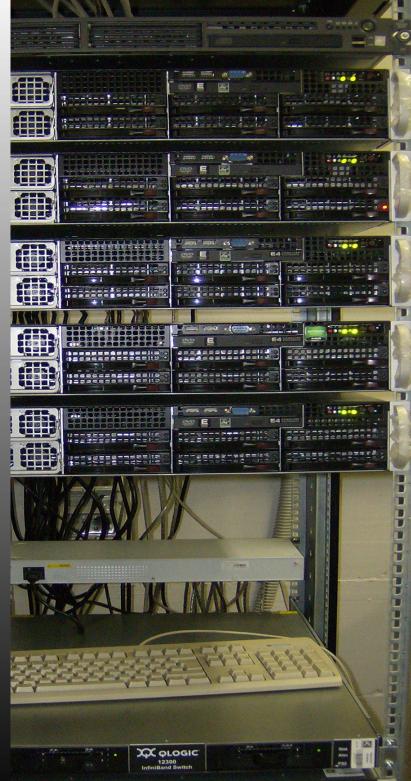
On the basis of density functional molecular dynamics simulations, we investigate the structural, dynamical and electronic properties of the amorphous and crystalline phases of materials in this class aiming at establishing correlations between the composition of the alloy and the electronic and optical 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, the microscopic mechanisms responsible for the fast crystallization and the properties of nanowires.

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 BONERA, EMANUELE GRILLI, FABIO PEZZOLI, STEFANO SANGUINETTI

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.

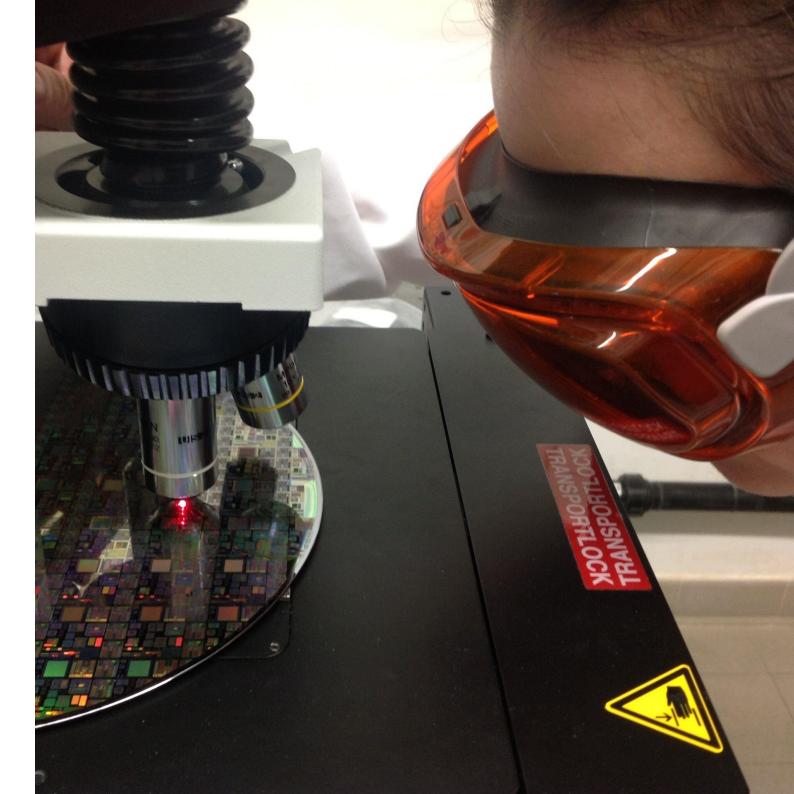
FACILITIES

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.









Optics and Optometry





SILVIA TAVAZZI

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

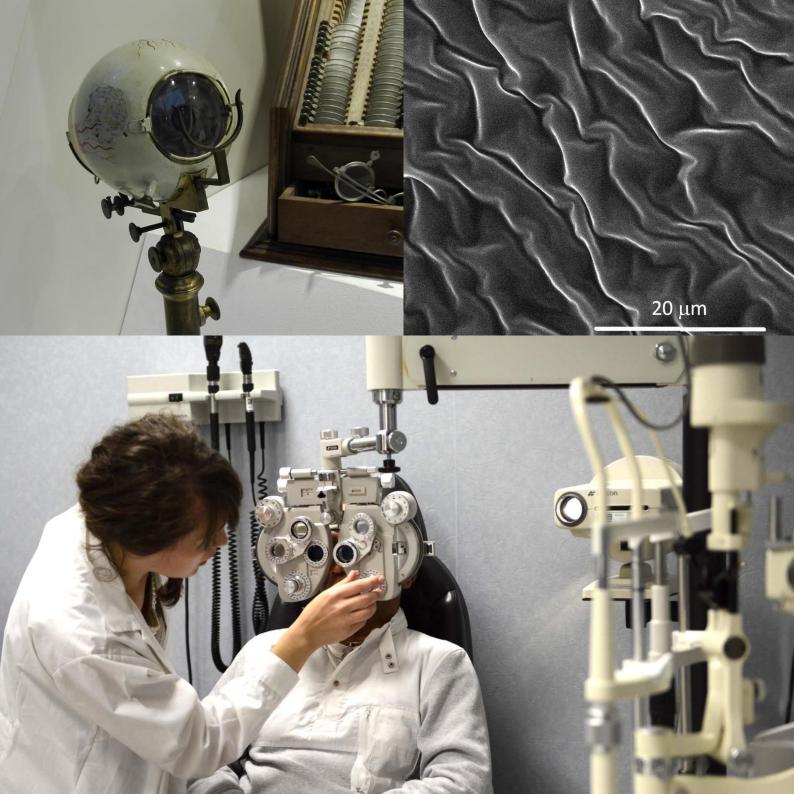
Recent studies were focused on the properties of materials for soft contact lenses in terms of microscopic structure and uptake/release of hyaluronan, lactoferrin, and drugs. Different materials were investigated. The uptake was studied in terms of loading capability, penetration depth in the lens, release 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 interface.

OPTICAL SYSTEMS

A method was recently developed, which allows the acquisition under a slit-lamp biomicroscope 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..



Organic molecular films and heterostructures





Adele Sassella

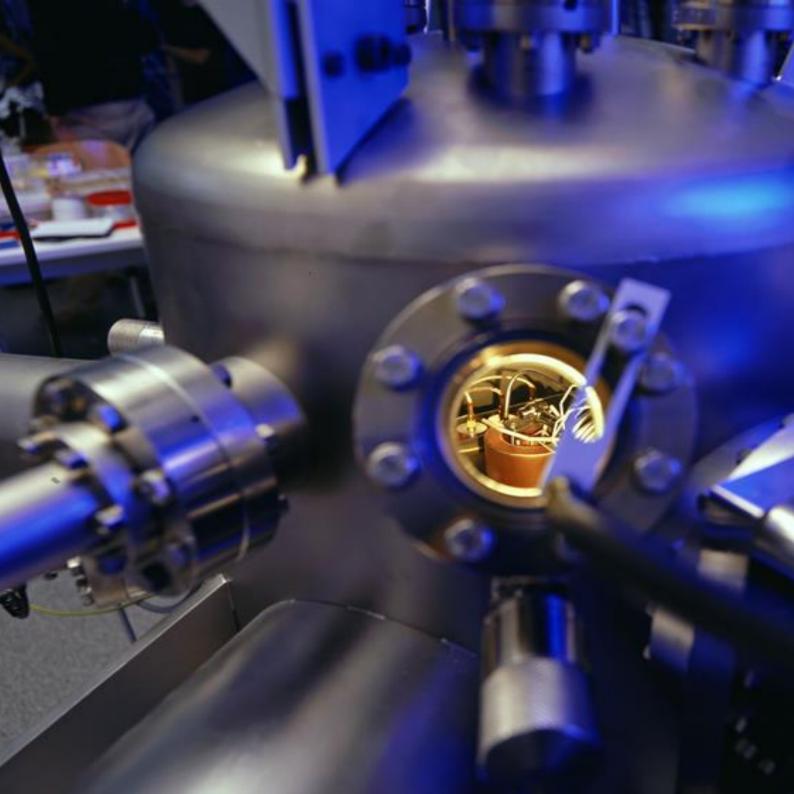
Thin film growth. Films of organic molecular semiconductors are grown by organic molecular beam epitaxy (OMBE) under different conditions, such as pressure, substrate type and temperature, absence or presence of external fields. The study of the OMBE growth process itself is carried out by detecting 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 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 insitu 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 μm^2 wide regions, while on crystalline samples molecular resolution is also achievable.



Photophysics of molecular semiconductors









SERGIO BROVELLI, ANGELO MONGUZZI, FRANCO MEINARDI

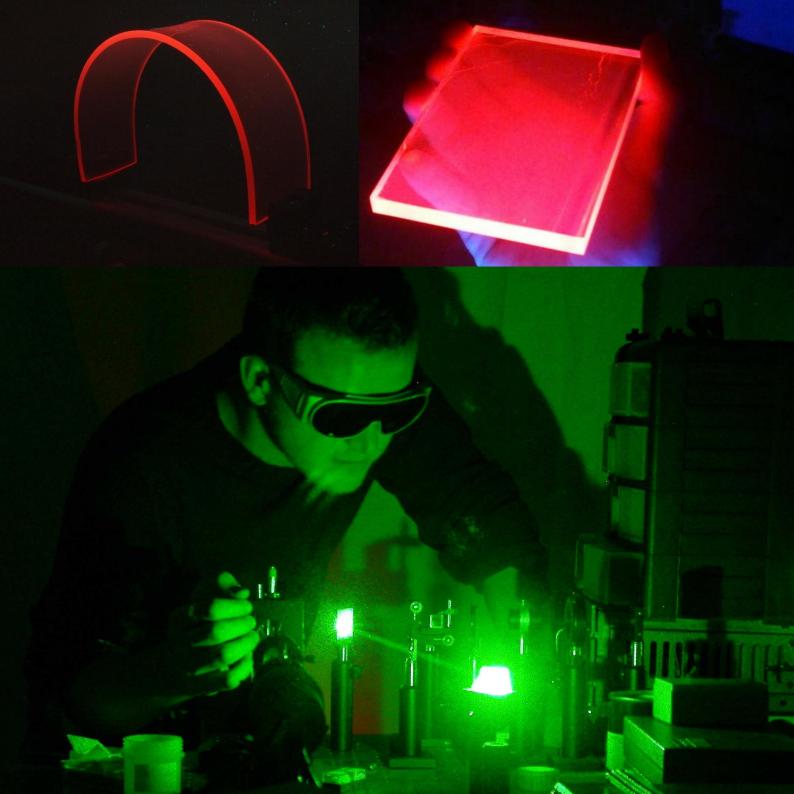
Non-Coherent Photons Up-conversion. The generation of photons of higher energy with respect to the excitation (up-conversion) through the non linear optical response of a material is a phenomenon useful to reach spectral regions otherwise not accessible. However, is appreciable only for coherent light sources delivering light intensity in the order of MW/cm². We are working on new routes to lower down to μ W/cm² the optical power requirements for non-coherent light up-conversion based on harnessing energy through bimolecular processes involving triplet-triplet annihilation indirectly excited via resonant energy transfer in organic multi-component systems. The blue-shift of the excitation energy has important applications in the field of solar energy photovoltaic conversion, as it allows collecting photons in the low energy tail of solar spectrum which cannot be efficiently converted. Moreover it can be exploited to develop novel blue and near UV light sources for light emitting technologies like WOLED and colour displays.

One Dimensional Photonic Crystals DFB Lasers. The avant-garde development of smart structures to provide optical feedback paves the way to the realization of novel laser emitters. An interesting approach is the distributed feedback (DFB) based on photonic crystals. In these systems a periodicity of the dielectric constant comparable to optical wavelengths generates stopgaps, photonic band gaps and slow photons. Gain materials, with which photonic crystals are doped, exhibit laser emission at wavelengths corresponding to the edges of the photonic band gap. In this field, we are pursuing the fabrication and the optical characterization of DFB lasers made with all-plastic and hybrid organic-inorganic one dimensional photonic crystals, even on flexible substrates. Possible applications for this kind of lasers are photonic and optoelectronic devices, such as optical switches, and sensors for a wide variety of analytes.

Nanochannels and Artificial Antennae. Inclusion of luminescent conjugated molecules in channelforming compounds allows the formation novel hybrid materials. In this research activity, artificial antennae are prepared by the inclusion of chromophores in a matrix with nanometric channels, imposing to the chromophore specific organization and interaction with the nanochanell surface. In particular, by using near infrared acceptor/emitters in these spatially confined systems, interesting applications in the field of telecom and phototherapy can be envisaged.

FACILITIES

Time Resolved Photoluminescence (PL). The main apparatus is based on a Ti:Sapphire laser coupled with a streak camera.



Oxide nanostructures and silica-based materials for optical technology









MAURO FASOLI, ALBERTO PALEARI, ANNA VEDDA

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





MARCO FANCIULLI

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

RESEARCH LINES

Si and Ge nanostructures

Silicon and germanium nanowires produced by MACE, VLS or by e-beam lithography (collaboration with the MDM IMM-CNR Lab.) are investigated using mainly spin dependent transport techniques aiming at the characterization of shallow donors, interface defects and electrostatically confined electrons.

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.

Point defects in semiconductors and oxides

Study of the electronic properties of point defects in semiconductors (Si, Ge), in high dielectric constant materials (transition metal oxides), and in 2D materials (MoS2, BN) using electron spin resonance techniques and inelastic electron tunneling spectroscopy.

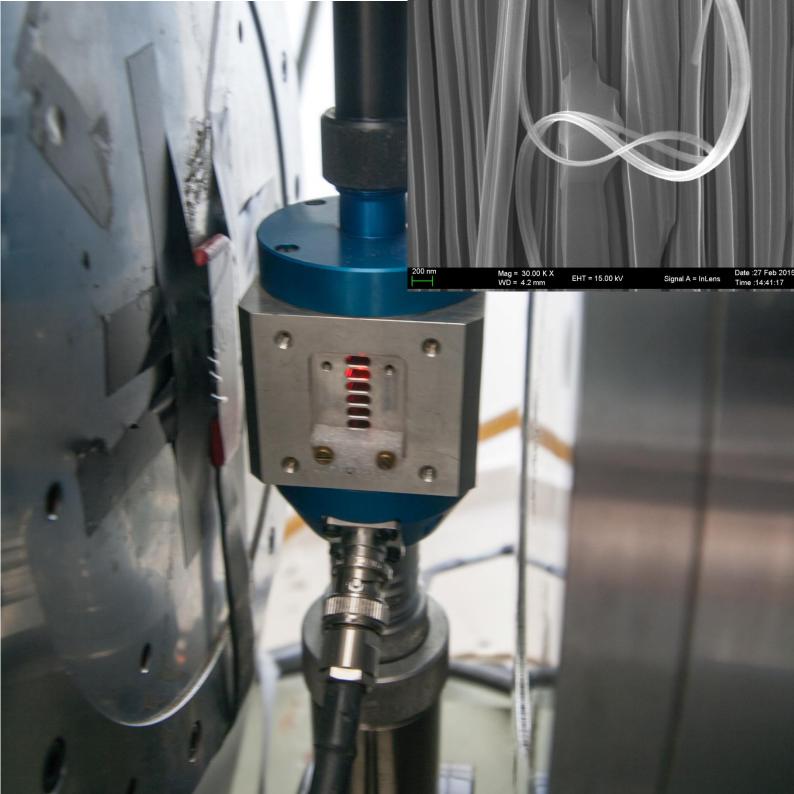
FACILITIES

Growth and processing

- Atomic Layer Deposition (ALD) mini-chamber with O3 line for *in-situ* characterization.
- Horizontal and vertical furnaces for annealing and diffusion
- Q-switched Ruby laser for laser annealing

Characterization

- Three 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 tunneling spectroscopy (IETS) working in the temperature range 4-300 K.
- Electrical measurements: I-V, C-V, C-t



Modeling and simulations of epitaxial semiconductor depositions and nanostructures





LEO MIGLIO, FRANCESCO MONTALENTI

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.



Photovoltaics and Thermoelectrics









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 power to wireless devices and (b) the development of novel mixed organic-inorganic nanocomposites to harvest body heat in portable (wearable) sensors.

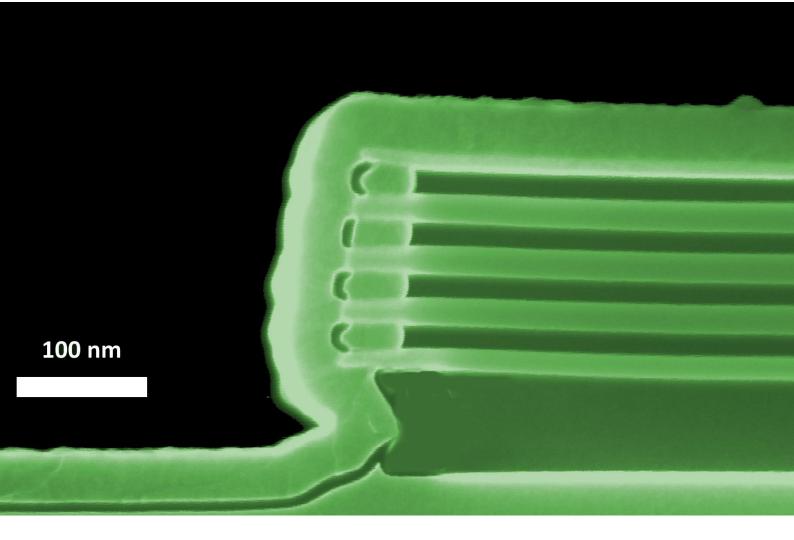


SILICON FOR SOLAR CELLS

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 low dimensional materials





GIAN PAOLO BRIVIO

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

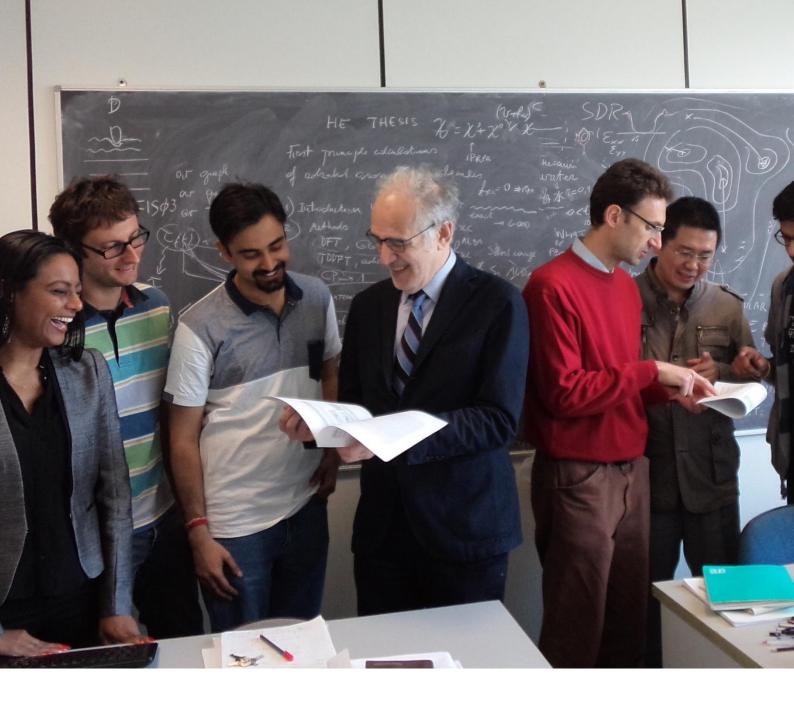
Charge transfer rates at metal/organic interfaces affect the efficiencies of devices for organic based electronics and photovoltaics. A study of electron transfer rates, which take place on the femtosecond timescale, is often difficult, especially since in most systems the molecular adsorption geometry 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.



Materials for gas storage and energy production: X-ray, neutron diffraction and physico-chemical properties

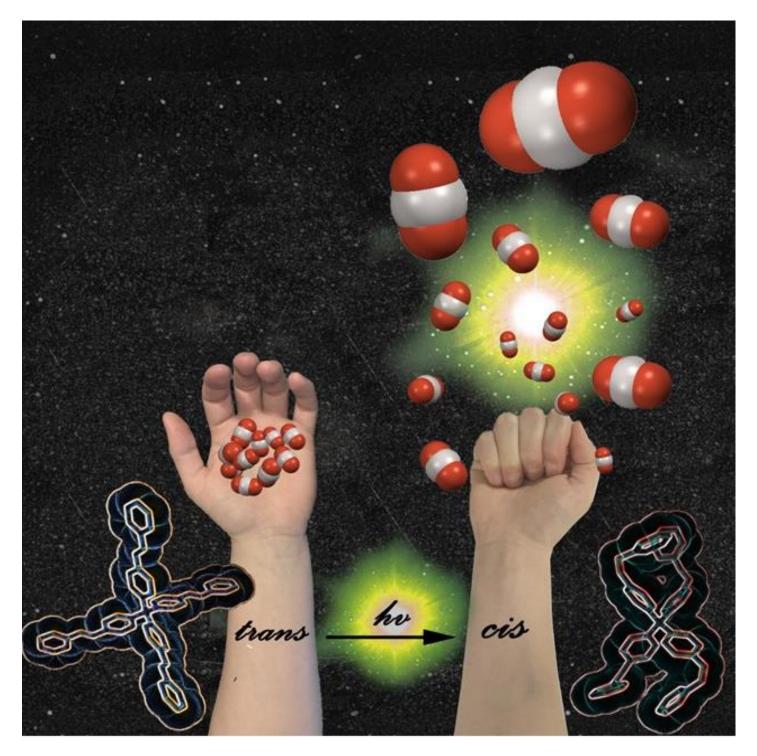




ANGIOLINA COMOTTI

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 storage 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, carbon dioxide that is an intermediate product in the hydrogen production processes, and pollutant vapours, especially benzene. The construction of stable and robust ionic, inorganic and hybrid frameworks with 3D periodic motifs can increase separation, capture and storage of small gases. These frameworks can arrange sites and receptors into arrays for controlling and interacting with gas species. The advantages of the novel materials will be compared with the conventional material properties for obtaining the basis of patent applications.

The research activity is mainly devoted to physico-chemical methods for the characterization of the porous structures and of the confined gases and vapours by X-ray and neutron diffraction techniques. Advanced experiments using synchrotron radiation and neutron sources will be performed at the European Facilities, especially at ESRF (Grenoble) and Rutherford Laboratory (Chilton). The synchrotron X-ray diffraction experiments enable the *in-situ* observations of the gas adsorption kinetics whilst neutron diffraction experiments can detect the localization of stored gases. The dynamics of gases and vapours in the confined state and the identification of ionic and weak interactions will be studied in depth by inelastic and deep inelastic neutron scattering.



Theory of oxide surfaces, interfaces, supported clusters





CRISTIANA DI VALENTIN, LIVIA GIORDANO, GIANFRANCO PACCHIONI, SERGIO TOSONI

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

UItrathin 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.

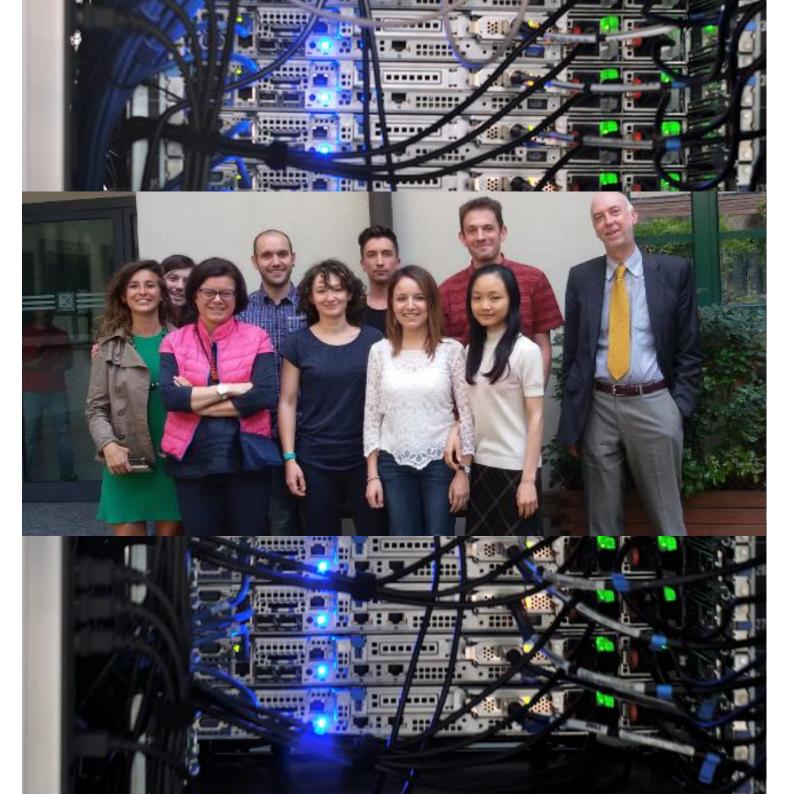


DEFECTS AND DOPANTS IN OXIDES

Nature of point defects in oxide materials for photocatalysis, photoelectrochemistry, microelectronics, fiber optics etc., in particular amorphous and crystalline TiO_2 , ZnO, WO₃, SiO₂, 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.

CHEMICALLY MODIFIED GRAPHENE AND CARBON BASED NANOSTRUCTURES

Doped graphene and graphene oxide are found to presents very interesting chemical properties which make them a new promising class of alternative materials for electrocatalysis. The activity is directed towards the characterization of the electronic properties, electrochemical activity, surface and interface chemistry of these systems when in the free-standing or metal-supported condition. Self-assembling or polymerization of tailored molecular precursors on metal surfaces is also investigated as an approach to obtained C-based wires, nanoribbons or two dimensional networks.



Electrochemical activities





CLAUDIO MARI, RICCARDO RUFFO

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 N₂ 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.



Chemistry of inorganic and organometallic materials





MASSIMILIANO D'ARIENZO, BARBARA DI CREDICO, ROBERTO SCOTTI

NANOSTRUCTURED OXIDES AND ORGANIC-INORGANIC HYBRID MATERIALS FOR PHOTOCATALYTIC APPLICATIONS

The research aims at the synthesis by soft-chemistry methods of shape controlled oxide nanocrystals (TiO₂, ZnO), oxide heterostructures and organic-inorganic hybrid materials, and at the study of the photocatalytic mechanism (formation and interfacial reactivity of charge trapping centers) by spectroscopic and spectromagnetic techniques. In fact, oxide nanocrystals with controlled polymorphism, defined morphology and specific exposed surfaces are able to provide selective sites for the photoxidation (i.e. organic, and pharmaceutical micropollutants degradation) and photoreduction reactions (i.e. H_2 production).

These features are exploited for developing innovative organic-inorganic hybrid materials which combine the intrinsic photocatalytic properties of the oxides with the ability of tuneable porous matrix (SiO₂ or Metal Organic Framework, MOF) to mediate the uptake of pollutants at the oxide surface and to generate a confined reactor around the catalytic sites simultaneously, where the photocatalytic degradation are controlled and enhanced.



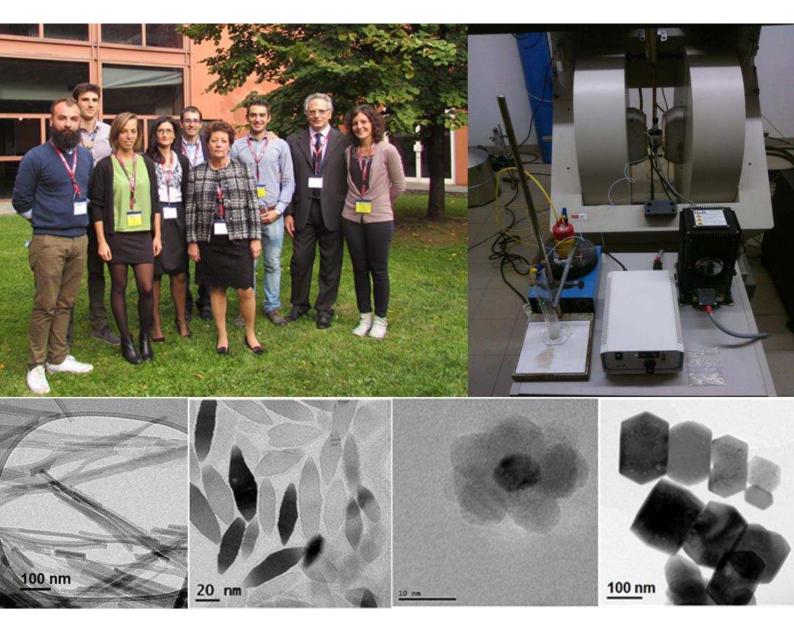
SHAPE CONTROLLED INORGANIC FILLERS FOR AUTOMOTIVE RUBBER NANOCOMPOSITES

The research focused on the synthesis of SiO_2 nanoparticles (NPs) with tailored isotropic/anisotropic shapes, surface-functionalized with groups able to physically or chemically interact with the polymer, used as filler in rubber nanocomposites. Different aqueous/non aqueous in/ex-situ sol-gel methods, also in the presence of surfactant as particle growth directing agent, are utilized to prepare SiO_2 NPs. The goal is to relate the surface and the morphological features of the filler NPs with their dispersion and networking, which influence the filler-filler and filler-rubber interaction, responsible for the improvement of the mechanical properties of the material. The research allows to introduce guidelines for optimizing the filler shape able to induce different rigidity in the polymer phase, through the investigation toward natural silicates as anisotropic fillers. A further objective of the research is the synthesis of ZnO NPs anchored to SiO₂, which act as reinforcing filler and curing activator simultaneously, for the improvement of the rubber curing process.

EQUIPMENTS

Total Organic Carbon Analyzer Shimadzu TOC-V CSH for liquid and gas samples. **S**urface Area and Pore Size Analyzer, Autosorb-1-MP Quantachrome Instrument. **E**lectron Spin Resonance (ESR) spectrometer, Brucker EMX

LINK: NanoMat-Lab Unimib - Facebook



Dating and characterization of ancient materials. Materials science and Cultural Heritage









ANNA GALLI, MARCO MARTINI, EMANUELA SIBILIA

THE ARCHAEOMETRY LAB

Since 1980 our activity focussed on the application of scientific techniques to archaeology, geology and cultural heritage, in particular in the field of absolute dating and characterisation of archaeological materials.

For what concerns the dating techniques, 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 (dating of wood) and radiocarbon (preparation of samples for Accelerator Mass Spectrometry, AMS, to evaluate the concentration of ¹⁴C atoms in organic remains). The laboratory is member of the CUDAM (Centro Universitario Datazioni e Archeometria Università di Milano Bicocca, http://cudam.mater.unimib.it).

For what concerns the characterisation of ancient materials, our research deals with non invasive spectroscopic methods, mainly performed using portable instruments, to study polychrome artefacts of various kind (paintings on boards, enamels, decorated ceramics, glass). Recently, we

RESEARCH LINES

Fundamental study of the low temperature TL peak in quartz and of the Pre-dose effect **S**tudy of the optical properties of mosaic glasses

Study of charge transfer phenomena in quartz and feldspars luminescence.

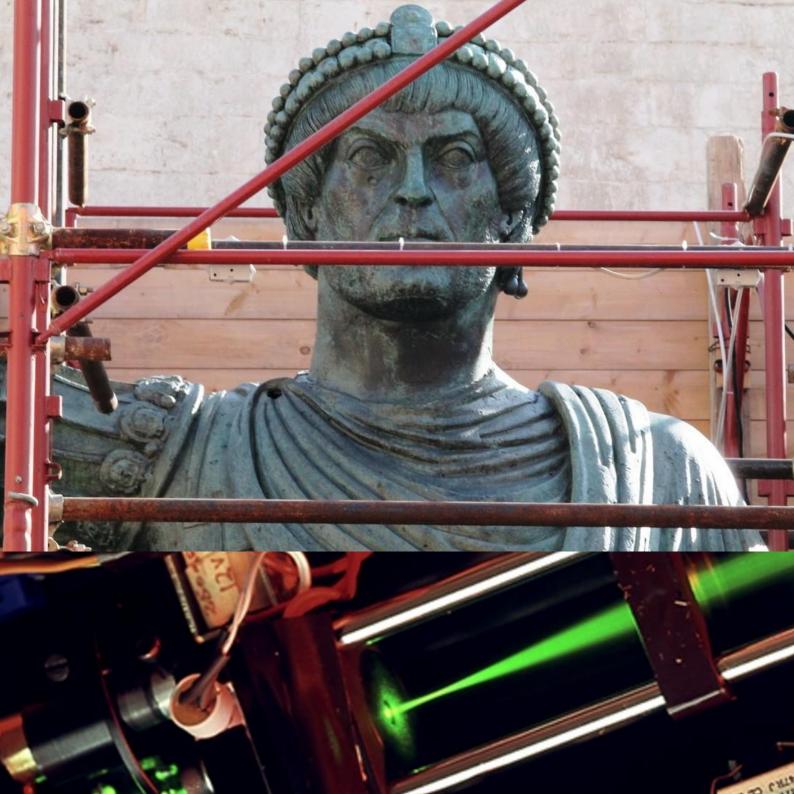
Studies of new procedures for the extraction of collagen from modern and archaeological bones for ¹⁴C dating

Studies of new procedures for identifying and selecting the anthropogenic calcite from the geogenic one in archaeological mortars; TL and OSL dating of mortars.

Surface dating

Study and characterisation of natural materials for accident dosimetry

Joined use of non invasive methods (EDXRF, FORS, Raman) on Renaissance pigments studies.



FUNDED PROJECTS

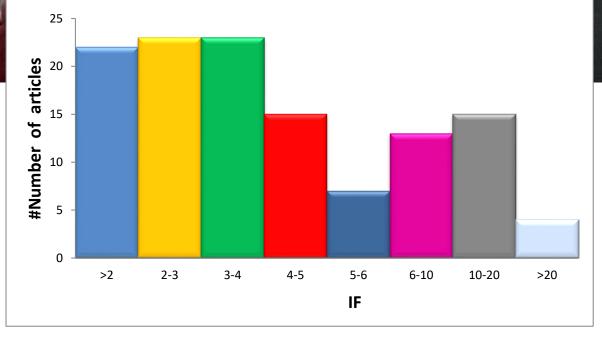
Coordinator	Project	Funded by
		REGIONE
A. ABBOTTO	Tessere Integrate di vetro Fotovoltaico per applicazioni Architettoniche INnovative	LOMBARDIA
A. ADDUTTU	Dispositivi Solari a Coloranti di Nuova Generazione: Sensibilizzatori e Conduttori	
	Nano-Ingegnerizzati (DSSCX)	MIUR
	SOLARDESIGN-On-the-fly alterable thin-film solar modules for design driven	
M. ACCIARRI	Applications	UE
	New materials with low environmental impact for thin film solar cells fabrication	MAE
M. BERNASCONI	SYNAPSE-SYnthesis and functionality of chalcogenide NAnostructures for	
IVI. DERINASCONI	PhaSE change memories	UE
L. BEVERINA	Exploitation of self-assembly and photochemistry for the straightforward, low cost	
L. DEVERINA	production of nanostructured organic photovoltaic devices	CARIPLO
	CHEETAH-Cost-reduction throughmaterial optimisation and Highrt EnErgy	
	outpuT of solAr pHotovoltaic modules-joining Europe's research and	
S. BINETTI	Development efforts in support of its PV industry	UE
	Caratterizzazione di silicio multicristallino cresciuto in condizione di microgravità,	
	a partire da silicio metallurgico	ASI
G. BRIVIO	THINFACE-Thin-film Hybrid Interfaces: a training initiative for the design of next-	
G. BRIVIO	generation energy devices	UE
S. BROVELLI	Electronic Doped Colloidal Nanocrystal Heterostructures for transformational	
3. DROVELLI	Breakthrought in solid-state lighting	CARIPLO
	Nanoporous materials with tailored structure for high performance methane	
	storage and purification	MIUR
	Biomethane low impact production and carbon dioxide bio-capture for circular	
A. COMOTTI	economy BALANCE	CARIPLO
	KiC-LIGHTBODY-Infrastructure and expertise network for Lightweight mobility :	EIT RAW
	body and chassis	MATERIALS
	Meccanismi di attivazione della CO2 per la progettazione di nuovi materiali per	
	l'efficienza dell'energia e delle risors	MIUR
	BIOINOHYB-Smart Bioinorganic Hybrids for Nanomedicine	UE
	DECORE-Direct ElectroChemical Oxidation Reaction of Ethanol: optimization of	
	the catalyst/support assembly for high temperature operation	UE
C. DI VALENTIN	Nuovi materiali fotocatalitici per la conversione di energia solare basati su	
	eterogiunzioni	CARIPLO
	Oltre il grafene: strati di carbonio nanostrutturati disegnati su misura per ottenere	
	nuovi materiali per la catalisi e la chimica sostenibile	MIUR

Coordinator	Project	Funded by
M. FANCIULLI	A new course on the Physics and technology of semiconductor devices with hand-on activity in a characterization and simulation lab	MICRON
V. FELLI	Variational methods, with applications to problems in mathematical physics and geometry	MIUR
R. LORENZI	Nanostructured oxide-in-oxide glasses for solar-blind UV-monitoring of work- safety and energy-saving in electric power distribution	CARIPLO
M. MARTINI	Studio e sviluppo applicativo di ossicarbonati e ossidi misti contenenti ioni lantanidi con proprietà luminescenti per applicazioni nel bio-imaging e nell'optoelettronica	MIUR
	Giotto, l'Italia: oltre l'immagine Sliding Doors: 600 anni di eccellenza tecnologica lombarda	CARIPLO REGIONE LOMBARDIA
F.MEINARDI	Nuove nanostrutture colloidali con molteplici funzionalità ottiche e magnetiche per applicazioni avanzate in elettronica, fotonica e diagnostica biomedica- II annualità Electronic Doped colloidal Nanocrystal Heterostructures with designed Interfacial composition: towards the development of new nano-device concepts for lighting	CRT TORTONA
A. MONGUZZI	and Energy Technologies Materiali per Up-conversion a bassa potenza con applicazione nel Solare e nella Bio-teranostica Multimodale	UE REGIONE LOMBARDIA
D. NARDUCCI	Advanced Simulation Design of Nanostructured Thermoelectric Materials with Enhanced Power Factors	UE
	Silicon Friendly Materials and device solutions for microenergy applications Solar driven chemistry: new materials for photo- and electro-catalysis (SMARTNESS) CASCADE DEOXYGENATION PROCESS USING TAILORED	UE MIUR
G. PACCHIONI	NANOCATALYSTS FOR THE PRODUCTION OF BIOFUELS FROM LIGNOCELLULOSIC BIOMASS CATSENSE	UE UE
A. PALEARI	Ossidi Nanostrutturati: multi-funzionalità e applicazioni KiC- IMAGINE- Development and implementation of EIT KIC Raw Materials Master Program(s) in Sustainable Materials	MIUR EIT RAW MATERIALS
F. PEZZOLI	Spin optoElectronics ARCHitectures based on group IV compounds – SEARCH IV	CARIPLO

Coordinator	Project	Funded by
	Sviluppo di materiali elettrodici per batterie ricaricabili a sodio ione	MAE
R. RUFFO	Give Sodium a Chance!Investigation of nanostructured mixed Na oxides as	
	electrode materials for energy storage	CARIPLO
	4PHOTON-Novel Quantum Emitters monolithically grown on Si, Ge and III-V	
	substrates	UE
	COSMITO - COmpressive Sampling Multispectral Imaging camera for remoTe	REGIONE
S. SANGUINETTI	Observation	LOMBARDIA
	COSMOS	CARIPLO
	FemToTera- Plasmon-enhanced Tera-Hertz emission by Femtosecond laser	
	pulses of nanostructuredsemiconductor/metal surfaces	UE
R. SCOTTI	Rational design of hybrid organic-inorganic interfaces: the next step towards	
K. 300111	advanced functional materials – Action MP1202	UE
A. SASSELLA	La sapienza è figliola della sperienzia. La fisica degli sperimentali da Pavia a	
A. OAGOLLLA	Milano Bicocca	MIUR
S. TAVAZZI	Augmented Environment for Control in amyotrophic lateral sclerosis	RICERCA SLA
	AIDA 2020-Advanced European Infrastructures for Detectors at Accelerators	UE
	INTELUM-International and intersectoral mobility to develop advanced scintillating	
A. VEDDA	fibres and Cerenkov fibres for new hadron and jet calorimeters for future colliders	UE
	KIC-OPTNEWOPT - MATERIALS SUBSTITUTION IN OPTOELECTRONIC	EIT RAW
	DEVICES	MATERIALS

PHD THESIS

Articles 2016 by impact factor (IF)



INTERNATIONAL JOURNALS

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	On the leading term of the eigenvalue variation for Aharonov-Bohm operators with a	
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2	Albanese, E; Leccese, M; Di Valentin, C; Pacchioni, G.	5,2
	Magnetic properties of nitrogen-doped ZrO2: Theoretical evidence of absence of room	
	temperature ferromagnetism.	
	SCIENTIFIC REPORTS 6, 31435.	
3	Albani, M; Bergamaschini, R; Montalenti, F. Dynamics of pit filling in heteroepitaxy via	3,7
	phase-field simulations. PHYSICAL REVIEW B 94, 075303.	
4	Bachman, J; Muy, S; Grimaud, A; Chang, H; Pour, N; Lux, S; Paschos, O; Maglia, F; Lupart, S;	37,4
	Lamp, P; Giordano, L; Shao-Horn, Y.	
	Inorganic Solid-State Electrolytes for Lithium Batteries: Mechanisms and Properties	
	Governing Ion Conduction. CHEMICAL REVIEWS 116, 140.	
5	Barget, M; Lodari, M; Borriello, M; Mondiali, V; Chrastina, D; Bollani, M; Bonera, E.	3,1
	Tensile strain in Ge membranes induced by SiGe nanostressors.	
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121	Zianni, X; Chantrenne, P; Narducci, D.	1,4
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122	Zulian, L; Segrado, F; Narducci, D.	1,4
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	ENERGY HARVESTING AND SYSTEMS 3, 329 .	

CONFERENCES AND SEMINARS

#	Authors And Title of Presentation	Conference/workshop
1	Albani, M; Bergamaschini, R; Montalenti, F. Dynamics of pit filling in heteroepitaxy via phase-field simulations.	32 European Conference on Surface Science (ECOSS-32); Grenoble (France)
2	Azadmand, M; Bietti, S; Barabani, L; Acciarri, M; Basso Basset, F; Bonera, E; Fedorov, A; Noetzel, R; Sanguinetti, S. Growth Suppression by Metal Droplets of In0.5Ga0.5N/Si(111) at Low Temperatures.	MBE 2016, 19th International Conference on Molecular-Beam Epitaxy; Montpellier (France)
3	Barget, M; Lodari, M; Mondiali, V; Chrastina, D; Bollani, M; Bonera, E. SiGe nanostructures inducing tensile strain in suspended germanium membranes	E-MRS Fall Meeting 2016; Varsavia, Polonia
4	Basso Basset, F; Bietti, S; Esposito, L; Bonera, E; Sanguinetti, S. Excitonic fine structure in GaAs/AlGaAs (111) quantum dots grown by droplet epitaxy.	Mauterndorf 2016, 19th International Winterschool, "New Developments in Solid State Physics"; Mauterndorf, Austria
5	Bergamaschini, R; Albani, M; Salvalaglio, M; Backofen, R; Voigt, A; Miglio, L; Montalenti F. Phase-Field modeling of semiconductor heteroepitaxy: elastic relaxation, surface energy minimization and intermixing.	International Conference on Molecular Beam Epitaxy; Montpellier (France)
6	Bergamaschini, R; Rovaris, F; Montalenti, F. Continuum model of cyclic growth induced by dislocations in SiGe/Si heteroepitaxy.	EDS Extended Defects in Semiconductors 2016; Les Issambres (Francia)
7	Bergamaschini, R; Rovaris, F; Montalenti, F. Continuum modeling of Ge/Si heteroepitaxy in the presence of misfit dislocations.	International Conference on Molecular Beam Epitaxy; Montpellier (France)
8	Bernasconi M. Atomistic simulations of phase change materials for data storage. (Invited)	New Horizons for Memory Storage: Advancing Non-volatile Memory with Atomistic Simulations; Dublino
9	Bernasconi, M. Atomistic simulations of thermal transport in phase change materials. (Invited)	European Phase Change and Ovonic Symposium; Cambridge
10	Beverina, L; Sassi, M; Galliani, D; Bruni, F; Scaccabarozzi, A; Campione, M; Ruffo, R; Giovanella, U; Luzzati, S; Meinardi, F; Stingelin, N; Brovelli, S. Latent hydrogen bond: a versatile tool enabling the facile preparation of organic devices. (Invited)	American Chemical Society Meeting; San Diego, California, USA

11	Binetti, S.	Advanced Characterization for PV, CHEETACH
	Photoluminescence and Raman spectroscopy for defect identification	workshop; Freiburg, Germany
	in Silicon, Cu(In,Ga)Se_2 and Cu_2ZnSnS_4. (Invited)	
12	Bracco, S.	Solid State NMR Spectroscopy School - Post 8th
	Molecular Motion in the Solid State: Determination Methods and	GERMN / 5th Iberian NMR Meeting; Valencia
	Relaxation Phenomena. (Invited)	
13	Brivio, G. Femtosecond charge transfer at hybrid interfaces.	The 15th International Workshop on dynamics,
	(Invited)	interactions and electronic transitions at
		surfaces; Shanghai (R.P. Cina)
14	Brivio, G; Zwick, C; Baby, A; Grunewald, M; Verwuster, E; Hofmann,	APS March Meeting; Baltimore
	OT; Forker, R; Fratesi, G; Zojer, E; Fritz, T. Complex Stoichiometry	
	reordering of PTCDA on Ag(111) upon K Intercalation.	
15	Castiglioni, F; Comotti, A; Bracco, S; Perego, J; Beretta, M; Gemmi,	XXII Convegno nazionale dell'Associazione
	M; Sozzani, P.	italiana di scienza e tencologia delle
	Polimerizzazioni confinate in organosilici mesoporose altamente	macromolecole – AIM; Genova
	ordinate.	
16	Comotti, A; Bracco, S; Negroni, M; Castiglioni, F; Sozzani, P.	8th GERMN / 5th Iberian NMR Meeting
	Structure, Dynamics and Gas Uptake of Porous Architectures: a Solid	27-29 June 2016, Valencia; Valencia
	State NMR Perspective.(Invited)	
17	Cvetko, D; Fratesi, G; Kladnik, G: Cossaro, A; Brivio, G;	Charge Carrier Dynamics at the Nanoscale
	Venkataraman, L; Morgant, A.	(CCDNano16); Berlino
40	Ultrafast Electron Injection to Photo-Excited Organic Adsorbates.	
18	De Cesari, S; Giorgioni, A; Isa, F; Grilli, E; Isella, G; Pezzoli, F.	E-MRS (European Materials Research Society),
	Optical Orientation of Spins in Ge/SiGe Multiple Quantum Wells	Spring Meeting; Lille (Francia)
10	grown (111) Si Substrate.	
19	Di Valentin, C.	2nd Sino-Italian Workshop on Graphene and
	Graphene/TiO2 interface in catalysis and photocatalysis. (Invited)	related 2D Materials; Genova, Italy
20	Di Valentin, C.	International Workshop on Ethanol Electro-
	Computational Electrocatalysis: Novel Materials for Direct Alcohol	oxidation; Florence
04	Fuel Cells. (Invited)	
21	Di Valentin, C; Ferrighi, L.	Spring ACS National Meeting; San Diego,
22	Graphene/ (101) anatase TiO2 interface: A DFT study. (Invited)	California, USA
22	Ferrighi, L; Datteo, M; Fazio, G; Di Valentin, C.	Congresso Nazionale della divisione di Chimica
	First-principles simulations of nanostructured materials: graphenic	Computazionale della società Chimica Italiana
	2D-sheets and semiconducting oxide nanoparticles. (Invited)	2016; Pisa
23	Ferrighi, L; Datteo, M; Fazio, G; Di Valentin, C.	MolSimEng 2016 (Molecular Simulation and
	First-principles simulations of nanostructured materials: graphenic	Engineering); Milano, Politecnico
	2D-sheets and semiconducting oxide nanoparticles. (Invited)	

24	Galliani, D.; Battiston, S; Narducci, D.	Giornate della Termoelettricità 2016 (GiTE); Pisa
	Tuning PEDOT:Tos thermoelectric properties through	
	nanoparticle inclusion.	
25	Galliani, D; Beverina, L; Narducci, D.	European Materials Research Society (E-MRS) Spring
	Conjugated Polymer Nanocomposite: Towards a Novel	Meeting 2016; Lille, Francia
	Material for Thermal Energy Microharversting.	
26	Galliani, D; Ruffo, R; Narducci, D.	European Conference on Thermoelectrics (ECT) 2016;
	Thermoelectric properties of PEDOT nanocomposites with	Lisbona (Portogallo)
	electrochemically tuned oxidation state.	
27	Giordano, L.	E-MRS fall meeting; Warsaw, Poland
	Charge transfers and unusual stoichiometries at oxide	
	ultrathin films on metal surfaces. (Invited)	
28	Giorgioni, A; Paleari, S; Cecchi, S; Golub, L; Grilli, E; Isella, G;	European Materials Research Society Spring Meeting
	Jantsch, W; Fanciulli, M; Pezzoli, F.	May 2-6; Lille, France
	Electron Spin Resonance of conduction electrons in Ge/SiGe	
	quantum wells.	
29	Gironi, L; Baldazzi, G; Bonvicini, V; Campana, R; Capelli, S;	14th International Conference on Topics in Astroparticle
	Evangelista, Y; Fasoli, M; Feroci, M; Fuschino, F; Labanti, C;	and Underground Physics, TAUP 2015; Congress Center
	Marisaldi, M; Previtali, E; Riganese, L; Rashevsky, A; Sisti, M;	of Unione Industriale, Torino, Italy
	Vacchi, A; Vedda, A; Zampa, G; Zampa, N; Zuffa, M. A flexible	
	scintillation light apparatus for rare events searches.	
30	Longoni, G; Mari, C; Ruffo, R; D'Arienzo, M.	229th ECS MEETING; Hilton Bayfront, San Diego,
	Morphology/Properties Correlations in TiO2 Nanostructured	California, USA
	Material As Negative Electrodes in SOdium Ion Batteries.	
31	Lorenzi, R; Golubev, N; Ignat'Eva, E; Sigaev, V; Azarbod, A;	International Symposium on SiO2, Advanced Dielectrics
	Mereu, R; Paleari, A.	and related Devices symposium 13-15 June; Nice, France
	Optical and electrical response of germanosilicate glass-	
	based films nanostructured by alkali-assisted incorporation	
	of gallium oxide.	
32	Marzegalli, A; Cortinovis, A; Basso Basset, F; Bonera, E;	2016 E-MRS Spring Meeting Simposium K; Lille
	Pezzoli, F; Scaccabarozzi, A; Isa, F; Isella, G; Zaumseil, P;	
	Capellini, G; Schröder, T; Miglio, L.	
	An exceptional thermal strain reduction in Ge suspended	
	layer grown on Si by a tilting pillar architecture.	
33	Meinardi, F.	The 1st International Symposium on Singlet Fission and
	Solid-State Sensitized Up-conversion Systems for Next	Photon Fusion: Emerging Solar Energy Technologies;
	Generation of Photon Managing Devices. (Invited)	Gothenburg
34	Monguzzi, A.	11th International Conference and Expo on Nanoscience
	Low power Up-conversion Nano-Materials for Solar	and Molecular Nanotechnology; Roma, Italy
	Applications and Bio-theranostics. (Invited)	
35	Monguzzi, A.	Energy Materials Nanotechnology - EMN Meeting on
	Low power Up-conversion Nano-Materials for Solar	Photonics; Barcelona, Spain
	Applications and Bio-theranostics. (Invited)	

36	Monguzzi, A; Braga, D; Oertel, A; Bianchi, A; Simonutti, R; Norris DJ; Meinardi, F. Effective Photocatalytic Water Splitting Enhancement by Broadband Solid-State TTA-UC.	1st International Symposium on Singlet Fission and Photon Fusion: Emerging Solar Energy Technologies; Goteborg, Svezia
37	Montalenti, F. Continuum Modeling of Ge/Si Heteroepitaxy: Interplay Between Elastic and Plastic Relaxation. (Invited)	ICSI VII ISTDM 2016; Nagoya (Japan)
38	Montalenti, F; Rovaris, F; Bergamaschini, R; Salvalaglio, M; Albani, M; Miglio, L; Backofen, R; Voigt, A. Continuum modeling of heteroepitaxial growth in semiconductors.(Invited)	MMM 2016; Dijon (France)
39	Moretti, F; Vedda, A; Chiodini, N; Cova, F; Fasoli, M; Pauwels, K; Tabarelli de Fatis, T; Auffray, E; Lucchini, M; Bourret- Courchesne, E; Baccaro, S; Cemmi, A. <i>Rare earth doped silica-based optical fibres for high energy</i> <i>physics detectors</i> .	EAGLES, International Conference on Rare-Earth Doped Glass Materials and Fibre Lasers; Trento
40	Muller; M; Lin, H; Sànchez-Portal, D; Fratesi, G; Brivio, G.; Sellon, A. Influence of Structural Fluctuations on the Lifetimes of Adsorbate States at hybrid organic-semiconductor interfaces.	APS March Meeting; Baltimore, Maryland
41	Narducci, D. Forging the impossible: the route to efficiency in thermoelectricity. (Invited)	Functional Energy Materials Conference 2016 (Zing Conferences); Dubrovnik, Croatia
42	Negroni, M; Bracco, S; Comotti, A; Sozzani, P. <i>Molecular</i> rotors in porous materials.	National Young Researchers' Forum on Materials Science and Technology July 11-13, 2016 - Ischia; Ischia
43	Pacchioni, G. CO oxidation on Au/TiO2 and Au/ZrO2 catalysts: role of oxide reducibility and nanostructuring. (Invited)	4th TYC-Energy Materials Workshop – Shaping nanocatalysis, King's College London; Londra
44	Pacchioni, G. From Erice 1987 to Erice 2016: 30 years of cluster research. (Invited)	Workshop on Delocalized electrons in atomic and molecular nanoclusters; Erice
45	Pacchioni, G. From reduction to reaction. TiO2 and ZrO2 catalytic materials in biomass conversion: hints from DFT. (Invited)	The 10th International Workshop on Oxide Surfaces; Dalian, Cina
46	Pacchioni, G. Interaction of metal atoms and clusters with insulating surfaces: charge transfer, diffusion, incorporation. (Invited)	Cluster Surface Interaction Workshop 2016, Argonne National Laboratory; Chicago
47	Pacchioni, G. Modern electronic structure theory and catalysis: towards the simulation of complex problems in chemistry. (Invited)	International Conference on "Concepts in catalysis: from heterogeneous to homogeneous and enzymatic catalysts"; Accademia Nazionale dei Lincei, Roma
48	Pacchioni, G. Modern electronic structure theory in predicting new materials with tailored properties. (Invited)	RAMSES: Advanced School on critical raw materials substitution for energetics and photonics; Milano
49	Pacchioni, G. Nanotechnologies and nanoscience through history. (Invited)	International Summer School Nanoscience meets Metrology; Torino

50	Pacchioni, G. Nature and consequences of electron localization and delocalization in oxide nanoparticles. (Invited)	Workshop on Delocalized electrons in atomic and molecular nanoclusters; Erice
51	Pacchioni, G. Oxide surfaces in catalysis: from size-selected clusters, to defects engineering and two-dimensional oxides. (Invited)	International Winter School Molecules@Surfaces; Bardonecchia
52	Pacchioni, G. <i>TiO2 and ZrO2 catalytic materials in biomass conversion. A computational chemistry perspective</i> . (Invited)	CASCATBEL Workshop Thermochemical lignocellulose conversion technologies; Salonicco, Grecia
53	Pacchioni, G. TiO2 and ZrO2 in biomass conversion: role of oxide reducibility. (Invited)	16th International Conference on Theoretical Aspects of Catalysis; Zakopane (Polonia)
54	Pacchioni, G. <i>Two-dimensional insulators: new materials, new structures, new functions</i> . (Invited)	Symposium on Functional Properties of Two- Dimensional Nanostructured Materials; Lovanio (Belgio)
55	Pacchioni, G. Two-dimensional oxides as new catalytic materials. (Invited)	Summer School on Energy Research at the Nanoscale: Devices, Materials, and Mechanisms; Berlino Elstal
56	Pacchioni, G. <i>Two-dimensional oxides: new structures, new functions and new materials</i> . (Invited)	Symposium on Progress in Science, Progress in Society – Ceremony of Awards of Blaise Pascal Medals 2016; Bruxelles
57	Perego, J; Comotti, A; Bracco, S; Piga, D; Sozzani, P. <i>Confined polymerization in porous materials</i> .	National Young Researchers' Forum on Materials Science and Technology July 11-13; Ischia, Italy
58	Pezzoli, F; Giorgioni, A; Gallacher, K; Isa, F; Biagioni, P; Millar, RW.; Gatti, E; Grilli, E; Isella, G; Paul, DJ; Miglio, L. Dislocation recombination and surface passivation of Ge micro-crystals on Si.	EMRS 2016 Spring Meeting, Symposium K: Group IV Semiconductors Materials Research: Growth, Characterization and Applications to Electronics and Spintronics; Lille, France
59	Pezzoli, F; Giorgioni, A; Myronov, M. Radiative recombination in GeSn epitaxial architectures.	EMRS 2016 Spring Meeting, Symposium O: Group IV semiconductors at the nanoscale - towards applications in photonics, electronics and life sciences; Lille, France
60	Piga, D; Sozzani, P; Comotti, A; Bassanetti, I; Bracco, S. Polimerizzazioni confinate in matrici organiche porose con elevata area superficiale.	XXII Convegno nazionale dell'Associazione italiana di Scienza e Tecnologia delle Macromolecole – AIM; Genova
61	Ravikumar, A.; Baby, A; Lin, H.; Brivio, G.; Fratesi G Transient magnetism in graphene induced by core level excitation of organic adsorbates.	APS March Meeting; Baltimore
62	Rovaris, F; Bergamaschini, R; Montalenti, F. Continuum Modeling of cyclic growth in Ge/Si(001) heteroepitaxy.(Invited)	GDR PULSE; Marseille (France)
63	Rovaris, F; Bergamaschini, R; Montalenti, F. Modeling simultaneous elastic and plastic relaxation during Ge deposition on Si(001). (Invited)	EMRS 2016 Fall Meeting; Warsaw (Poland)

64	Sassi, M; Mattiello, S; Rooney, M; Brazzo, P; Sanzone, A; Beverina, L. <i>Tackling materials science with the tools of organic</i> <i>chemistry: dyes, pigments and all there is in between</i> . (Invited)	Convegno della divisione organica della società chimica italiana 2016; Venezia
65	Scarpellini, D; Bietti, S; Elborg, M; Kuroda, T; Nemcsics, A; Basso Basset, F; Vozzi, C; Manzoni, C; Sanguinetti, S. Nanostructured Surfaces for Teraherz Generation.	MBE 2016, 19th International Conference on Molecular- Beam Epitaxy; Montpellier (France)
66	Sozzani, P. Molecular rotors built in porous materials. (Invited)	Molecular Rotors, Motors, and Switches; Telluride CO (USA)
67	Vedda, A. Characterization of defects in scintillators. (Invited)	ASCIMAT school on advanced scintillator materials; Milano
68	Vedda, A. Performances and applications of rare-earth doped silica-based scintillating fibers. (Invited)	CIMTEC 2016. 5th International Conference "Smart and Multifunctional Materials, Structures and Systems"; Perugia
69	Vedda, A. Rare-earth incorporation in oxide scintillator crystals, glasses, and nanostructures: Optical emission and beyond. (Invited)	7th International Symposium on Optical Materials; Lione
70	Vedda, A. Towards substitution of rare-earth ions in scintillator materials. (Invited)	E-MRS Spring Conference - Symposium E - Substitution of Critical Raw Materials: Synthesis, Characterization and Processing of New Advanced Materials in optoelectronic and magnetic devices.; Lille (Francia)
71	Vedda, A; Chiodini, N; Cova, F; Fasoli, M; Moretti, F; Pauwels, K; Tabarelli de Fatis, T; Auffray, E; Lucchini, M; Bourret- Courchesne, E; Baccaro, S; Cemmi, A. <i>Rare earth doped silica-based optical fibres for high energy</i> <i>physics detectors</i> . (Invited)	Fifth International Conference Engineering of Scintillation Materials and Radiation Technologies, ISMART 2016; Minsk
72	Vedda, A; Fasoli, M; Lorenzi, R; Villa, I; Lauria, A; Niederberger, M; Dujardin, C; Moretti, F. Hafnium dioxide luminescent nanoparticles: structure and emission control through doping and thermal treatments.	2016 International Conference on Defects in Insulating Materials (ICDIM 2016); Lyon (F)
73	Vitiello, E; Giorgioni, A; Virgilio, M; Frigerio, J; Gatti, E; De Cesari, S; Bonera, E; Grilli,E; Isella, G; Pezzoli, F.	102° Congresso SIF; Padova Spin-dependent direct gap emission in tensile-strained Ge-on-Si heterostructures.
74	Vitiello, E; Virgilio, M; Giorgioni, A; Frigerio, J; Gatti, E; De Cesari, S; Bonera, E; Grilli, E; Isella, G; Pezzoli, F. Spin-dependent direct gap emission in tensile-strained Ge films on Si substrates.	E-MRS Spring Meeting 2016; Lille (France)
75	Vitiello, E; Virgilio, M; Giorgioni, A; Frigerio, J; Gatti, E; De Cesari, S; Bonera, E; Grilli, E; Isella, G; Pezzoli, F. Spin-dependent direct gap emission in tensile-strained Ge films on Si substrates.	Mauterndorf Winterschool; Mauterndorf (Austria)

PHD THESIS

DOCTORATE IN MATERIALS SCIENCE AND NANOTECHNOLOGY EUROPEAN DOCTORATE IN PHYSICS AND CHEMISTRY OF ADVANCED MATERIALS

http://www.scuoladottorato.scienze.unimib.it/

Anu BABY: Hybrid Interfaces: Adsorption of Aromatic Molecules on Metals

Simone BONETTI: Polymer Nanoparticles: A New Technological Platform for Emerging Applications

Nunzio BUCCHERI: Design and synthesis of small molecules for NIR-operating light emitting and sensing devices

Davide CAMPI: Atomistic simulations of thermal transport and vibrational properties in phasechange materials

Bianca CECCONI: Artificial Photosynthesis: Molecular Approaches for Photocatalytic Hydrogen Production

Alessandro CRIPPA: High frequency physics and broadband instrumentation in CMOS silicon quantum devices

Roberta DAL MAGRO: Enhanced Brain Targeting of ApoE – functionalized Lipid Nanoparticles

Matteo FARINA: Nuclear Magnetic Resonance: structural characterisation of polymers and biochars

Hong Sheng LIN: Ab initio study of organic molecules adsorbed on technologically relevant surfaces

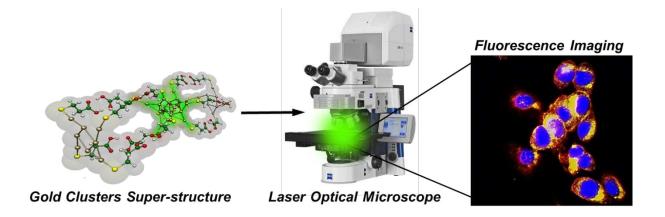
Marco SALVALAGLIO: Continuum modeling of vertical heterostructures: elastic properties and morphological evolution

Antonio SUSANNA: Highly Efficient MeO Nanoparticles as Curing Activator for Rubber Composites

Marco TAGLIAFERRI: Charge detection in silicon double quantum dot nanodevices

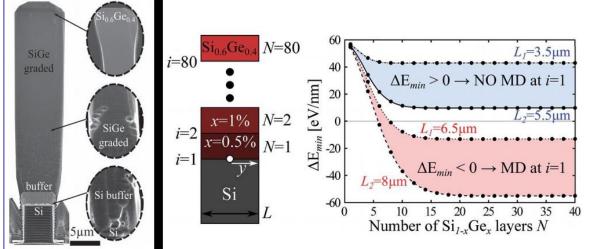
B. Santiago-Gonzalez, A. Monguzzi, J. M. Azpiroz, M. Prato, S. Erratico, M. Campione, R. Lorenzi, J. Pedrini, C. Santambrogio, Y. Torrente, F. De Angelis, F. Meinardi, S. Brovelli, *Permanent excimer superstructures by supramolecular networking of metal quantum clusters* Science **353**, 571-575 (2016)

Metal quantum clusters have ideal properties for medical applications such as imaging. The challenge is to prolong their transient properties for the fabrication of useful devices. We arranged gold clusters in a supramolecular lattice held together by hydrogen bonding and showed that this material can be used for imaging of fibroblast cells. In the superstructure, the gold molecules can come together in the excited state as excimers and then dissociate to emit radiation. Because they are within a lattice, this behavior shows long-term stability. Furthermore, the lattice superstructure scavenges reactive oxygen species and reduces cell damage.



Isa, F; Salvalaglio, M; Dasilva, Y; Meduňa, M; Barget, M; Jung, A; Kreiliger, T; Isella, G; Erni, R; Pezzoli, F; Bonera, E; Niedermann, P; Gröning, P; Montalenti, F; von Känel, H. Highly Mismatched, Dislocation-Free SiGe/Si Heterostructures. ADVANCED MATERIALS 28, 884 (2016).

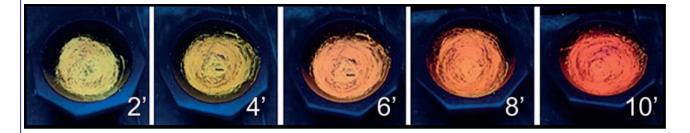
Above a certain critical thickness, dislocations are unavoidably introduced in latticemismatched heteroepitaxial films. As such defects can be detrimental in affecting devices' performances, lowering their density is a key issue in present optics and microelectronics. Thanks to their huge height to base aspect ratio, small (width below 50 nm) nanowires can be grown dislocation-free, as the abundance of free surfaces allows for a massive elastic relaxation of the misfit-strain. In this work it is shown that total absence of dislocations can be achieved also at the micron scale, provided that (a) vertical heteroepitaxy can be achieved (b) the content of the stressor is slowly increased during deposition.



Left: SiGe dislocation-free, micrometer-sized vertical crystal grown by Low-Energy Plasma Enhanced Chemical Vapour Deposition. Right: theoretical calculations predicting the absence of dislocations for widths up to $\sim 5\mu m$.

Toma, O; Allain, M; Meinardi, F; Forni, A; Botta, C; Mercier, N. Bismuth-Based Coordination Polymers with Efficient Aggregation-Induced Phosphorescence and Reversible Mechanochromic Luminescence. ANGEWANDTE CHEMIE INTERNATIONAL EDITION 55, 7998. (2016).

Coordination polymers (CPs) are very promising luminogens for lighting technologies and chemical sensors, but their emission efficiency usually decreases dramatically upon aggregation as a result of concentration quenching processes. Here we report the first bismuth-based CPs showing not only a solid-state phosphorescence quantum yield as high as 85%, due to an aggregation induced phosphorescence process, but also mechanochromic luminescence (MCL). In particular, upon grinding the samples, their amorphisation induce a shift of the emission from the yellow to the orange-red while the color of the powders remained unchanged. The total wavelength shift (more than 100 nm) is the largest ever observed for MCL complexes and it is fully reversible upon heating. Starting from this results, a new family of MCL materials is actually under development.



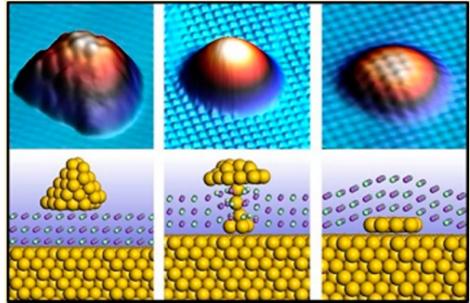
In the figure: UV-excited luminescence of one of the synthesized CPs upon grinding for different times.

Z. Li, H.Y. T. Chen, K. Schouteden, T. Picot, K. Houben, T.W. Liao, C. van Haesendonck, G. Pacchioni, P. Lievens, E. Janssens,

Size-dependent penetratin of gold nanoclusters through a defect-free, nonporous NaCl membrane,

Nano Letters 16, 3063 (2016).

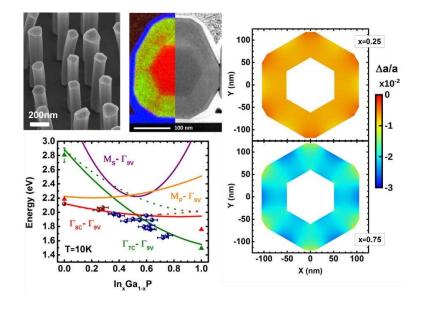
Metal quantum clusters have ideal properties for medical applications such as imaging. The challenge is to prolong their transient properties for the fabrication of useful devices. We arranged gold clusters in a supramolecular lattice held together by hydrogen bonding and showed that this material can be used for imaging of fibroblast cells.



In the superstructure, the gold molecules can come together in the excited state as excimers and then dissociate to emit radiation. Because they are within a lattice, this behavior shows long-term stability. Furthermore, the lattice superstructure scavenges reactive oxygen species and reduces cell damage.

Gagliano, L; Belabbes, A; Albani, M; Assali, S; Verheijen, M; Miglio, L; Bechstedt, F; Haverkort, J; Bakkers, E., *Pseudodirect to Direct Compositional Crossover in Wurtzite GaP/InxGa1-xP Core-Shell Nanowires*, Nano Letters 16, 7930 (2016).

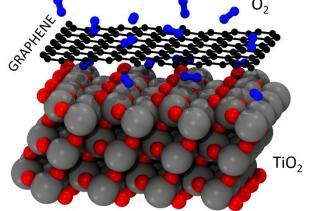
Thanks to their geometry, core-shell nanowires allow the realization of novel semiconductor crystal structures with yet unexplored properties, such as to induce in the shell a crystal structure different from the bulk one. In fact, we obtained the growth of wurtzite GaP/In_xGa_{1-x}P core-shell nanowires, with tunable indium concentration *x*, suitable for optical emission in the visible region, from 590 nm to 760 nm. We demonstrate a crossover from pseudodirect ($\Gamma_{8c}-\Gamma_{9v}$) to direct ($\Gamma_{7c}-\Gamma_{9v}$) transition with *x*, both experimentally and by Density Functional Theory calculations. As the increasing strain in the shell with *x* too does affect the electronic band structure, Finite Element Method calculation of the strain in the system has been performed. This work opens the way applications in solid state lighting, tandem solar cells, and solar hydrogen production.



Ferrighi, L; Datteo, M; Fazio, G; Di Valentin, C. *Catalysis under Cover: Enhanced Reactivity at the Interface between (Doped) Graphene and Anatase TiO2*. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 138, 7365 (2016).

The "catalysis under cover" involves chemical processes which take place in the confined zone between a 2D material, such as graphene, and the surface of an underlying support, such as a metal oxide. The hybrid interface between graphene and anatase TiO_2 is extremely important for photocatalytic and catalytic applications.

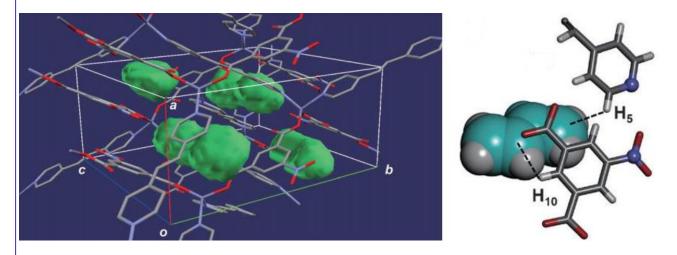
We investigate and discuss the reactivity of O₂ and H₂O on top and at the interface of this system by means of dispersioncorrected hybrid density functional calculations. Pure and boron- or nitrogendoped graphene are interfaced with the most stable (101) anatase surface of TiO2 in order to improve the chemical activity of the C-layer. Especially in the case of boron, enhanced reactivity toward an O_2 dissociation is observed as a result of both



the contribution of the dopant and of the confinement effect in the bidimensional area between the two surfaces. Stable dissociation products are observed where the boron atom bridges the two systems by forming B-O covalent bonds. On the contrary, the same conditions are not found to favor water dissociation, proving that the "catalysis under cover" is not a general effect, but rather highly depends on the interfacing material properties, on the presence of defects and impurities and on the specific reaction involved.

Kishida, K; Okumura, Y; Watanabe, Y; Mukoyoshi, M; Bracco, S; Comotti, A; Sozzani, P; Horike, S; Kitagawa, S. *Recognition of 1,3-Butadiene by a Porous Coordination Polymer*. ANGEWANDTE CHEMIE INTERNATIONAL EDITION 55, 13784 (2016).

Metal Organic Frameworks (MOFs) retail in their porous structure such a specific room for butadiene, a precursor of synthetic elastomers, that this molecule can be separated from similar hydrocarbon mixtures with unprecedented efficiency.



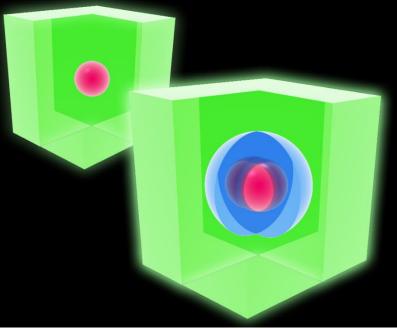
The new purification process contributes to the relevant issue of using functional absorptive materials for important industrial applications. The host-guest steric interaction could be recognized by magic angle spinning NMR, which highlighted host-guest close proximity in the crystal.

From the viewpoint of materials design for specific gas separation under ambient conditions, the results of this study suggest that the key is to combine both narrow voids and structural flexibility for the separation of light gas mixtures.

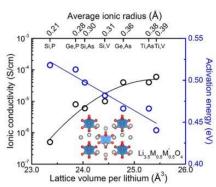
Pinchetti, V; Meinardi, F; Camellini, A; Sirigu, G; Christodoulou, S; Bae, W; De Donato, F; Manna, L; Zavelani-Rossi, M; Moreels, I; Klimov, V; Brovelli, S. *Effect of Core/Shell Interface on Carrier Dynamics and Optical Gain Properties of Dual-Color Emitting CdSe/CdS Nanocrystals*. ACS NANO 10, 6877 (2016).

Two-color emitting colloidal semiconductor nanocrystals (NCs) are of interest for applications in multimodal imaging, sensing, lighting, and integrated photonics. In this study, we elucidate the effect of the interface morphology on the dual emission property of a special class of CdSe/CdS NCs consisting of a small core and a bulk-like shell.

Side-by-side comparison between NCs with identical dimensions but different core/shell interface reveal that systems with a zincblende core

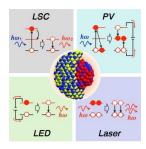


show a faster growth of shell luminescence with excitation fluence and a more readily realized regime of amplified spontaneous emission (ASE) even under "slow" nanosecond excitation. These distinctions are ascribed to the creation of a potential barrier (blue in figure) for photoexcited shell holes inhibiting their relaxation into the core that helps maintain a higher population of shell states and simplifies the realization of dual emission and ASE involving shell-based optical transitions.



Reviews/focus papers

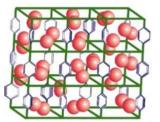
Bachman, J; Muy, S; Grimaud, A; Chang, H; Pour, N; Lux, S; Paschos, O; Maglia, F; Lupart, S; Lamp, P; Giordano, L; Shao-Horn, Y. *Inorganic Solid-State Electrolytes for Lithium Batteries: Mechanisms and Properties Governing Ion Conduction.* CHEMICAL REVIEWS 116, 140 (2016).



Pietryga, J; Park, Y; Lim, J; Fidler, A; Bae, W; Brovelli, S; Klimov, V.

Spectroscopic and Device Aspects of Nanocrystal Quantum Dots.

CHEMICAL REVIEWS 116, 10513 (2016).



Comotti, A; Bracco, S; Sozzani, P. *Molecular Rotors Built in Porous Materials*. ACCOUNTS OF CHEMICAL RESEARCH 49, 1701 (2016).

PEOPLE

0

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Paola **PALERMO** Chemistry Course

Claudio LAGRASTA

Bruno VODOPIVEC

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Umberto PASOTTI



Lorenzo FERRARO

Carmen CANEVALI Luisa RAIMONDO

Enterprise Services/Conto terzi

http://www.mater.unimib.it/it/sezioni/servizi-alle-imprese

The Department of Materials Science has a range of specialist equipment for providing services to external companies and other public or private organizations. It offers a comprehensive service for the investigation of materials and materials-related problems. The expertise of the research staff and extensive facilities can be used in a variety of ways to support industries, including:

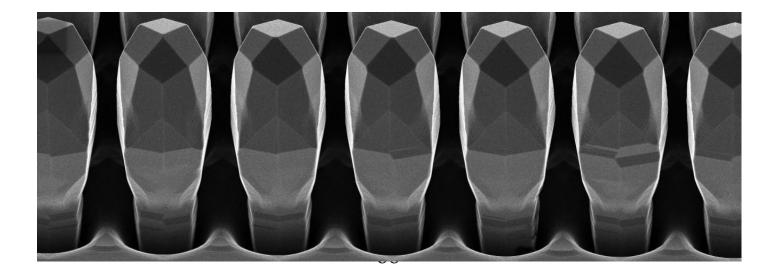
- Materials characterization
- Research projects
- Consultancy
- Training

Materials Characterization - Investigating the properties of a materials such as:

- Structure/microstructure
- Composition
- Thermal behavior
- Morphology
- Optical, electric, electro-optical, magnetic properties
- Dating and characterization of ancient materials

Consultancy – Assisting in any materials-related problem such as effect of processing, compatibility with other materials

Research Projects – Providing technical and creative solutions to specific materials-related problems, designing and projecting new materials, working at the forefront of ground-breaking technologies in the areas of Materials Science, Nanotechnology, Photonics and Biophotonics, Optics, Electronics and Optoelectronics, Spintronics, Energy and Environments, Cultural Heritage.



Facilities Spin off

CUDAM, CENTRO UNIVERSITARIO DATAZIONI E ARCHEOMETRIA MILANO BICOCCA

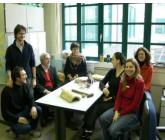


www.cudam.mater.unimib.it

All the UNIMIB Laboratories involved in geological and archaeological dating are members of CUDaM. The Centre presently counts about 30 members from the four

participating departments:

DEPARTMENT OF MATERIALS SCIENCES DEPARTMENT OF EARTH AND ENVIRONMENTAL SCIENCES DEPARTMENT OF PHYSICS "G. OCCHIALINI" DEPARTMENT OF COMPUTER SCIENCES



Aims of the CUDAM are:

- Promotion of studies and researches on dating techniques in geology, environmental science and cultural heritage
- Promotion of interdisciplinary cooperations
- Support and participation in national and international projects devoted to the improvement and application of dating techniques;
- Dating service for public and private customers

Dating techniques:

Thermoluminescence: measurement through thermal stimulation of the electronic charges trapped since last firing

Applications: Authentication of ceramics; Dating of ceramics, bricks, hearths, clay cores, burnt flints, metallurgical slags....

Optically Stimulated Luminescence: measurement through optical stimulation of the electric charges trapped since last light exposure

Applications: Geological and geoarchaeological dating of sediments.

Dendrochronology: measurement of the relative thickness of the annual rings in wood Applications: Dating of wood (archaeology, history of the art, architecture, wood paintings, ancient musical instruments...

Radiocarbon: measurement of the residual concentration of ¹⁴C in organic remains Applications: Dating of organic materials (wood, charcoal, shells, textiles....) The laboratory is equipped for sample preparation to be measured in AMS dating laboratories (University of Florence, Lecce and Neaples).



INTER-UNIVERSITY CENTER FOR NANOMETRIC EPITAXIAL STRUCTURES ON SILICON AND SPINTRONICS

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 microelectronic, 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.:

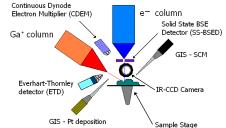
• electron imaging of the sample during navigation without erosion or gallium implantation produced by the ion beam;

• 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 **RI**CERCA 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 interuniversity center. It aims at developing, licensing, or selling innovative technologies manufacturing semiconductor structures and devices, with specific application to thick-film systems, such as highefficiency 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

Galateabiotechwww.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. **T**ECNOLOGIE 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 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



	CHIMICA ORGANICA	SCIENZA DEI MATERIALI
A. ABBOTTO	CHIMICA ORGANICA II E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
MACCIADDI	FISICA III CON LABORATORIO	OTTICA E OPTOMETRIA
M. ACCIARRI	LABORATORIO DI FISICA APPLICATA	FISICA
	COMPLEMENTI DI STRUTTURA DELLA MATERIA	SCIENZA DEI MATERIALI
M. BERNASCONI	STRUTTURA DELLA MATERIA	FISICA
	NANOTECNOLOGIE	SCIENZA DEI MATERIALI
L. BEVERINA	CHIMICA ORGANICA II E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
S. BINETTI	MATERIALI E DISPOSITIVI PER L'ENERGIA	SCIENZA DEI MATERIALI
E. BONERA	FISICA DEI MATERIALI CON LABORATORIO	SCIENZA DEI MATERIALI
A. BORGHESI	FISICA II	OTTICA E OPTOMETRIA
G.P. BRIVIO	TEORIA DELLA MATERIA CONDENSATA I e II	FISICA
S. BROVELLI	LABORATORIO DI FISICA II	SCIENZA DEI MATERIALI
M. CATTI	CHIMICA FISICA DEI MATERIALI	SCIENZA DEI MATERIALI
	LABORATORIO DI CHIMICA ANALITICA STRUMENTALE	SCIENZA DEI MATERIALI
A. COMOTTI	LABORATORIO DI TECNOLOGIA DEI MATERIALI II	SCIENZA DEI MATERIALI
M. D'ARIENZO	CHIMICA GENERALE E INORGANICA CON LABORATORIO	SCIENZA DEI MATERIALI
	CHIMICA GENERALE E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
C. DI VALENTIN	SPETTROSCOPIA E SINTESI DI COMPOSTI INORGANICI	SCIENZE E TECNOLOGIE CHIMICHE
	METODI COMPUTAZIONALI IN CHIMICA INORGANICA	SCIENZE E TECNOLOGIE CHIMICHE
M. FANCIULLI	DISPOSITIVI ELETTRONICI	SCIENZA DEI MATERIALI
E. GRILLI	LABORATORIO DI STATO SOLIDO ED ELETTRONICA I	FISICA
	SPETTROSCOPIA OTTICA DELLO STATO SOLIDO	FISICA
	CHIMICA FISICA APPLICATA CON LABORATORIO	SCIENZA DEI MATERIALI
C. M. MARI	CHIMICA FISICA II E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
M. MARTINI	FISICA I CON LABORATORIO	SCIENZA DEI MATERIALI
PL PARTINI	INTERAZIONE RADIAZIONE IONIZZANTE-MATERIA	SCIENZA DEI MATERIALI
F. MEINARDI	INTERAZIONE LUCE MATERIA	OTTICA E OPTOMETRIA
	ELETTRONICA E FOTONICA MOLECOLARE	SCIENZA DEI MATERIALI

	NANOTECNOLOGIE	SCIENZA DEI MATERIALI
L. MIGLIO	FISICA DELLO STATO SOLIDO	SCIENZA DEI MATERIALI
	STRUTTURA DELLA MATERIA II	SCIENZA DEI MATERIALI
F. MONTALENTI	TERMODINAMICA STATISTICA COMPUTAZIONALE DEI SOLIDI	FISICA
	TERMODINAMICA STATISTICA DEI MATERIALI	FISICA
	CHIMICA GENERALE E INORGANICA CON LABORATORIO	SCIENZA DEI MATERIALI
F. MORAZZONI	CHIMICA DI COORDINAZIONE E METALLORGANICA	SCIENZE E TECNOLOGIE CHIMICHE
	METODI FISICI IN CHIMICA INORGANICA	SCIENZE E TECNOLOGIE CHIMICHE
	CHIMICA INORGANICA II E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
M. MORET	CHIMICA	FISICA
	CHIMICA GENERALE E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
D. 114 D. 116 CT	CHIMICA FISICA	SCIENZA DEI MATERIALI
D. NARDUCCI	CHIMICA FISICA SUPERIORE	SCIENZE E TECNOLOGIE CHIMICHE
G. PACCHIONI	CHIMICA INORGANICA II E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
	CHIMICA DEI MATERIALI CERAMICI	SCIENZA DEI MATERIALI
	FISICA	SCIENZE BIOLOGICHE
A. PALEARI	FISICA II	OTTICA E OPTOMETRIA
	FISICA DEI DIELETTRICI	SCIENZA DEI MATERIALI
	LABORATORIO DI CHIMICA ORGANICA	SCIENZA DEI MATERIALI
A. PAPAGNI	CHIMICA	OTTICA E OPTOMETRIA
	SINTESI E TECNICHE SPECIALI DI MATERIALI ORGANICI	SCIENZA DEI MATERIALI
	CHIMICA FISICA APPLICATA CON LABORATORIO	SCIENZA DEI MATERIALI
R. RUFFO	CHIMICA FISICA II E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
	FISICA DEI MATERIALI CON LABORATORIO	SCIENZA DEI MATERIALI
S. SANGUINETTI	LABORATORIO DI STATO SOLIDO ED ELETTRONICA II	FISICA
	STRUTTURA DELLA MATERIA I	SCIENZA DEI MATERIALI
A. SASSELLA	FISICA II	SCIENZA DEI MATERIALI
	FISICA I	OTTICA E OPTOMETRIA
	CHIMICA DEI MATERIALI INORGANICI	SCIENZA DEI MATERIALI
R. SCOTTI	CHIMICA INORGANICA I E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE

E. SIBILIA	LABORATORIO DI TECNOLOGIA DEI MATERIALI I	SCIENZA DEI MATERIALI
	FISICA I CON LABORATORIO	SCIENZA DEI MATERIALI
	CHIMICA DEI MATERIALI POLIMERICI	SCIENZA DEI MATERIALI
R. SIMONUTTI	CHIMICA ANALITICA STRUMENTALE E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
P. SOZZANI	CHIMICA MACROMOLECOLARE	SCIENZE E TECNOLOGIE CHIMICHE
	CHIMICA MACROMOLECOLARE CON LABORATORIO	SCIENZA DEI MATERIALI
S. TAVAZZI	OTTICA GEOMETRICA E OFTALMICA CON LABORATORIO	OTTICA E OPTOMETRIA
	FISICA I CON LABORATORIO	SCIENZA DEI MATERIALI
A. VEDDA	CARATTERIZZAZIONE FISICA DEI MATERIALI CON LABORATORIO	SCIENZA DEI MATERIALI



GRADUATE STUDENTS 2016



Materials Science

Triennale

DAVIDE ANTONIO ALICINO, DARIO BARNI, FULVIO BELLATO, CAMILLA BONALDO, SILVIO BONAMIGO, MAURA BONZI, VALENTINA CAPROTTI, LUCA CEPPI, ALESSANDRO CHIODI, LORENZO MARIA COGLIATI, FRANCESCA CORBELLA, ROBERTA CRAPANZANO, ANDREA DE CAPITANI, STEFANO DE MARCO, GIANNI D'IMPERIO, STEFANO EUGENIO DREI, ERIC MICHELE FANTUZZI, DOMENICO ANTONIO FLORENZANO, DAVIDE GAGLIARDI, LORENZO MAZZOLENI, SARA MECCA, FABIO MELZI, ANDREA OLDANI, EDOARDO CLAUDIO PADOVANI, ANDREA PALPELLA, SALVATORE PESCIO, ALBERTO PINZO, MARCO PIROVANO, ROBERTA SIPALA, ELIA VILLA, LORENZO VILLA, MARCO VISCONTI

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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 2016 edition, we were present with LEGO-LIGHT stand to discover the magic of colours with the help of Emiliano Bonera and his group. Sergio Brovelli had a public talk about *A window of energy*.









Miriam Ferrari Award

The Miriam Ferrari award is assigned each year to two students who have graduated in the course of Materials Science at the University of Milano-Bicocca, in recognition of the quality of their studies and in order to favour the continuation of their education career.

The award consists of 2,000 Euro and is granted thanks to a donation of the family in memory of Miriam Ferrari, a former student of the Materials Science course.

This year, the awards were granted to Marianna DITERLIZZI and Chiara CAPITANI

Lunedì 30 Maggio 2016 Aula 7 - Edificio U6 Università degli studi di Milano - Bicocca

ore 14:30 *Cerimonia di premiazione*

ore 15:00 Concerto in Memoriam di "Miriam Ferrari" musiche di Ravel, Piazzola, Garson, Repilado, Yadar, Kovacs Stefania Mormone, pianoforte Alberto Serrapiglio, clarinetto



per informazioni sul concerto: Centro QUA SI

per informazioni sulla cerimonia:

Anna Vedda

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