Scienza dei Materiali Materials Science

ANNUAL REPORT 2014

Università degli Studi di Milano-Bicocca



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Matematica Scienza del Materiali

THE MATERIALS SCIENCE DEPARTMENT

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

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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

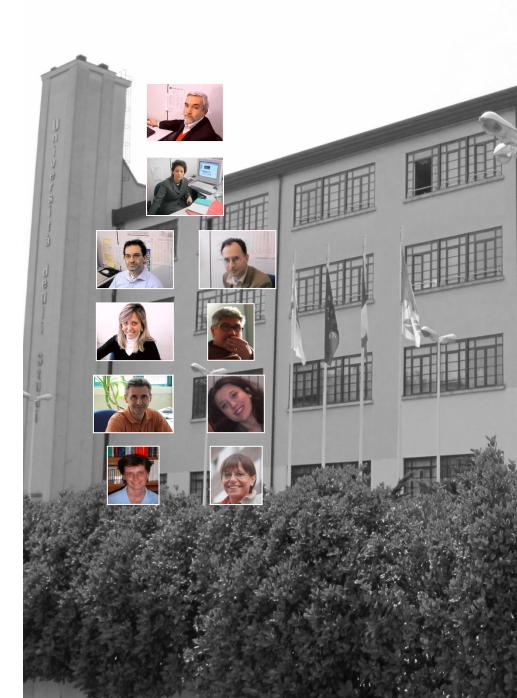
DEPUTY DIRECTOR Franca Morazzoni

Alessandro Abbotto Marco Bernasconi

Simona Binetti Francesco Maggio

Alberto Paleari Luisa Raimondo

Adele Sassella Emanuela Sibilia





DIDACTICS

Alessandro Abbotto Chemical Science Courses, Chairman

> Marco Bernasconi Student career commission

Farncesco Montalenti Study advisory

Dario Narducci Library Board, Chairman

Alberto Paleari Materials Science Courses, Chairman

Antonio Papagni Optics and Optometry Course, Coordinator

> Piero Sozzani Erasmus

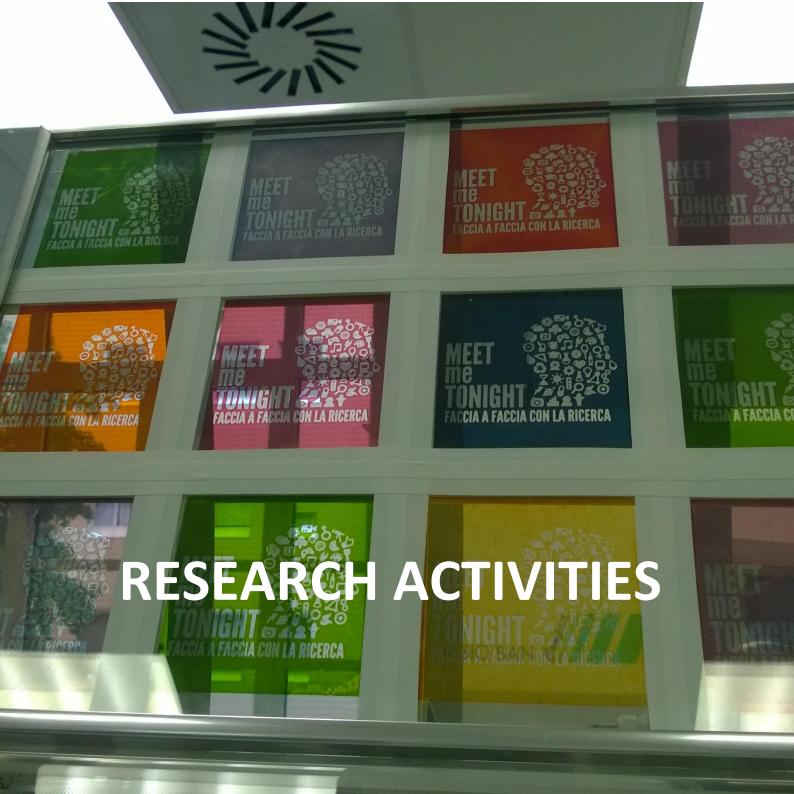
Anna Vedda Thesis commission



NUMBERS 2014

PERSONNEL	#
Researchers	38
Administration	8
Technical personnel	8
Post graduate	63
Total	117

FUNDINGS	€
Contracts	417.000
European Community	528.000
CARIPLO and Regione Lombardia	693.000
Other	493.000
Ordinary financial resources	105.000
Funding for didactics	86.000
Private contributions	194.000
Total	2.516.000



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

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, Stefano Sanguinetti

Optical spectroscopy and fabrication of semiconductors and semiconductor quantum structures

Alessandro Borghesi, Silvia Tavazzi

Optics and optometry

Adele Sassella Organic molecular semiconductors

Sergio Brovelli, Francesco Meinardi Photophysics of molecular semiconductors

Norberto Chiodini, 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

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

Michele Catti

Energy storage materials. Chemical synthesis, crystal structure, theoretical models

Angiolina Comotti

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

Cristiana Di Valentin, Livia Giordano, Gianfranco Pacchioni

Theory of oxide surfaces, interfaces, and supported clusters

Claudio Maria Mari, Riccardo Ruffo

Electrochemical activities

Franca Morazzoni, 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.

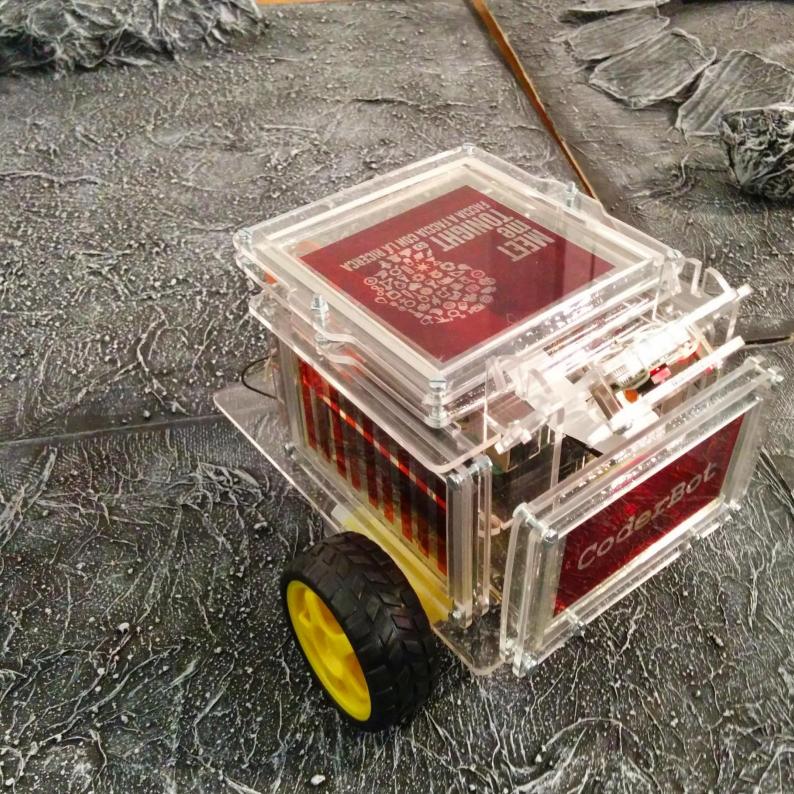
ARTIFICIAL PHOTOSYNTHESIS: CLEAN AND RENEWABLE SOLAR FUELS

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





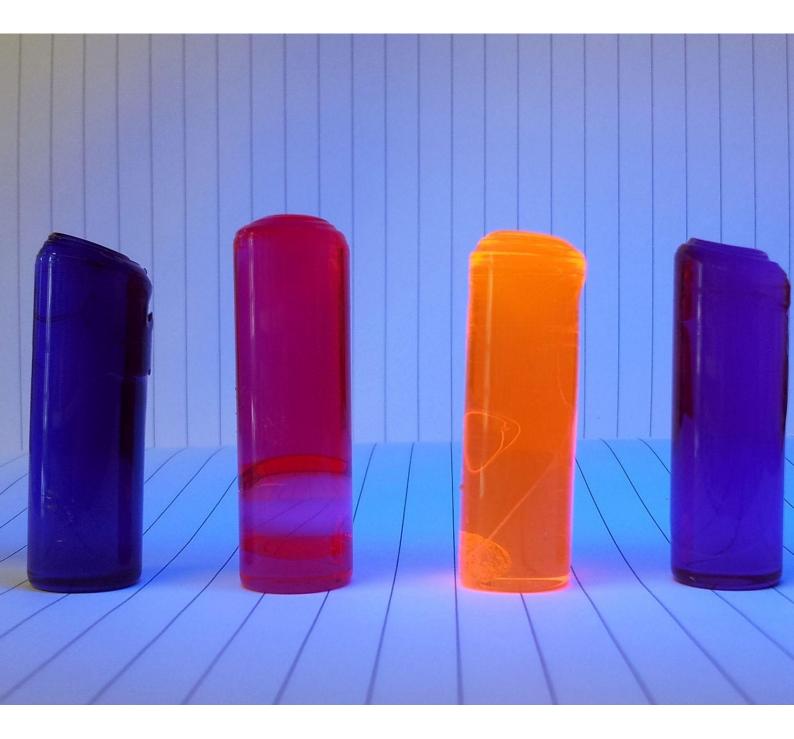
LUCA BEVERINA

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, 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 synthons. The fabrication of solar cells and their analysis is carried out in collaboration with Italian and European research centres and companies.

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

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



Synthesis and characterization of novel polymeric nanostructures





ROBERTO 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.

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

Another possible application of these nanocomposites is in the conservation of cultural heritage, as protective layer that can protect the painting surface from UV radiation, preserving the aesthetics.



Nanostructured materials and magic angle spinning NMR





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 wide-line spectroscopy, including deuterium. High vacuum (10⁻⁹ torr) pump and equipment for hyperpolarized Xenon spectroscopy -laser excited NMR). Dynamic Mechanical Analyzer, Differential Scanning Calorimetry Gel Permeation Cromatography and access to large NMR facilities.



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





MARCO BERNASCONI

PHASE CHANGE MATERIALS FOR DATA STORAGE

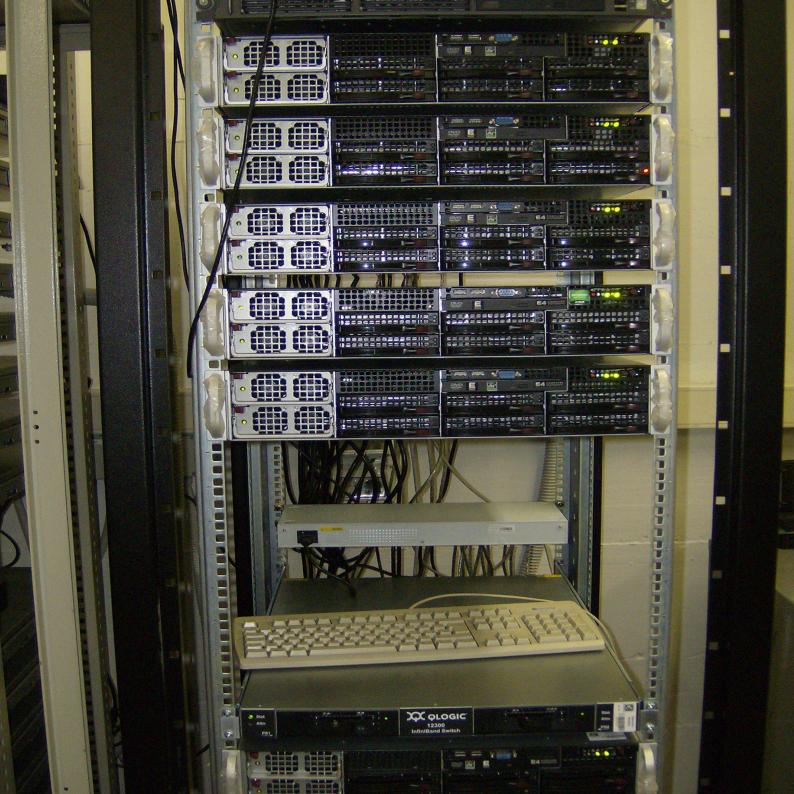
Phase change materials ($Ge_2Sb_2Te_5$ and related telluride alloys) are attracting an increasing interest worldwide for applications in optical disks (DVDs) and in a novel non volatile electronic memory, the phase change memory cell. Both applications rely on a fast (10-100 ns) and reversible transformation 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 abinitio 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 PHONON 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 Sb2Te3, Bi_2Te_3 and the related semimetal elements Sb, Bi. The results are compared with measurements from inelastic He atom scattering from experimental partner groups.



Optical spectroscopy and fabrication of semiconductors and semiconductor quantum structures





EMILIANO BONERA, EMANUELE GRILLI, 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;

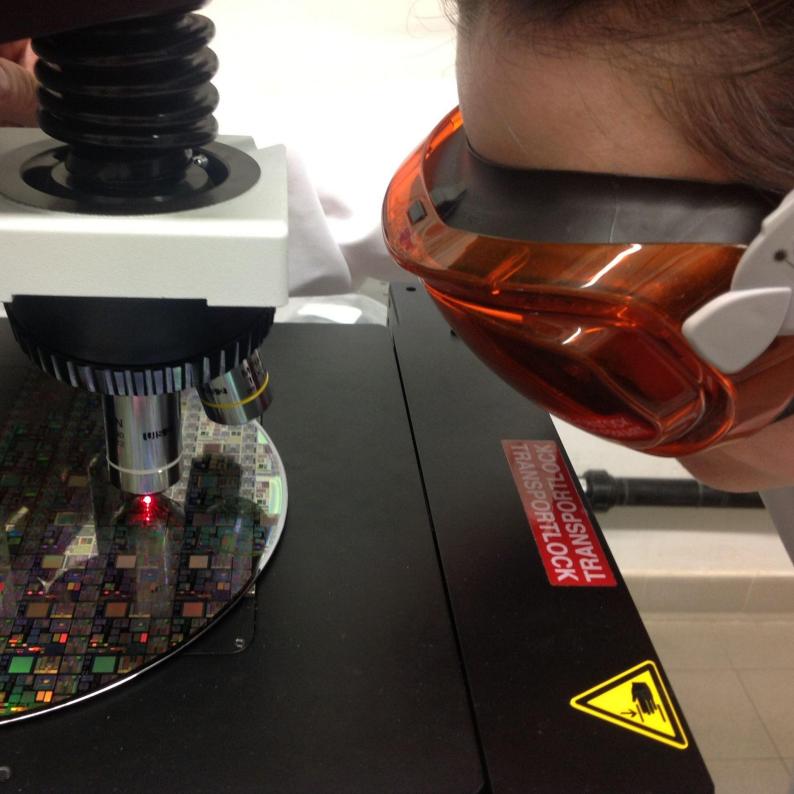
2. We study the nanostructure properties via spectroscopic measurements addressing electronic structure and carrier relaxation mechanisms;

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





ALESSANDRO BORGHESI, 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.

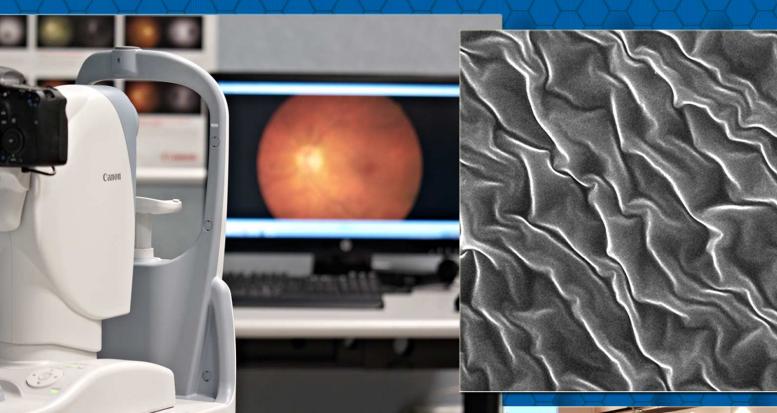
OPTICAL SYSTEMS

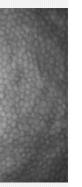
A method was recently developed, which allows the acquisition under a slit-lamp biomicroscope of images of the corneal endothelium cells, which can be automatically recognized by a new procedure of morphometric analysis. The method provides data of the investigated endothelium area, the cell density, 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.

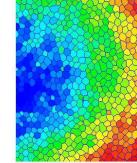
FACILITIES

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..









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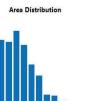
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Distribution





200 300 400 500 600 686

Total Area (mm²) 0,2151

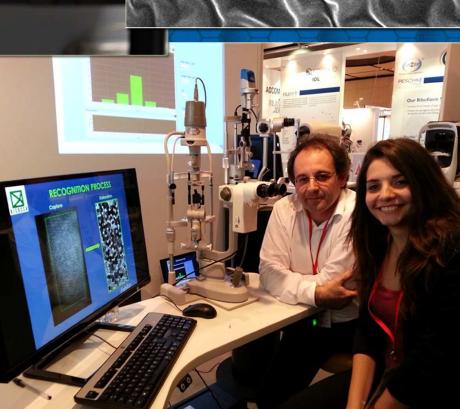
#Cells 603 CD (cells / mm²) 2548

Mean Area ± SD (µm²) 357±93

CV

218

26 Max Area (µm²) 678 Min Area (µm²)



Organic molecular semiconductors





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, for the study of the growth process itself and of the intrinsic properties of the molecular materials in the solid state and, in particular, in the form of thin layers, suitable for device applications. Several molecules, such as oligothiophenes, oligocenes, acridines, and porphyrines are studied. The OMBE growth process is monitored in-situ by reflectance anisotropy spectroscopy (RAS), which also gives insight on the evolution of the electronic properties of the films during growth. The morphology and structural properties of the samples, closely related to the growth mode, are then studied ex-situ, mainly by atomic force microscopy; finally, the optical and transport properties of the molecular films are studied in comparison with the single crystal properties.

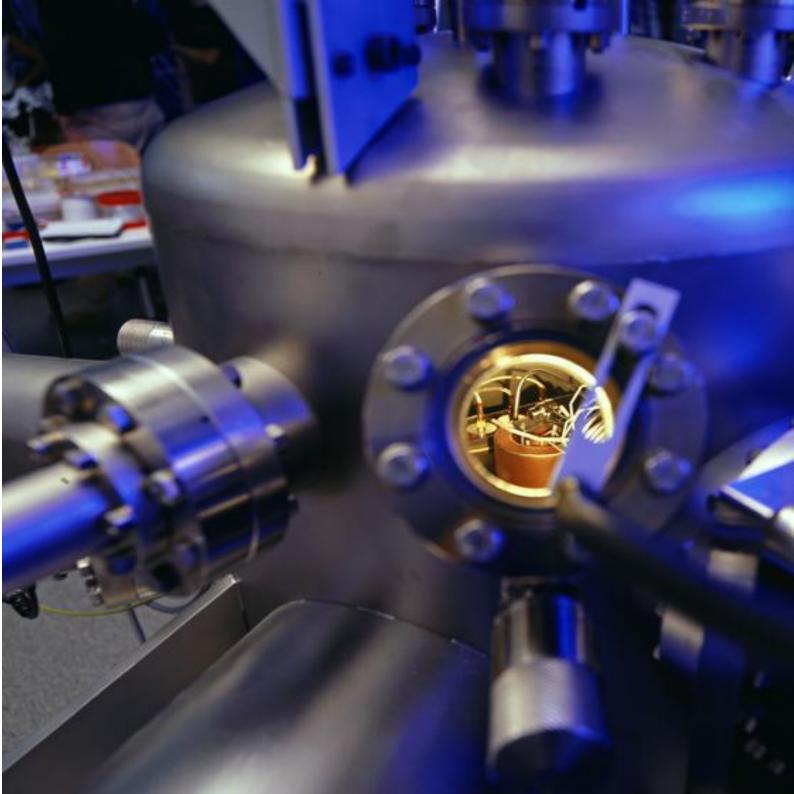
Nanostructures. Films of different molecules are grown on high quality single crystals of the same or similar molecular organic compounds, so as to reach homo- and hetero-epitaxy, therefore preparing artificial structures with high quality interfaces and controlled properties. Thin films are also stacked 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.

Modelling. After the investigation of the single molecule characteristics from ab-initio calculations, the results are used as microscopic ingredients for building the Frenkel exciton Hamiltonian of single crystals of the same materials studied experimentally. Thus, the dielectric tensor is calculated in order to simulate the crystal and thin film optical spectra under different experimental configurations taking into consideration optical anisotropy and directional dispersion.

FACILITIES

The OMBE apparatus consists of the introduction chamber, a second chamber for the sample metallization, and the deposition chamber, where six sources are installed for different compounds, a quartz microbalance controls the film thickness, and the RAS apparatus is installed; a fourth chamber for *in-situ* optical characterization is also available. Optical spectroscopies, such as absorption, reflection, photoluminescence and ellipsometry, are used for the study of thin films and multilayers down to few K, also in comparison with the properties detected *in-situ* by RAS. Atomic force microscopy is used for the morphology characterization of all the samples and for the study of the film growth process.



Photophysics of molecular semiconductors







SERGIO BROVELLI, FRANCO MEINARDI

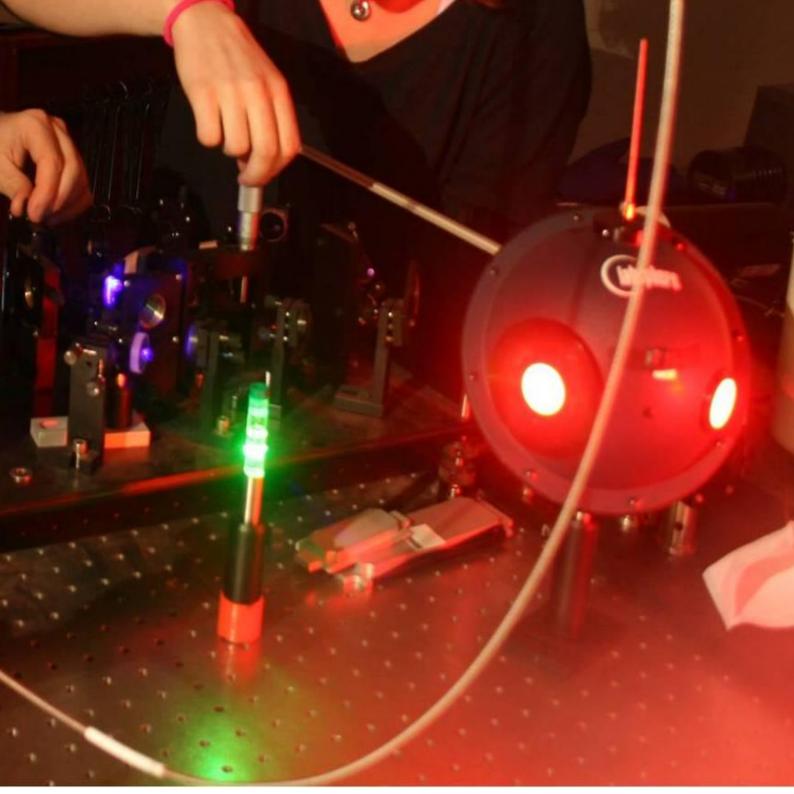
Non-Coherent Photons Up-conversion. The generation of photons of higher energy with respect to the excitation (up-conversion) through the non linear optical response of a material is a phenomenon useful to reach spectral regions otherwise not accessible. However, is appreciable only for coherent light 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









NORBERTO CHIODINI, ALBERTO PALEARI, ANNA VEDDA

Our research is focused on the physical properties of silica-based glass and glassceramics 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 radioluminescence 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 strong collaboration with the CNR-IMM, MDM Laboratory and leading semiconductor industries, Micron and STMicroelectronics.

POINT DEFECTS IN SEMICONDUCTORS AND OXIDES

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

SEMICONDUCTOR/OXIDE INTERFACES

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

Si AND Ge NANOSTRUCTURES

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.

FACILITIES

Growth and processing: Atomic Layer Deposition (ALD) mini-chamber with O3 line for *insitu* characterization; horizontal and vertical furnaces for annealing and diffusion; Q-switched Ruby laser for laser annealing

Characterization: two CW X-band systems for electron spin resonance (ESR) spectroscopy, electrically detected spin resonance spectroscopy (EDMR) and electron nuclear double resonance spectroscopy (ENDOR), variable temperature measurements (4-600 K); multi-frequency (0.1-40 GHz) EDMR; set-up for inelastic electron tunneling spectroscopy (IETS) working in the temperature range 4-300 K.



Modeling and simulations of epitaxial semiconductor depositions and nanostructures







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











MAURIZIO ACCIARRI, SIMONA BINETTI, DARIO NARDUCCI

NANOTECHNOLOGY FOR THERMOELECTRICITY

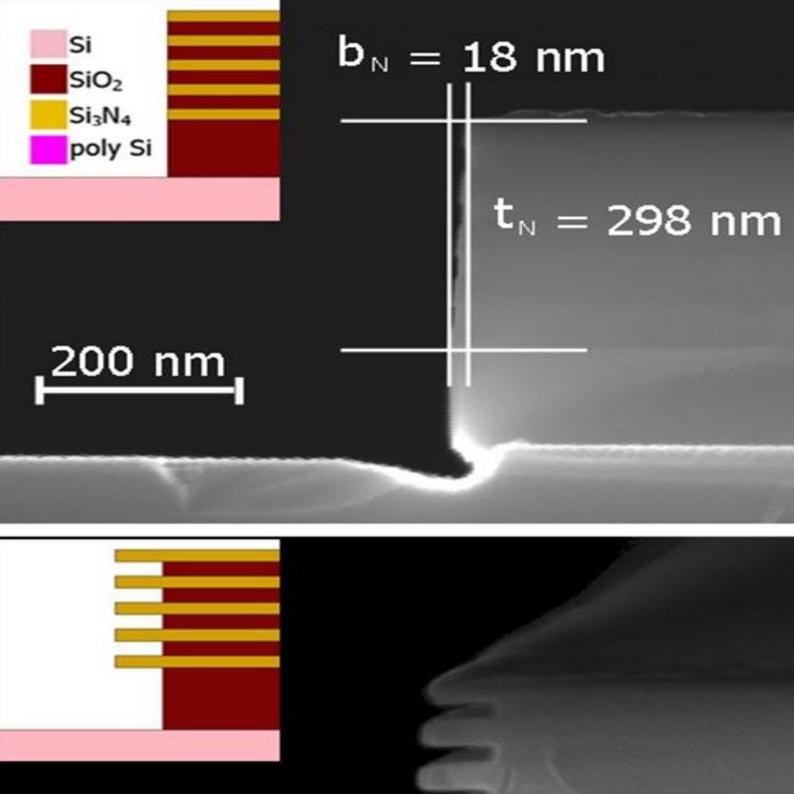
Thermoelectricity is a way to convert heat into electricity without the use of any movable part. As such, thermoelectric generators are suitable, especially when miniaturized, to harvest low-temperature heat and to make it available as electric power to distributed sensor networks or to other portable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

SILICON FOR SOLAR CELLS

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

INORGANIC SEMICONDUCTOR THIN FILMS FOR PHOTOVOLTAICS

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



Theory and computations of 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 34 Universities and research Laboratories, aims at advancing computational spectroscopy. In our studies we make use and contribute to quantum codes both for the supercell geometry and for non periodic systems within the density functional theory framework. Our results are relevant to basic knowledge and to device implementations, such as photovoltaics and nanoelectronics.

CORE LEVEL SPECTROSCOPY

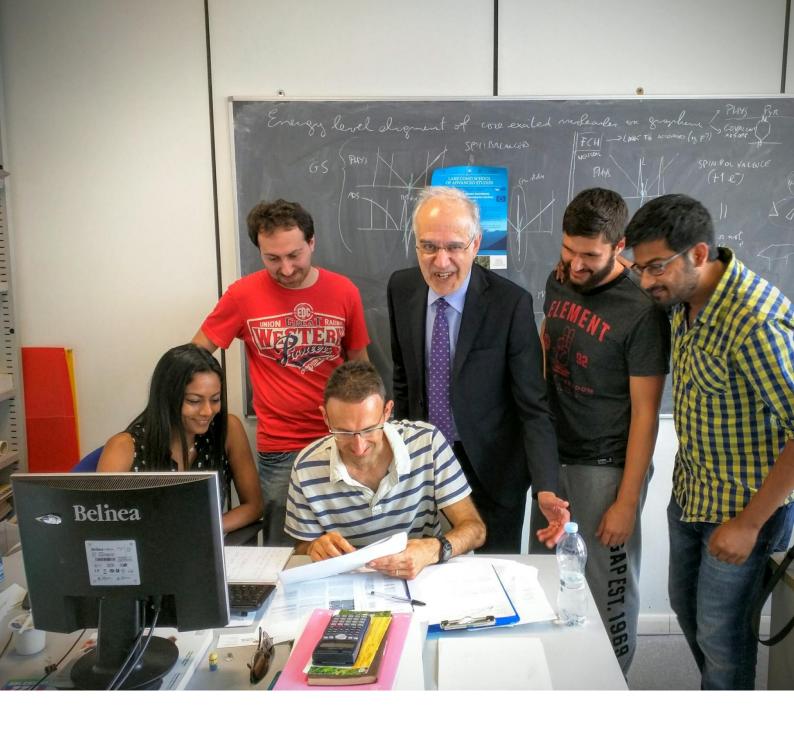
The near edge X-ray absorption fine structure spectroscopy (NEXAFS), the x-ray photoelectron spectroscopy (XPS) and the scanning tunneling microscopy (STM) of aromatic molecules adsorbed on insulators and metals were computed and our results compared with the experimental measurements at the synchrotron ELETTRA. The molecular orbitals symmetry of perylene derivatives were analyzed by surface science approaches adopting highly ordered samples. For pentacene on Al(001) we have discovered an unusual V-shape adsorbate structure.

MAGNETIC NANOSTRUCTURES

We investigated by first principles the adsorption of aromatic radicals on graphene. Taking into account the radicals of benzene and of the extrema of standard lists of charge donating and accepting groups, we found that the carbon atom on the adsorption site A is lifted out of the graphene plane. At the same time its p_z orbital is removed from the p band system leaving the electrons in the other sublattice B unpaired, which results in nonzero magnetism universally for the investigated species.

CHARGE TRANSFER TIMES OF ORGANIC ADSORBATES

Charge transfer from an organic adsorbed molecule is a very important process in surface reaction dynamics, photocatalysis, molecular electronics and photovoltaics by dye sensitized solar cells. In this field we have developed a theory to deal with a semi-infinite substrate and computed the lifetimes of the excited resonant states of few molecules adsorbed on metals and on graphene. Our model for a core electron excited system remark the relevance of the electronic effects in charge transfer processes and provide quantitative estimates of lifetimes between 10-100 fms.



Energy storage materials. Chemical synthesis, crystal structure, theoretical models





Michele Catti

Inorganic materials of interest for ionic conductivity in lithium batteries and for hydrogen storage (also in collaboration with Pirelli) are presently studied. The focus is on relationships between structural properties, chemical composition, ionic mobility and reactivity with hydrogen, in the frame of a more general study of phase transformations in the solid state. Both experimental and computational methods are employed.

EXPERIMENTAL

Chemical synthesis is performed by a variety of techniques, including high-temperature treatments in controlled atmosphere. A thorough crystallographic characterization is then carried out by X-ray powder diffractometry. For the purpose of fully determining the crystal structure of the phases obtained, neutron diffraction data are often collected in several European centres (e.g., the ISIS facility at the neutron spallation source of the Rutherford Appleton Laboratory, U.K.). The reactions of hydrogen absorption and desorption are studied by a PCI (Pressure-Composition-Temperature) apparatus from the thermodynamic and the kinetic point of view. Measurements of electrical (complex impedance spectroscopy) and electrochemical properties are performed in the laboratory of Prof. C.M. Mari within a collaboration.

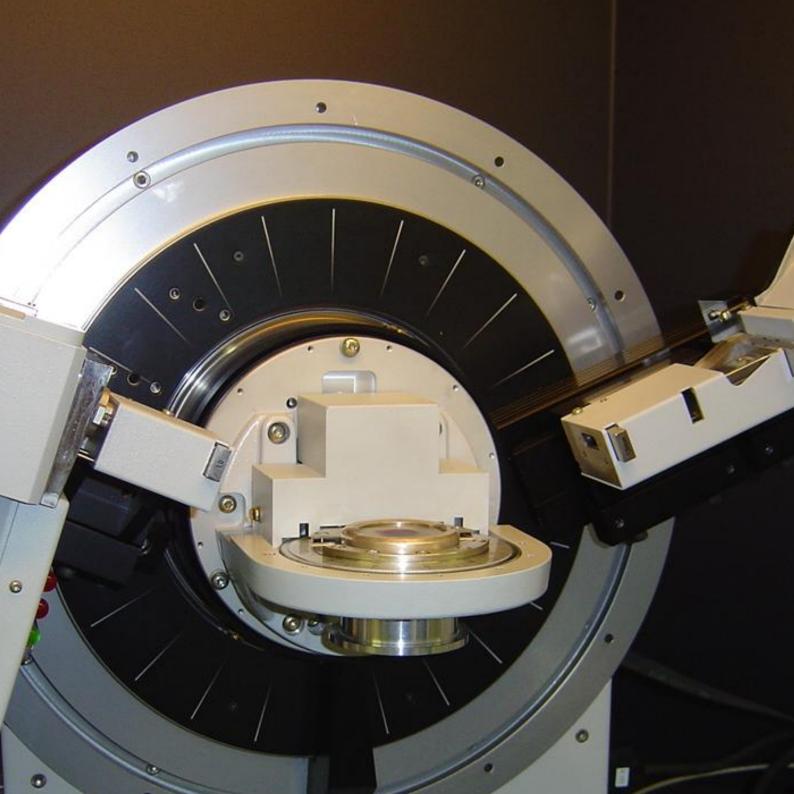
COMPUTATIONAL

The theoretical investigations are based on quantum-mechanical periodic DFT methods, with the aim of modelling the relative stability, the structural properties and the ionic transport of crystalline phases.

RESULTS

Recently studied materials are the fast lithium ion conductors of the LLTO family $(Li_{0.3}La_{0.567}TiO_3)$ with perovskite structure. Neutron diffraction data, electrical measurements and ab-initio simulations allowed us to clarify the mechanism of Li⁺ ion diffusion in this material. A complex series of phase transformations, also dependent on the thermal history, was revealed by Rietveld refinements from neutron data. The Li⁺ ion disorder explains the two-dimensional high ionic mobility in the (001) plane. By DFT calculations, it was possible to interpret the long-range structural results on the basis of local models of the Li⁺ ion environment. The least-energy ion mobility pathways are also under investigation, with the aim of calculating the activation energy for the lithium transport process. The study of other classes of lithium ion conductors has been now undertaken.

Mg-based alloys and borohydrides are being presently investigated for their hydrogen storage properties, in collaboration with CORIMAV-Pirelli. The materials, synthesized by the ball milling technique, show promising H-absorption behaviour for particular compositions and crystal structures.



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

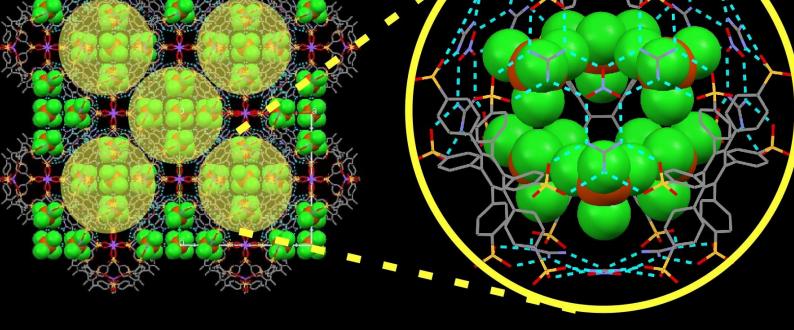


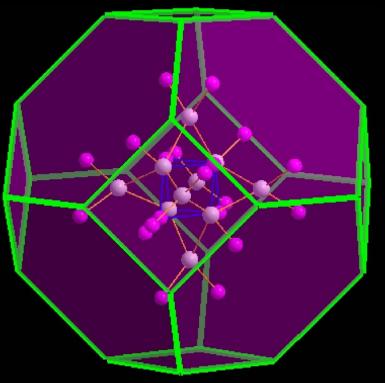


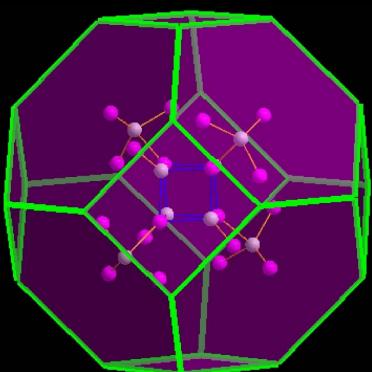
ANGIOLINA COMOTTI

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







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.



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



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

arrays of adsorption and reactive sites, etc.

Nature of point defects in oxide materials for photocatalysis, photoelectrochemistry, microelectronics, fiber optics etc., in particular amorphous and crystalline TiO₂, 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 CI_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, FRANCA MORAZZONI, ROBERTO SCOTTI

FOR PHOTOCATALYTIC APPLICATIONS The research aims at the synthesis by soft-chemistry methods of shape controlled oxide nanocrystals (TiO₂, ZnO, WO₃), 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 (H₂)

production and CO₂ photoconversion in renewable fuels) reactions. 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 can be 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 modulation of the amount of entrapped rubber and it is the basis for extending the investigation toward natural silicates as anisotropic fillers. A further objective of the research is the synthesis of ZnO NPs anchored to SiO₂, which acts as reinforcing filler and curing activator simultaneously, for the improvement of the rubber curing process.

EQUIPMENTS

Chemistry laboratories, fully equipped for the synthesis and the processing of the compounds. Total Organic Carbon Analyzer Shimadzu TOC-V CSH for liquid and gas samples. Surface Area and Pore Size Analyzer, Autosorb-1-MP Quantachrome Instrument. Electron Spin Resonance (ESR) spectrometer, Brucker EMX



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







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 14 C atoms in organic remains). The laboratory is member of the CUDaM (Centro Universitario Datazioni 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,...).



MAIN ACTIVITIES

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 14 C 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.



PUBLICATIONS TALKS PHD THESIS PATENTS

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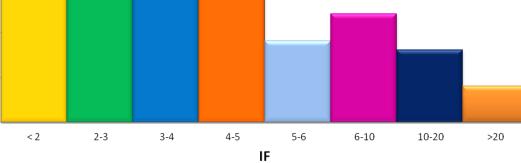
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M. MUCCINI

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PUBLICATIONS ON INTERNATIONAL JOURNALS

#	Citation	IF (ISI)
1	Andreucci S. , Panzeri L . , Martini I.P., Martini M. , Maspero F. , Pascucci V. Evolution and architecture of a west Mediterranean upper Pleistocene to Holocene coastal apron-fan system. SEDIMENTOLOGY, 61, 333-361; doi: 10.1111/sed.12058.	2,741
2	Backofen, R; Bergamaschini, R ; Voigt, A. The interplay of morphological and compositional evolution in crystal growth: a phase-field model. PHILOSOPHICAL MAGAZINE 94, 2162.	1,427
3	Bassanetti, I; Comotti, A ; Sozzani, P ; Bracco, S; Calestani, G; Mezzadri, F; Marchiò, L. Porous molecular crystals by macrocyclic coordination supramolecules. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 136, 14883.	11,444
4	Bassinet, C; Woda, C; Bortolin, E; Della Monaca, S; Fattibene, P; Quattrini, MC; Bulanek, B; Ekendahl, D; Burbidge, CI; Cauwels, V; Kouroukla, E; Geber-Bergstrand, T; Mrozik, A; Marczewska, B; Bilski, B; Sholom, S; McKeever, SWS; Smith, RW; Veronese, I; Galli, A; Panzeri, L ; Martini, M. <i>Retrospective radiation dosimetry using OSL of electronic components: results of an inter-laboratory</i> <i>comparison.</i> RADIATION MEASUREMENTS 71, 475.	1,14
5	Belli, M ; Fanciulli, M ; Batani, D. Electron spin resonance of substitutional nitrogen in silicon. PHYSICAL REVIEW B 89, 115207.	3,664
6	Benedek, G; Bernasconi, M ; Bohnen, K; Campi, D; Chulkov, E; Echenique, P; Heid, R; Sklyadneva, I; Toennies, J Unveiling mode-selected electron-phonon interactions in metal films by helium atom scattering. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 16, 7159.	4,198
7	Bergantin, S; Moret, M ; Buth, G; Fabbiani, F.P.A. Pressure-Induced Conformational Change in Organic Semiconductors: Triggering a Reversible Phase Transition in Rubrene. JOURNAL OF PHYSICAL CHEMISTRY C 118, 13476.	4,772
8	Beverina, L ; Pagani, G. π -conjugated zwitterions as paradigm of donor-acceptor building blocks in organic-based materials. ACCOUNTS OF CHEMICAL RESEARCH 47, 319.	24,348
9	Beverina, L ; Pagani, G; Sassi, M. Multichromophoric electrochromic polymers: Colour tuning of conjugated polymers through the side chain functionalization approach. CHEMICAL COMMUNICATIONS 50, 5413.	6,718
10	Beverina, L ; Sassi, M. Twists and turns around a square: The many faces of Squaraine chemistry.	2,463

	SYNLETT 25, 477.	
11	Bianchi, A; Mauri, M; Bonetti, S; Koynov, K; Kappl, M; Lieberwirth, I; Butt, H; Simonutti, R. Hierarchical self-assembly of PDMA-b-PS chains into granular nanoparticles: Genesis and fate. MACROMOLECULAR RAPID COMMUNICATIONS 35, 1994.	4,608
12	Bietti, S; Somaschini, C; Esposito, L; Fedorov, A; Sanguinetti, S. Gallium surface diffusion on GaAs (001) surfaces measured by crystallization dynamics of Ga droplets. JOURNAL OF APPLIED PHYSICS 116, 114311	2,185
13	Bietti, S; Somaschini, C; Frigeri, C; Fedorov, A; Esposito, L; Geelhaar, L; Sanguinetti, S Self-assisted GaAs nanowires with selectable number density on Silicon without oxide layer. JOURNAL OF PHYSICS D 47, 394002	2,521
14	Bigia, F; Piscopo, CG; Predieri, G; Sartori, G; Scotti, R ; Zanoni, R; Maggi, R Molybdenum-MCM-41 silica as heterogeneous catalyst for olefin epoxidation. JOURNAL OF MOLECULAR CATALYSIS A 386, 108.	3,679
15	Binetti, S; Le Donne, A; Sassella, A. Photoluminescence and infrared spectroscopy for the study of defects in silicon for photovoltaic applications. SOLAR ENERGY MATERIALS AND SOLAR CELLS 130, 696.	5,03
16	Bollani, M; Bietti, S; Frigeri, C; Chrastina, D; Reyes, K; Smereka, P; Millunchick, J; Vanacore, G; Burghammer, M; Tagliaferri, A; Sanguinetti, S. Ordered arrays of embedded Ga nanoparticles on patterned silicon substrates. NANOTECHNOLOGY 25, 205301.	3,672
17	Brovelli, S ; Bae, W; Galland, C; Giovanella, U; Meinardi, F ; Klimov, V. Dual-Color Electroluminescence from Dot-in-Bulk Nanocrystals. NANO LETTERS 14, 486	12,94
18	Brovelli, S ; Bae, W; Meinardi, F; Santiago González, B; Lorenzon, M; Galland, C; Klimov, V. Electrochemical control of two-color emission from colloidal dot-in-bulk nanocrystals. NANO LETTERS 14, 3855.	12,94
19	Brown, M; Arrigoni, M; Héroguel, F; Beloqui Redondo, A; Giordano, L ; Van Bokhoven, J; Pacchioni, G. <i>PH dependent electronic and geometric structures at the water-silica nanoparticle interface.</i> JOURNAL OF PHYSICAL CHEMISTRY C 118, 29007	4,835
20	Brown, R; Hund, Z; Campi, D; O'Leary, L; Lewis, N; Bernasconi, M ; Benedek, G; Sibener, S. The interaction of organic adsorbate vibrations with substrate lattice waves in methyl-Si(111)-(1 × 1). THE JOURNAL OF CHEMICAL PHYSICS 141, 024702	3,122
21	Bruni, F; Sassi, M; Campione, M; Giovanella, U; Ruffo, R ; Luzzati, S; Meinardi, F ; Beverina, L ; Brovelli, S. Post-deposition Activation of Latent Hydrogen-Bonding: A New Paradigm for Enhancing the Performances of Bulk Heterojunction Solar Cells. ADVANCED FUNCTIONAL MATERIALS 24, 7410.	10,439
22	Buechner, C; Lichtenstein, L; Stuckenholz, S; Heyde, M; Ringleb, F; Sterrer, M; Kaden, WE; Giordano, L ; Pacchioni, G ; Freund, H-J. Adsorption of Au and Pd on Ruthenium-Supported Bilayer Silica. JOURNAL OF PHYSICAL CHEMISTRY C, 118, 20959.	4,835
23	Bussetti, G; Campione, M; Ferraro, L; Raimondo, L; Bonanni, B; Goletti, C; Palummo, M; Hogan, C; Duò, L; Finazzi, M; Sassella, A. Probing Two-Dimensional vs Three-Dimensional Molecular Aggregation in Metal-Free Tetraphenylporphyrin	4,835

	Thin Films by Optical Anisotropy.	
	JOURNAL OF PHYSICAL CHEMISTRY C 118, 15649.	
24	Bussetti, G; Campione, M; Raimondo, L; Yivlialin, R; Finazzi, M; Ciccacci, F; Sassella, A ; Duò, L. Unconventional post-deposition chemical treatment on ultra-thin H2TPP film grown on graphite. CRYSTAL RESEARCH AND TECHNOLOGY 49, 581.	1,164
25	Bussetti, G; Trabattoni, S; Uttiya, S; Sassella, A ; Riva, M; Picone, A; Brambilla, A; Duò, L; Ciccacci, F; Finazzi, M. Controlling drop-casting deposition of 2D Pt-octaethyl porphyrin layers on graphite. SYNTHETIC METALS 195, 201.	2,222
26	Calvillo, L; Fittipaldi, D; Rüdiger, C; Agnoli, S; Favaro, M; Valero-Vidal, C; Di Valentin, C ; Vittadini, A; Bozzolo, N; Jacomet, S; Gregoratti, L; Kunze-Liebhäuser, J; Pacchioni, G ; Granozzi, G. Carbothermal transformation of TiO2 into TiOxCy in UHV: Tracking intrinsic chemical stabilities. JOURNAL OF PHYSICAL CHEMISTRY C 118, 22601.	4,835
27	Camposeo, A; Polo, M; Del Carro, P; Silvestri, L; Tavazzi, S ; Pisignano, D. Random lasing in an organic light-emitting crystal and its interplay with vertical cavity feedback. LASER & PHOTONICS REVIEWS 8, 785.	9,313
28	Caratto, V; Locardi, F; Costa, G; Masini, R; Fasoli, M; Panzeri, L; Martini, M ; Bottinelli, E; Gianotti, E; Miletto, I. NIR persistent luminescence of lanthanide ion-doped rare-earth oxycarbonates: The effect of dopants. ACS APPLIED MATERIALS & INTERFACES 6, 17346.	5,9
29	Carrara, M; Tenconi, C; Guilizzoni, R; Borroni, M; Cerrotta, A; Fallai, C; Gambarini, G; Vedda, A ; Pignoli, E. Stem effect of a Ce3+ doped SiO2 optical dosimeter irradiated with a 192Ir HDR brachytherapy source. RADIATION PHYSICS AND CHEMISTRY 104, 175.	1,189
30	Carrara, M; Tenconi,C; Rossi, G; Guilizzoni, R; Borroni, M; Cerrotta, A; Fallai, C; Gambarini, G; Vedda, A ; Pignoli, E. Temperature dependence of a Ce3+ doped SiO2 radioluminescent dosimeter for in vivo dose measurements in HDR brachytherapy. RADIATION MEASUREMENTS 71, 324.	1,14
31	Catti, M ; Ghaani, M. On the lithiation reaction of niobium oxide: structural and electronic properties of Li1.714Nb2O5. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 16, 1385.	4,198
32	Cecchi, S; Gatti, E; Chrastina, D; Frigerio, J; Müller Gubler, E; Paul, D; Guzzi, M ; Isella, G. Thin SiGe virtual substrates for Ge heterostructures integration on silicon. JOURNAL OF APPLIED PHYSICS 115, 0935022,185.	
33	Chen, H; Giordano, L; Pacchioni, G. Adsorption Properties of Two-Dimensional NaCl: A Density Functional Theory Study of the Interaction of Co, Ag, and Au Atoms with NaCl/Au(111) Ultrathin Films. JOURNAL OF PHYSICAL CHEMISTRY C 118, 12353.	4,835
34	Chen, H; Pacchioni, G. Properties of two-dimensional insulators: A DFT study of Co adsorption on NaCl and MgO ultrathin films. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 16, 21838.	4,198
35	Chen, P; Zhang, J; Feser, J ; Pezzoli, F ; Moutanabbir, O; Cecchi, S; Isella, G; Gemming, T; Baunack, S; Chen, G; Schmidt, O; Rastelli, A. Thermal transport through short-period SiGe nanodot superlattices.	2,185

	JOURNAL OF APPLIED PHYSICS 115, 044312.	
36	Chiodini, N; Vedda, A; Veronese, I. Rare Earth Doped Silica Optical Fibre Sensors for Dosimetry in Medical and Technical Applications. ADVANCES IN OPTICS 2014, 974584	NA
37	Cianci, E; Molle, A; Lamperti, A; Wiemer, C; Spiga, S; Fanciulli, M. Phase Stabilization of Al:HfO2 Grown on In(x)Gal(1-x)As Substrates (x=0, 0.15, 0.53) via Trimethylaluminum-Based Atomic Layer Deposition. ACS APPLIED MATERIALS & INTERFACES 6, 3455.	5,9
38	Colombo, A; Dragonetti, C; Valore, A; Coluccini, C; Manfredi, N; Abbotto, A. Thiocyanate-free ruthenium(II) 2,2'-bipyridyl complexes for dye-sensitized solar cells. POLYHEDRON 82, 50.	2,047
39	Comotti, A ; Bracco, S;Ben, T; Qiu, S; Sozzani, P. Molecular Rotors in Porous Organic Frameworks. ANGEWANDTE CHEMIE 53, 1043.	11,336
40	Conesa-Boj, S; Boioli, F; Russo-Averchi, E; Dunand, S; Heiss, M; Ruffer, D; Wyrsch, N; Ballif, C; Miglio, L ; Morral, A.F. <i>Plastic and Elastic Strain Fields in GaAs/Si Core-Shell Nanowires.</i> NANO LETTERS 14, 1859.	12,94
41	Coscia, U; Ambrosone, G; Basa, D; Rigato, V; Binetti, S. Structural and photoconductivity properties of silicon carbon thin films. PHYSICA STATUS SOLIDI C 11, 1669.	NA
42	Costa, D; Ribeiro, T; Mercuri, F; Pacchioni, G ; Marcus, P. Atomistic Modeling of Corrosion Resistance: A First Principles Study of O-2 Reduction on the Al(111) Surface Covered with a Thin Hydroxylated Alumina Film. ADVANCED MATERIALS INTERFACES 1, 1300072.	NA
43	Cui, Y; Shao, X; Prada, S; Giordano, L; Pacchioni, G ; Freund, H; Nilius, N. Surface defects and their impact on the electronic structure of Mo-doped CaO films: an STM and DFT study. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 16, 12764.	4,198
44	D'Arienzo , M; Armelao, L; Mari, C ; Polizzi, S; Ruffo, R ; Scotti, R ; Morazzoni, F. Surface interaction of WO3 nanocrystals with NH3: Role of the exposed crystal surfaces and porous structure in enhancing the electrical response. RSC ADVANCES 4, 11012.	3,708
45	De Angelis, F; Di Valentin, C ; Fantacci, S; Vittadini, A; Selloni, A. Theoretical studies on anatase and less common TiO2phases: Bulk, surfaces, and nanomaterials. CHEMICAL REVIEWS 114, 9708.	45,661
46	Di Carlo, G; Orbelli Biroli, A; Tessore, F; Pizzotti, M; Mussini, P; Amat, A; De Angelis, F; Abbotto, A ; Trifiletti, V; Ruffo, R. Physicochemical Investigation of the Panchromatic Effect on β -Substituted ZnIIPorphyrinates for DSSCs: The Role of the π Bridge between a Dithienylethylene Unit and the Porphyrinic Ring. JOURNAL OF PHYSICAL CHEMISTRY C 118, 7307.	4,835
47	Di Martino, D; Beverina, L ; Sassi, M; Brovelli, S ; Tubino, R; Meinardi, F. Straightforward fabrication of stable white LEDs by embedding of inorganic UV-LEDs into bulk polymerized polymethyl-methacrylate doped with organic dyes. SCIENTIFIC REPORTS 4, 4400.	5,078

	DiVelentin C. Deschieni C	
	Di Valentin, C; Pacchioni, G.	
48	Spectroscopic properties of doped and defective semiconducting oxides from hybrid density functional	24,348
•	calculations	1/2 1
	ACCOUNTS OF CHEMICAL RESEARCH 47, 3233.	
	Errahali, M; Gatti, G; Tei, L; Paul, G; Rolla, G; Canti, L; Fraccarollo, A; Cossi, M; Comotti, A ; Sozzani, P ;	
49	Marchese, L.	4,835
49	Microporous hyper-cross-linked aromatic polymers designed for methane and carbon dioxide adsorption.	4,055
	JOURNAL OF PHYSICAL CHEMISTRY C 118, 28699.	
	Fanciulli, M; Scalise, E.	
50	Vibrational properties of epitaxial silicene layers on (111) Ag.	2,538
	APPLIED SURFACE SCIENCE 291, 113.	
	Fathi, R ; Ruffo, R; Mari, C.M.	
	Electrochemical Behavior of Electrodeposited Sn Films: Possible Negative Electrode for Na+ Rechargeable	
51	Batteries.	NA
	JOURNAL OF CHEMISTRY AND CHEMICAL ENGINEERING 8, 358.	
	Favaro, M; Agnoli, S; Di Valentin, C ; Mattevi, C; Cattelan, M; Artiglia, L; Magnano, E; Bondino, F; Nappini,	
	S; Granozzi, G.	
52	TiO2/graphene nanocomposites from direct reduction of graphene oxide by metal evaporation.	6,16
	CARBON 68, 319.	
	Fazio, G; Ferrighi, L; Di Valentin, C.	
53	Boron-doped graphene as active electrocatalyst for oxygen reduction reaction at a fuel-cell cathode.	6,073
رر	JOURNAL OF CATALYSIS 318, 203.	0,075
	Ferraro, E; De Michielis, M; Mazzeo, G; Fanciulli, M ; Prati, E.	
54	Effective Hamiltonian for the hybrid double quantum dot qubit.	2,96
7	QUANTUM INFORMATION PROCESSING 13, 1155.	2,90
	Ferrighi, L; Datteo, M; Di Valentin, C.	
	Boosting graphene reactivity with oxygen by boron doping: Density functional theory modeling of the	
55	reaction path.	4,835
	JOURNAL OF PHYSICAL CHEMISTRY C 118, 223.	
	Fratesi, G; Lanzillotto, V; Floreano, L; Brivio, G.	
	Correction to "Azimuthal Dicroism in Near-Edge X-ray Absorption Fine Structure Spectra of Planar	
56	Molecules".	4,835
	JOURNAL OF PHYSICAL CHEMISTRY C 118, 2236.	
	Fratesi, G; Lanzilotto, V; Stranges, S; Alagia, M; Brivio, G ; Floreano, L.	0
57	High resolution NEXAFS of perylene and PTCDI: a surface science approach to molecular orbital analysis.	4,198
	PHYSICAL CHEMISTRY CHEMICAL PHYSICS 16, 14834.	
- 0	Fratesi, G; Motta, C; Trioni, MI; Brivio, G ; Sanchez-Portal, D.	
58	Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles.	4,835
	JOURNAL OF PHYSICAL CHEMISTRY C 118, 8775	
	Frigeri, C; Bietti, S; Scaccabarozzi, A; Bergamaschini, R; Falub, C; Grillo, V; Bollani, M; Bonera, E;	
59	Niedermann, P; von Känel, H; Sanguinetti, S; Miglio, L.	0,604
~ ~ ~	A Structural Characterization of GaAs MBE Grown on Si Pillars.	
	ACTA PHYSICA POLONICA A 125, 986.	
60	Galli, A; Bonizzoni, L.	1,348

	True versus forged in the cultural heritage materials: the role of PXRF analysis.	
	X-RAY SPECTROMETRY - ISSN:0049-8246 vol. 43 (1).	
	Galli, A., Martini, M., Maspero, F., Sibilia. E.	
61	Surface dating of bricks, an application of luminescence techniques.	1,337
	European Physical Journal Plus, 129	
	Galli, S; Maspero, A; Giacobbe, C; Palmisano, G.; Nardo, L; Comotti, A ; Bassanetti, I; Sozzani, P ;	
()	Masciocchi, N.	4.229
62	When Long Bis (pyrazolates) Meet Late Transition Metals: Structure, Stability and Adsorption of MOFs Featuring Large Parallel Channels.	1,238
	JOURNAL OF MATERIALS CHEMISTRY A 2, 12208.	
	Gatti, E; Isa, F; Chrastina, D; Müller Gubler, E; Pezzoli, F; Grilli, E ; Isella, G.	
63	Ge/SiGe quantum wells on Si(111): Growth, structural, and optical properties.	2,185
e)	JOURNAL OF APPLIED PHYSICS 116, 043518.	2,105
	Gionco, C; Paganini, M; Giamello, E; Burgess, R; Di Valentin, C; Pacchioni, G.	
64	Cerium-doped zirconium dioxide, a visible-light-sensitive photoactive material of third generation.	6,687
•	THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS 5, 447.	, ,
	Giordano, L; Pacchioni, G; Noguera, C; Goniakowski, J.	
65	Identification of Active Sites in a Realistic Model of Strong Metal-Support Interaction Catalysts: The Case of	5 0 4 4
05	Platinum (111)-Supported Iron Oxide Film.	5,044
	CHEMCATCHEM 6, 185.	
	Giorgioni, A; Vitiello, E; Grilli, E; Guzzi, M ; Pezzoli, F.	
66	Valley-dependent spin polarization and long-lived electron spins in germanium.	3,515
	APPLIED PHYSICS LETTERS 105, 152404.	
-	Giovanella, U; Leone, G; Galeotti, F; Mróz, W; Meinardi, F ; Botta, C.	
67	FRET-Assisted Deep-Blue Electroluminescence in Intercalated Polymer Hybrids.	8,535
	CHEMISTRY OF MATERIALS 26, 4572.	
68	Grazianetti, C; Chiappe, D; Cinquanta, E; Tallarida, G; Fanciulli, M ; Molle, A. Exploring the morphological and electronic properties of 63ilicone superstructures.	2 5 2 8
00	APPLIED SURFACE SCIENCE 291, 109.	2,538
	Ha, N; Liu, X; Mano, T; Kuroda, T; Mitsuishi, K; Castellano, A; Sanguinetti, S ; Noda, T; Sakuma, Y; Sakoda, K.	
	Droplet epitaxial growth of highly symmetric quantum dots emitting at telecommunication wavelengths	
69	on InP(111)A.	3,515
	APPLIED PHYSICS LETTERS 104, 143106.	
	He, L; Fratesi, G; Brivio, G.	
70	Graphene magnetism induced by covalent adsorption of aromatic radicals	4,198
	PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 2210.	-
	Houssa, M; van den Broek, B; Scalise, E; Ealet, B; Pourtois, G; Chiappe, D; Cinquanta, E; Grazianetti, C;	
71	Fanciulli, M; Molle, A; Afanas'ev, VV; Stesmans, A.	2,538
<i>/</i> '	Theoretical aspects of graphene-like group IV semiconductors.	2,550
	APPLIED SURFACE SCIENCE 291, 98.	
	Kaden, W; Büchner, C; Lichtenstein, L; Stuckenholz, S; Ringleb, F; Heyde, M; Sterrer, M; Freund, H;	
72	Giordano, L; Pacchioni, G; Nelin, C; Bagus, P.	3,664
•	Understanding surface core-level shifts using the Auger parameter: A study of Pd atoms adsorbed on	
	ultrathin SiO 2 films, PHYSICAL REVIEW B 89, 115436.	

73	Khung, Y; Ngalim, S; Meda, L; Narducci, D. Preferential formation of Si-O-C over Si-C linkage upon thermal grafting on hydrogen-terminated silicon (111). CHEMISTRY-A EUROPEAN JOURNAL 20, 15151.	5,696
74	Kreiliger, T; Falub CV; Isa, F; Isella, G; Chrastina, G; Bergamaschini, R; Marzegalli, A; Kaufmann, R; Niedermann, P; Neels, A; Muller, E; Meduna, M; Dommann, A; Miglio, L ; von Kanel, H. Epitaxial Ge-crystal arrays for X-ray detection. JOURNAL OF INSTRUMENTATION 9, C03019.	1,526
75	Lamperti, A; Molle, A; Cianci, E; Wiemer, C; Spiga, S; Fanciulli, M . Effect on Al:MO2/Ino.53Gao.47As interface (M = Hf, Zr) of trimethyl-aluminum pre-treatment during atomic layer deposition. THIN SOLID FILMS 563, 44.	1,867
76	Lee, H; Pasta, M; Wang, R; Ruffo, R; Cui, Y. Effect of the alkali insertion ion on the electrochemical properties of nickel hexacyanoferrate electrodes. FARADAY DISCUSSIONS 176, 69.	4,194
77	Li, Z; Chen, HY; Schouteden, K; Lauwaet, K; Giordano, L ; Trioni, MI; Janssens, E; Iancu, V; Van Haesendonck, C; Lievens, P; Pacchioni, G. <i>Self-Doping of Ultrathin Insulating Films by Transition Metal Atoms.</i> PHYSICAL REVIEW LETTERS 112, 026102.	7,728
78	Lobello, M; Fantacci, S; Manfredi, N; Coluccini, C ; Abbotto, A ; Nazeeruddin, M; De Angelis, F. Design of Ru(II) sensitizers endowed by three anchoring units for adsorption mode and light harvesting optimization. THIN SOLID FILMS 560, 86.	1,867
79	Lorenzi, B; Frabboni, S; Gazzadi, G; Tonini, R; Ottaviani, G; Narducci, D. Nanovoid Formation and Dynamics in He+-Implanted Nanocrystalline Silicon. JOURNAL OF ELECTRONIC MATERIALS 43, 3852.	1,675
80	Lorenzi, B; Narducci, D ; Tonini, R; Frabboni, S; Gazzadi, G; Ottaviani, G; Neophytou, N; Zianni, X. Paradoxical Enhancement of the Power Factor of Polycrystalline Silicon as a Result of the Formation of Nanovoids. JOURNAL OF ELECTRONIC MATERIALS 43, 3812.	1,675
81	Lorenzi, R; Paleari, A ; Golubev, NV; Ignat'eva, ES; Sigaev, VN; Niederberger, M; Lauria, A. Non-aqueous sol–gel synthesis of hybrid rareearth-doped γ-Ga2O3 nanoparticles with multiple organic– inorganic-ionic light-emission features. JOURNAL OF MATERIALS CHEMISTRY C 3, 41.	4,696
82	Lotarev, SV; Lipatiev, AS; Golubev, NV; Ignat'eva, ES; Usmanova, LZ; Priseko, YuS; Lepekhin, NM; Paleari, A ; Sigaev, VN. Space-selective enhancement of blue photoluminescence in gallium germanosilicate glass through laser- induced nanostructuring. MATERIALS LETTERS 122, 174.	2,269
83	Manfredi, N; Bianchi, A; Causin, V; Ruffo, R; Simonutti, R; Abbotto, A. Electrolytes for quasi solid-state dye-sensitized solar cells based on block copolymers. JOURNAL OF POLYMER SCIENCE. PART A, POLYMER CHEMISTRY 52, 719.	3,245
84	Manfredi, N; Cecconi, B; Abbotto, A. Multi-Branched Multi-Anchoring Metal-Free Dyes for Dye-Sensitized Solar Cells. EUROPEAN JOURNAL OF ORGANIC CHEMISTRY 2014, 7069.	3,154

85	Mantovan, R; Vangelista, S; Kutrzeba-Kotowska, B; Lamperti, A; Manca, N; Pellegrino, L; Fanciulli, M. <i>Fe3-delta O4/MgO/Co magnetic tunnel junctions synthesized by full in situ atomic layer and chemical vapour deposition.</i> JOURNAL OF PHYSICS D 47, 102002.	2,521
86	Mantovan, R; Vangelista, S; Wiemer, C; Lamperti, A; Tallarida, G; Chikoidze, E; Dumont, Y; Fanciulli, M. Synthesis of multiferroic Er-Fe-O thin films by atomic layer and chemical vapor deposition. JOURNAL OF APPLIED PHYSICS 115, 17D907.	2,185
87	Martini, M ; Fasoli, M; Villa, I. Defect studies in quartz: Composite nature of the blue and UV emissions. NUCLEAR INSTRUMENTS & METHODS B 327, 15.	1,186
88	Meinardi, F ; Colombo, A; Velizhanin, KA; Simonutti, R ; Lorenzon, M; Beverina, L ; Viswanatha, R; Klimov, VI; Brovelli, S. Large-area luminescent solar concentrators based on 'Stokes-shift-engineered' nanocrystals in a mass- polymerized PMMA matrix. NATURE PHOTONICS 8, 392.	29,958
89	Mereu, R; Marchionna, S; Le Donne, A; Ciontea, L; Binetti, S ; Acciarri, M. ZnO:Al/i-ZnO bi-layers deposited on large substrates by pulsed D.C. magnetron sputtering for chalcogenide photovoltaics. CERAMICS INTERNATIONAL 40, 14595.	2,086
90	Mereu, R; Marchionna, S; Le Donne, A; Ciontea, L; Binetti, S ; Acciarri, M. Optical and electrical studies of transparent conductive AZO and ITO sputtered thin films for CIGS photovoltaics. PHYSICA STATUS SOLIDI C 11, 1464.	NA
91	Molholt, TE; Mantovan, R; Gunnlaugsson, HP; Svane, A; Masenda, H; Naidoo, D; Bharuth-Ram, K; Fanciulli, M ; Gislason, HP; Johnston, K; Langouche, G; Olafsson, S; Sielemann, R; Weyer, G. Interstitial Fe in MgO. JOURNAL OF APPLIED PHYSICS 115, 023508.	2,185
92	Mondiali, V; Bollani, M; Chrastina, D; Rubert, R; Chahine, G; Richard, M; Cecchi, S; Gagliano, L; Bonera, E; Schülli, T; Miglio, L. Strain release management in SiGe/Si films by substrate patterning. APPLIED PHYSICS LETTERS 105, 242103.	3,515
93	Monguzzi, A; Braga, D; Gandini, M; Holmberg, V; Kim, D; Sahu, A; Norris, D; Meinardi, F. Broadband up-conversion at subsolar irradiance: Triplet-triplet annihilation boosted by fluorescent semiconductor nanocrystals. NANO LETTERS 14, 6644.	12,94
94	Monguzzi, A; Meinardi, F. Second-Order Photochemical Upconversion in Organic Systems. JOURNAL OF PHYSICAL CHEMISTRY A 118, 1439.	2,775
95	Montalenti, F ; Salvalaglio, M; Marzegalli, A; Zaumseil, P; Capellini, G; Schülli, T; Schubert, M; Yamamoto, Y; Tillack, B; Schroeder, T. Fully coherent growth of Ge on free-standing Si(001) nanomesas. PHYSICAL REVIEW B 89, 014101.	3,664
96	Moretti, E; Talon, A; Storaro, L; Le Donne, A; Binetti, S ; Benedetti, A; Polizzi, S. Concentration quenching and photostability in Eu(dbm)3phen embedded in mesoporous silica	2,367

	nanoparticles.	
	JOURNAL OF LUMINESCENCE 146, 178.	
97	Moretti, F; Patton, G; Bleski, A; Fasoli, M; Vedda, A ; Trevisani, M; Bettinelli, M; Dujardin, C. Radioluminescence Sensitization in Scintillators and Phosphors: Trap Engineering and Modeling. JOURNAL OF PHYSICAL CHEMISTRY C 118, 9670.	4,835
98	Narducci, D ; Lorenzi, B; Zianni, X; Neophytou, N; Frabboni, S; Gazzadi, G; Roncaglia, A; Suriano, F. Enhancement of the power factor in two-phase silicon-boron nanocrystalline alloys. PHYSICA STATUS SOLIDI A, 211, 1255.	1,525
99	Neophytou, N; Zianni, X; Kosina, H; Frabboni, S; Lorenzi, B; Narducci, D. Power Factor Enhancement by Inhomogeneous Distribution of Dopants in Two-Phase Nanocrystalline Systems. JOURNAL OF ELECTRONIC MATERIALS 43, 1896.	1,675
100	Nicolini, T; Famulari, A; Gatti, T; Martí Rujas, J; Villafiorita Monteleone, F; Canesi, E; Meinardi, F ; Botta, C; Parisini, E; Meille, S; Bertarelli, C Structure–Photoluminescence Correlation for Two Crystalline Polymorphs of a Thiophene–Phenylene Co- Oligomer with Bulky Terminal Substituents. THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS 5, 2171.	6,687
101	Pacchioni, G. Ketonization of Carboxylic Acids in Biomass Conversion over TiO2 and ZrO2 Surfaces: A DFT Perspective. ACS CATALYSIS 4, 2874.	7,572
102	Pacchioni, G. Two-Dimensional Oxides and Their Role in Electron Transfer Mechanisms with Adsorbed Species. THE CHEMICAL RECORD 14, 910.	5,577
103	Pagonis, V; Chithambo, M; Chen, R; Chruścińska, A; Fasoli, M; Li, S; Martini, M ; Ramseyer, K. Thermal dependence of luminescence lifetimes and radioluminescence in quartz. JOURNAL OF LUMINESCENCE 145, 38.	2,367
104	Pal, J; Smerieri, M; Celasco, E; Savio, L; Vattuone, L; Ferrando, R; Tosoni, S; Giordano, L; Pacchioni, G ; Rocca, M. How Growing Conditions and Interfacial Oxygen Affect the Final Morphology of MgO/Ag(100) Films. JOURNAL OF PHYSICAL CHEMISTRY C 118, 26091.	4,835
105	Paleari, A ; Sigaev, V; Golubev, N; Ignat'eva, E; Bracco, S; Comotti, A ; Azarbod, A; Lorenzi, R. Crystallization of nanoheterogeneities in Ga-containing germanosilicate glass: Dielectric and refractive response changes. ACTA MATERIALIA 70, 19.	3,94
106	Paleari, S; Molle, A; Accetta, F; Lamperti, A; Cianci, E; Fanciulli, M. Electrically detected magnetic resonance study of the Ge dangling bonds at the Ge(111)/GeO2 interface after capping with Al2O3 layer. APPLIED SURFACE SCIENCE 291, 3.	2,538
107	Persano, L; Camposeo, A; Pisignano, D; Burini, A; Spearman, P; Tavazzi, S. Electron-beam nanopatterning and spectral modulation of organic molecular light-emitting single crystals LANGMUIR 30, 1643.	4,384
108	Pezzoli, F; Isa, F; Isella, G; Falub, CV; Kreiliger, T; Salvalaglio, M; Bergamaschini, R; Grilli, E; Guzzi, M ; von Kanel, H; Miglio, L. Ge Crystals on Si Show Their Light.	NA

	PHYSICAL REVIEW APPLIED 1, 044005.	
109	Pichler, A; Resel, R; Neuhold, A; Dingemans, T; Schwabegger, G; Moret, M ; Simbrunner, C; Salzmann I. Crystal structure determination of organic thin-films: the example of 2,2':6',2''-ternaphthalene. ZEITSCHRIFT FUR KRISTALLOGRAPHIE 229, 385.	1,255
110	Pinus, I; Catti, M ; Ruffo, R ; Salamone, M; Mari, C.M. Neutron Diffraction and Electrochemical Study of FeNb11O29/Li11FeNb11O29for Lithium Battery Anode Applications CHEMISTRY OF MATERIALS 26, 2203.	8,535
111	Prada, S; Giordano, L; Pacchioni, G. Nb-doped CaO: An efficient electron donor system. JOURNAL OF PHYSICS. :CONDENSED MATTER 26, 315004.	2,223
112	Prada, S; Giordano, L ; Pacchioni, G ; Noguera, C; Goniakowski, J. Properties of Pt-supported iron oxide ultra-thin films: Similarity of Hubbard-corrected and hybrid density functional theory description THE JOURNAL OF CHEMICAL PHYSICS 141, 144702.	3,122
113	Ribolini, A; Bini, M; Consoloni, I; Isola, I; Pappalardo, M; Zanchetta, G; Fucks, E; Panzeri, L; Martini, M ; Terrasi, F. <i>Late-pleistocene wedge structures along the patagonian coast (argentina): Chronological constraints and palaeo-environmental implications.</i> GEOGRAFISKA ANNALER A 96, 161.	1,564
114	Ros, I; Placido, T; Amendola, V; Marinzi, C; Manfredi, N; Comparelli, R; Striccoli, M; Agostiano, A; Abbotto, A ; Pedron, D; Pilot, R; Bozio, R. SERS Properties of Gold Nanorods at Resonance with Molecular, Transverse, and Longitudinal Plasmon Excitations. PLASMONICS 9, 581.	2,738
115	Rotta, D; Vellei, A; Mazzeo, G; Belli, M; Cocco, S; Tagliaferri, M; Crippa, A; Prati, E; Fanciulli, M. Spin-dependent recombination and single charge dynamics in silicon nanostructrures. THE EUROPEAN PHYSICAL JOURNAL PLUS 129, 121.	1,475
116	Russo, L; Battocchio, C; Secchi, V; Magnano, E; Nappini, S; Taraballi, F; Gabrielli, L; Comelli, F; Papagni, A ; Costa, B; Polzonetti, G; Nicotra, F; Natalello, A; Doglia, S; Cipolla, L. <i>Thiol–ene Mediated Neoglycosylation of Collagen Patches: A Preliminary Study.</i> LANGMUIR 30, 1336.	4,384
117	Saielli, G; Bagno, A; Castiglione, F; Simonutti, R ; Mauri, M; Mele, A. Understanding cage effects in Imidazolium ionic liquids by 129XE NMR: MD simulations and relativistic DFT calculations. JOURNAL OF PHYSICAL CHEMISTRY B 118, 13963.	3,377
118	Sala, EM; Bollani, M; Bietti, S; Fedorov, A; Esposito, L; Sanguinetti, S. Ordered array of Ga droplets on GaAs(001) by local anodic oxidation. JOURNAL OF VACUUM SCIENCE & TECHNOLOGY B 32, 061206.	1,358
119	Salamone, M; Sassi, M; Beverina, L; Mari, C; Ruffo, R. Investigation of redox activity in the napthalenediimide-poly(3,4- ethylenedioxythiophene) cross-linked polymers. ELECTROCHIMICA ACTA 140, 152.	4,086
120	Salvalaglio, M; Montalenti, F.	2,185

	Fine control of plastic and elastic relaxation in Ge/Si vertical heterostructures. JOURNAL OF APPLIED PHYSICS 116, 104306.	
121	Scaccabarozzi, A; Bietti, S; Fedorov, A; von Känel, H; Miglio, L ; Sanguinetti, S. Photoluminescence study of the strain relaxation of GaAs crystals grown on deeply patterned Si substrates. JOURNAL OF CRYSTAL GROWTH 401, 559.	1,693
122	Scalise, E; Houssa, M; Cinquanta, E; Grazianetti, C; van den Broek, B; Pourtois, G; Stesmans, A; Fanciulli , M ; Molle, A. Engineering the electronic properties of silicene by tuning the composition of MoX2 and GaX (X = S,Se,Te) chalchogenide templates. 2D MATERIALS, 1, 011010.	NA
123	Schlexer, P; Giordano, L; Pacchioni, G. Adsorption of Li, Na, K, and Mg Atoms on Amorphous and Crystalline Silica Bilayers on Ru(0001): A DFT Study. JOURNAL OF PHYSICAL CHEMISTRY C 118, 15884.	4,835
124	Scopece, D; Montalenti, F ; Bonera, E ; Bollani, M; Chrastina, D. Straining Ge bulk and nanomembranes for optoelectronic applications: a systematic numerical analysis. SEMICONDUCTOR SCIENCE AND TECHNOLOGY 29, 095012.	2,206
125	Scotti, R ; Conzatti, L; D'Arienzo , M; Di Credico, B; Giannini, L; Hanel, T; Stagnaro, P; Susanna, A; Tadiello, L; Morazzoni, F. Shape controlled spherical (oD) and rod-like (1D) silica nanoparticles in silica/styrene butadiene rubber nanocomposites: Role of the particle morphology on the filler reinforcing effect. POLYMER 55, 1497.	3,766
126	Sezen, H; Buchholz, M; Nefedov, A; Natzeck, C; Heissler, S; Di Valentin, C ; Wöll, C. Probing electrons in TiO2 polaronic trap states by IR-absorption: Evidence for the existence of hydrogenic states. SCIENTIFIC REPORTS 4, 03808.	5,078
127	Sforazzini, G; Kahnt, A; Wykes, M; Sprafke, J; Brovelli, S ; Montarnal, D; Meinardi, F; Cacialli, F; Beljonne, D; Albinsson, B; Anderson, H Synthesis and Photophysics of Coaxial Threaded Molecular Wires: Polyrotaxanes with Triarylamine Jackets. JOURNAL OF PHYSICAL CHEMISTRY C 118, 4553.	4,835
128	Shen, Y; Feng, X; Shi,Y; Vedda, A ; Moretti, F; Pan, Y. The radiation hardness of Pr:LuAG scintillating ceramics. CERAMICS INTERNATIONAL 40, 3715.	2,086
129	Sigaev, V; Golubev, N; Ignat'eva, E; Paleari, A ; Lorenzi, R. Light-emitting Ga-oxide nanocrystals in glass: a new paradigm for low-cost and robust UV-to-visible solar- blind converters and UV emitters. NANOSCALE 6, 1763.	6,739
130	Somaschini, C; Biermanns, A; Bietti, S; Bussone, G; Trampert, A; Sanguinetti, S ; Riechert, H; Pietsch, U; Geelhaar, L. Axial InAs/GaAs heterostructures on silicon in a nanowire geometry. NANOTECHNOLOGY 25, 485602.	3,672
131	Sosso, G; Colombo, J; Behler, J; Del Gado, E; Bernasconi, M. Dynamical heterogeneity in the supercooled liquid state of the phase change material GeTe.	3,377

	JOURNAL OF PHYSICAL CHEMISTRY B 118, 13621.	
132	Suriano, F; Ferri, M; Moscatelli, F; Mancarella, F; Belsito, L; Solmi, S; Roncaglia, A; Frabboni, S; Gazzadi, G; Narducci, D. Influence of Grain Size on the Thermoelectric Properties of Polycrystalline Silicon Nanowires. JOURNAL OF ELECTRONIC MATERIALS 44, 371.	1,675
133	Taboada, A; Kreiliger, T; Falub, C; Isa, F; Salvalaglio, M; Wewior, L; Fuster, D; Richter, M; Uccelli, E; Niedermann, P; Neels, A; Mancarella, F; Alen, B; Miglio, L ; Dommann, A; Isella, G; von Kanel, H. Strain relaxation of GaAs/Ge crystals on patterned Si substrates. APPLIED PHYSICS LETTERS 104, 022112.	3,515
134	Taddei, M; Costantino, F; Marmottini, F; Comotti, A ; Sozzani, P ; Vivani, R. The first route to highly stable crystalline microporous zirconium phosphonate metal–organic frameworks. CHEMICAL COMMUNICATIONS 50, 14831.	6,718
135	Tavazzi, S ; Camposeo, A; Pisignano, D; Silvestri, L. Molecular packing versus strength and effective mass of the emitting exciton of β-1,1,4,4-tetraphenyl-1,3- butadiene. JOURNAL OF PHYSICAL CHEMISTRY C 118, 8588.	4,835
136	Tavazzi, S ; Ferraro, L; Cozza, F; Pastori, V; Lecchi, M; Farris, S; Borghesi, A. Hydrogen peroxide mechanosynthesis in siloxane-hydrogel contact lenses. ACS APPLIED MATERIALS & INTERFACES 6, 19606.	5,9
137	Tosoni, S; Di Valentin, C; Pacchioni, G. Effect of alkali metals interstitial doping on structural and electronic properties of WO3. JOURNAL OF PHYSICAL CHEMISTRY C 118, 3000.	4,835
138	Uttiya, S; Miozzo, L; Fumagalli, E; Bergantin, S; Ruffo, R ; Parravicini, M; Papagni, A ; Moret, M ; Sassella, A . Connecting molecule oxidation to single crystal structural and charge transport properties in rubrene derivatives. JOURNAL OF MATERIALS CHEMISTRY C 2, 4147.	0,951
139	Vanacore, G; Hu, J; Liang, W; Bietti, S; Sanguinetti, S ; Zewail, A. Diffraction of quantum dots reveals nanoscale ultrafast energy localization. NANO LETTERS 14, 6148.	12,94
140	Vanacore, G; Zani, M; Bollani, M; Bonera, E ; Nicotra, G; Osmond, J; Capellini, G; Isella, G; Tagliaferri, A. Monitoring the kinetic evolution of self-assembled SiGe islands grown by Ge surface thermal diffusion from a local source. NANOTECHNOLOGY, 25, 135606.	3,672
141	Veronese, I; Mattia, C; Fasoli, M; Chiodini, N; Mones, E; Cantone, M; Vedda, A. Infrared luminescence for real time ionizing radiation detection. APPLIED PHYSICS LETTERS 105, 061103.	3,515
142	von Känel, H; Isa, F; Falub, CV; Barthazy, EJ; Müller, E; Chrastina, D; Isella, G; Kreiliger, T; Taboada, AG; Meduňa, M; Kaufmann, R; Neels, A; Dommann, A; Niedermann, P; Mancarella, F; Mauceri, M; Puglisi, M; Crippa, D; La Via, F; Anzalone, R; Piluso, N; Bergamaschini, R.Marzegalli, A; Miglio, L. <i>Three-dimensional EpitaxialSi1-xGex, Ge and SiC Crystals on Deeply Patterned Si substrates.</i> ECS TRANSACTIONS 64, 631.	NA
143	Wagner, A; Cröll, A; Gonik, M; Hillebrecht, H; Binetti, S ; Ledonne, A. Si1-xGex(x≥0.2) crystal growth in the absence of a crucible.	1,693

	JOURNAL OF CRYSTAL GROWTH 401, 762.	
	Wahba, L; D'Arienzo, M; Dirè, S; Donetti, R; Hanel, T; Morazzoni, F; Niederberger, M; Santo, N; Tadiello,	
	L; Scotti, R.	
144	A novel non-aqueous sol–gel route for the in situ synthesis of high loaded silica–rubber	4,151
	nanocomposites.	
	SOFT MATTER 10, 2234.	

COMMUNICATIONS AT CONFERENCES & SEMINARS

#	Authors	Title	Conference
1	Abhilash, R.; Lin, H.; Fratesi, G.; Brivio, GP.	Adsorption of pyridine on graphene (invited)	XIX ETSF Workshop on Electronic Excitations. Zaragoza (Spain)
2	Acciarri, M; Le Donne, A; Mereu, R; Garattini, P; Falcone, M; Marchionna, S; Meschia, M; Moneta, R; Gasparotto, A; Binetti, S.	Cu(In,Ga)Se2 Solar Cells on Flexible Substrate Fabricated by an Innovative Roll to Roll Hybrid Sputtering and Evaporation Process (invited)	29th European Photovoltaic Solar Energy Conference and Exhibition. Paris (France)
3	Asnaghi, D; Sormani, G; Piga, D; Denaro, F; Beretta, M; Comotti, A ; Bracco, S; Sozzani, P.	Polymerization in Nanoporous Materials (invited)	ISMAC Workshop "Catalytic Olefin Polymerization and High Performance Materials" Milano
4	Baby, A; Fratesi, G; Floreano, L; Brivio, GP.	Molecular adsorption of pentacene on Aluminum (001) (invited)	Workshop on Surfaces, Interfaces and Functionalization Processes in Organic Compounds and Applications - SINFO II - Trieste
5	Basiricò, L; Ciavatti, A; Grande, S; Raimondo, L; Trabattoni, S; Sassella, A ; Braga, D; Campione, M; Fraboni, B.	Optoelectronic characterization of highly oriented rubrene crystalline thin films (invited)	10th International Conference on Organic Electronics (ICOE) Modena
6	Bernasconi, M.	Molecular Dynamics Simulation of the Crystallization Kinetics of Phase Change Materials for Data Storage	Cecam Workshop on "Molecular Simulations of Crystallization from Solution" Lugano (Switzerland)
7	Bernasconi, M.	Neural Network Simulation of Phase Change Materials: Handling Large Models with DFT Accuracy. (invited)	CIMTEC 2014 - 13th International Conference on Modern Materials and Technologies – 6th Forum on new Material.Montecatini Terme
8	Bernasconi, M.	Atomistic simulations of phase change materials for data storage	Congresso Nazionale della Società Italiana di Fisica, Pisa
9	Bernasconi, M.	Thermal transport in phase change materials (invited)	International Workshop on Characterization and Modeling of Memory Devices. Micron Semiconductors Italy
10	Bernasconi, M.	Tutorial of Symposium HH: Atomistic simulations of structural and functional properties of phase change materials (invited)	Materials Reserach Society Spring Meeting- Symposium HH: Phase-Change Materials From Basic Properties to Applications San Francisco, CA (USA)
11	Bernasconi, M ; Sosso, GC; Gabardi, S; Caravati, S; Colombo, J; Del Gado, E; Behler, J; Parrinello, M.	Fragility, dynamical heterogeneity, crystallization kinetics and structural relaxation of the phase change compound GeTe from large scale molecular dynamics simulations (invited)	Materials Research Society Fall Meeting Boston (USA)

12	Bietti, S.	Droplet Epitaxy Growth of Nanostructures on Patterned and (111) Substrates (invited)	10th International Workshop on Epitaxial Semiconductors on Patterned Substrates and Novel Index Surfaces (ESPS-NIS) Traunkirchen (Austria)
13	Bietti, S.	Droplet epitaxy nanostructures for device applications (invited)	5th International Conference on NANO- structures SElf-Assembly (NANOSEA 2014), Marseille (France)
14	Bietti, S.	Droplet Epitaxy and applications (invited)	Materiaux et applications aux dispositifs et capteurs - MADICA 2014 Mahdia (Tunisie)
15	Bietti, S ; Esposito, L; Scaccabarozzi, A; Fedorov, A; Sanguinetti, S.	Size control of GaAs quantum dots grown by droplet epitaxy for device applications .(invited)	MBE International Conference on Molecular Beam Epitaxy - September 7-12 Flagstaff, Arizona (USA)
16	Bietti, S ; Tiburzi, G; Esposito, L; Fedorov, A; Sanguinetti, S.	Size Dispersion Control of GaAs Quantum Dots Grown by Droplet Epitaxy. (invited)	18th International Conference on Molecular Beam Epitaxy (MBE 2014).Flagstaff (USA)
17	Binetti , S ; P. Garattini, S. Tombolato, R. Mereu, A. Le Donne, M. Acciarri , S. Marchionna, M. Meschia	Chalcogenide thin film solar cells on flexible substrates. (invited)	Congresso Nazionale della Società Chimica Italiana.Arcavacata di Rende (Cosenza)
18	Binetti S. , Gonik M, Le Donne A. , Croel A.	"Silicon sample for PV application grown under reduced melt convection".(invited)	E- MRS Spring Meeting 2014. Lille (France).
19	Binetti, S; Acciarri, M ; Meschia, M; Gasparotto, A.	Cu(In,Ga)Se2 solar cells fabricated by an innovative roll to roll hybrid sputtering and evaporation process. .(invited)	Bilateral activities between CNR (Italian National Research Center) and CAS (Chinese Academy of Science) on CIGS-based thin film solar cells - CNR-CAS Joint workshop, IMEM-CNR.Parma
20	Binetti, S; Catti, M.	La Scienza dei Materiali per la scuola secondaria: interdisciplinarietà del progetto PLS .(invited)	Smart Education & Tecnology Days - 3 giorni per la scuola" - XII edizione.Napoli.
21	Bonera, E	Group IV membranes.(invited)	Epioptics-13.Erice.
22	Bonfiglio, G; Caroselli, M; Martini, M; Sibilia, E. et al.	Datazione assoluta e caratterizzazione di laterizi e malte dal sito UNESCO di Modena	100° Congresso SIF, PISA
23	Bracco, S; Comotti, A ; Beretta, M; Sozzani, P.	Modulation of Rotor Dynamics and Recognition of Host-Guest Interactions in Highly Porous Materials. (invited)	GIDRM Gruppo Italiano Discussione Risonanze Magneticge National Congress.Bari.
24	Bracco, S; Comotti, A ; Beretta, M; Sozzani, P.	Materiali ad alta porosità come nano- reattori per polimerizzazioni. (invited)	XXI Convegno Italiano di Scienza delle Macromolecole. Torino.
25	Colombo, A; Simonutti, R.	Polymer based nanocomposites with tailorable optical properties (invited)	SPIE NANOPHOTONICS Materials XI San Diego (USA).
26	Comotti, A.	Porous Materials for the Manipulation of Gases, Vapors and Polymers: Synthesis, Structural Characterization and Rotor Dynamic. (invited)	Seminario, Università degli Studi di Roma "Tor Vergata".Roma.
27	Comotti, A ; Bracco, S; Beretta, M; Sozzani, P.	Confined Polymerization in highly Porous Frameworks to Construct Novel Polymeric Architectures and	EUPOC Precision Polymers: Synthesis, Folding and Function - May 25 - 29. Gargnano, Lago di Garda (BS).

		Morphological Replica. (invited)	
28	Comotti, A; Bracco, S; Sozzani, P.	Hybrid Porous Materials for the Manipulation of Gases, Vapors and Polymers: Structural Characterization and Rotor Dynamics. (invited)	Joint AIC-SILS Conference. Firenze.
29	Comotti, A; Bracco, S; Sozzani, P.	Porous organic materials to fabricate polymer architectures and fast rotors modulated by vapors	Mof - International Conference on Metal Organic Frameworks & Open Framework Compounds - September 28/October 1. Kobe (Japan)
30	Costantino, F; Taddei, M; Marmottini, F; Vivani, R; Comotti, A ; Cohen, SM.	New structural archetypes in zirconium phosphonates chemistry: first routes towards open framework compounds	Joint AIC-SILS Conference. Firenze
31	De Mattia, C; Mones, E; Veronese, I; Fasoli, M; Chiodini,N ; Cantone, MC.; Vedda, A.	Recent progresses in scintillating doped silica fiber optics	SPIE Conference on Hard X-Ray, Gamma-Ray and Neutron Detector Physics XVI. San Diego(USA).
32	Di Valentin, C.	Modelling doped graphene for the electrocatalysis of the oxygen reduction reaction (ORR)	China-Italy Bilateral Symposium on Graphene, 2014.Dalian (China)
33	Di Valentin, C.	Modelling photoinduced redox processes in the bulk and at the surface of TiO2	Materials Challenges in Devices for Fuel Solar Production and Employment.ICTP/SISSA Trieste.
34	Fasoli, M.	Looking at the bright side of defects	EURODIM 2014, Canterbury (UK)
35	Fasoli, M.	Band gap engineering in garnets	WGMCS-1 Shangai (Cina)
36	Fasoli, M., Cantone M. C. , Chiodini N. , C. De Mattia, E. Mones, I. Veronese, Vedda A.	Scintillating fibers for in-vivo radiation dosimetry	E-MRS 2014 Varsavia (Polonia)
37	Fasoli M., Martini M.	Detailed investigation of natural and synthetic quartz luminescence	SiO ₂ 2014 Cagliari
38	Fasoli M., Martini M.	The composite nature of the thermoluminescence UV emission in quartz	LED 2014 Montreal (Canada)
39	Fratesi, G; Motta, C; Trioni, MI; Brivio, GP ; Sanchez-Portal, D.	Resonant Lifetime of Core Excited Organic Adsorbates from First Principles	Worshop on Dynamical Phenomena at Surfaces (WDPS16). Madrid (Spain).
40	Fratesi, G; Motta, C; Trioni, MI; Sanchez Portal, D; Brivio, G.	Fast electron transfer at molecule- substrate interfaces (invited)	American Physical Society March Meeting Denver (USA).
41	Gagliano, L; Rossetto, L; Scopece, D; Mondiali, V; Lodari, M; Giorgioni, A; Pezzoli, F; Bollani, M; Chrastina, D; Montalenti, F; Bonera, E.	Local uniaxial tensile deformation of germanium up to the 4% threshold by epitaxial nanostructures. (invited)	European Material Research Society Fall Meeting Warsaw (Poland).
42	Galli, A; Martini,, M; Sibilia, E; Maspero, F.	Datazione di superfici di laterizi antichi con al tecnica di "surface dating"	100° Congresso SIF Pisa
43	Galli, S; Maspero, A; Giacobbe, C; Palmisano, G.; Masciocchi, N; Comotti, A ; Bassanetti, I; Sozzani, P.	Long Bis(pyrazolates) Meet Transition Metals: Structural Features, Stability and Adsorption Performances of MOFs Featuring Large Parallel	Joint AIC-SILS Conference - 15/18 September.Florence.

		Channels. (invited)	
44	Giordano, L, Prada, S; Pacchioni, G.	Charging phenomena on doped wide-gap oxides: identifying the key parameters by DFT calculations.	9th International Workshop on Oxide Surfaces (IWOX-IX).Tahoe City, California (USA).
45	Giorgioni, A; Vitiello, E; Grilli, E ; Bonera, E; Guzzi, M ; Pezzoli, F.	Addressing spin-optoelectronic properties of Ge by polarization and time-resolved PL investigations	European Material Research Society 2014 Fall Meeting - 16/19 September.Warsaw (Poland).
46	Golubev, NV; Ignat'eva, ES; Sigaev, VN; Paleari, A ; Lorenzi, R.	Nanostructured gallium germanosilicate glasses: light emission spectroscopy and applications	Наука будущего - Science of the future.St. Petersburg (Russia).
47	Guibert P., Bailiff I., Blain S., Bouvier A., Chauvin A., Dufresne Ph., Gueli A., Lanos Ph., Martini M. , Prigent D., Sapin Chr., Sibilia E. , Troja O.	L'apport des methodes de datation physique à la caractèrisation et à la datation de matériaux de construction et de structures architecturales : un bilan et des perspectives.	The Archaeology of Buildings in Perspective. How to Better Understand, Preserve and Restore Buildings, Lion
48	Lin, H; Fratesi, G; LIN, H; Brivio, GP.	Graphene magnetism induced by aromatic molecule adsorption	XIX ETSF Workshop on Electronic Excitations.Zaragoza (Spain).
49	Lorenzi, R ; Brovelli, S ; Meinardi, F; Paleari, A.	Band-to-Band Excitation and Decay in SiO2 – Can We Get Evidences of such a Path? (invited)	SiO2 2014, Advanced Dielectrics and Related Devices.Cagliari .
50	Lorenzi, R; Sigaev, V; Golubev, N; Ignat'eva, E; Azarbod, A; Paleari, A.	Blue-emitting Ga2O3 QDs in glass for solar-blind UV-converters	International Conference on Quantum Dots (QD 2014).Pisa
51	Marchiò, L; Bassanetti, I; Atzeri, C; Comotti, A; Sozzani, P.	Sorption Properties of Silver Coordination Polymers with Bis(pyrazolyl)methane Ligands	IUCr - Congress and General Assembly of the International union of Crystallography Montreal, Québec (Canada).
52	Marzegalli, A.	Understanding complex dislocation behavior and reactions in advanced GeSi epitaxy	E-MRS European Materials Research Society Fall Meeting. Warsaw (Poland).
53	Mereu, RA; Le Donne, A; Binetti, S ; Acciarri, M.	Studies of the Zn2SnO4 and InxSy as Alternative Buffer Layers Deposited via R.F. Sputtering for Chalcogenide Photovoltaics	29th European Photovoltaic Solar Energy Conference and Exhibition. Paris (France).
54	Miglio, L; Bergamaschini, R; Bietti, S; Bonera, E; Grilli, E; Guzzi, M; Marzegalli, A; Montalenti, F; Pezzoli, F; Salvalaglio, M; Sanguinetti, S; et al.	Epitaxial self-assembly of 3-D semiconductor structures on deeply patterned Si substrates at the microscale	International conference on quantum dots (QD-2014).Pisa.
55	Monguzzi, A.	Low Power Photon Up-Conversion in Multicomponent Organic Systems: Photophysics and Materials.	1st CMS International Symposium Fukuoka (Japan).
56	Monguzzi, A.	Low Power Photon Up-Conversion in Multicomponent Organic Systems: Photophysics and Materials	ISECM 201, 2nd International Symposium on Energy Challenges and Mechanics. Aberdeen (Scotland).
57	Montalenti, F; Salvalaglio, M; Marzegalli, A; Zaumseil, P; Capellini, G; Schülli, T; Schubert,	Si CMOS compatible, compliant integration of lattice-mismatched semiconductors on Si(001): Example of	7th International Silicon-Germanium Technology and Device Meeting, ISTDM 2014. Singapore

	M; Yamamoto, Y; Tillack, B; Schroeder, T.	fully coherent Ge/Si nanostructures	
58	Moret, M ; Zolotarev, PN; Proserpio, D.M.	To cleave or not to cleave: topological analysis of organic crystal structures	Second joint AIC-SILS Conference - 15/18 september. Firenze
59	Moretti, F; Patton,G; Belsky, A; Fasoli, M; Vedda, A ; Trevisani, M; Bettinelli, M; Dujardin, C.	Trap Engineering Approach for a Theory of X-ray Induced Memory Effects in Scintillators and Phosphors	Eurodim 2014. University of Kent - Canterbury (UK)
60	Pacchioni, G.	Two-dimensional oxides: from microelectronics to nanocatalysis	14e Rencontre des Chimistes Théoriciens Francophones. Paris (France).
61	Pacchioni, G.	Third generation photocatlysts: Ce- doped ZrO2	247th American Chemical Society Meeting - Surface and catalytic reactions for energy efficiency. Dallas (Texas, USA)
62	Pacchioni, G.	Strategies to induce charge transfer to supported Au clusters on oxide surfaces	American Chemical Society Meeting - Clusters in catalysis. Dallas (Texas, USA).
63	Pacchioni, G.	From second to third generation of photocatalysts: Ce-doped ZrO2	Chalmers annual materials science initiative: Materials for tomorrow. Goteborg (Svezia).
64	Pacchioni, G.	Modern electronic structure approaches for heterogeneous catalysis	Eni S.p.A. Division Refining & Marketing - Centro Ricerche. San Donato Milanese.
65	Pacchioni, G.	Two-dimensional oxides: new structures, new functions, and new materials	Institute of Materials Science. EPFL, Lausanne (Switzerland).
66	Pacchioni, G.	Strategies to induce charge transfer to supported Au clusters on oxide surfaces	Workshop Cluster Surface Interaction 2014 Villa Cagnola (Varese)
67	Pacchioni, G.	WO3 and ZrO2 in photocatalysis: hints from DFT	XXV Congresso Nazionale della Società Chimica Italiana. Arcavacata di Rende (Cosenza).
68	Paleari, A ; Sigaev, V; Golubev, N; Ignat'eva, E; Lauria, A; Azarbod, A; Lorenzi, R.	Phase changes and ripening of Ga-oxide QDs in solid host . (invited)	International Conference on Quantum Dots (QD 2014). Pisa.
69	Zolotarev P.; Moret M., Proserpio D., Blatov V.	Search for the cleavable organic crystals: topological and energetic aspects	International scientific conference "Science of the Future". St. Petersburg, Russia.
70	Raimondo, L; Trabattoni, S; Campione, M; Braga, D; Holmberg, VC; Norris, D; Moret, M ; Ciavatti, A; Fraboni, B; Sassella, A .	Growth and FET integration of free- standing crystalline rubrene thin films	International Conference on Synthetic Metals (ICSM 2014). Turku (Finland).
71	Ruffo, R; Mari, CM ; Salamone, MM; Longoni, G.	Investigation of NaxMno.5Feo.5O2 Cathode Materials from Low Cost Preparation Routes. (invited)	IMLB 2014 17th International Meeting on Lithium Ion Batteries. Como.
72	S.Binetti, P. Garattini, R. Mereu , A. Le Donne, S. Marchionna, M. Meschia, A. Gasparotto, M. Acciarri.	"Cu(In, Ga) Se2 solar cells on flexible substrate fabricated by an innovative roll to roll hybrid sputtering and evaporation process"	E- MRS Spring Meeting. Lille (France).
73	Sassella, A ; Bussetti,G, Campione, M; Riva, A; et al.	Stable alignment of tautomers at room temperature in porphyrin 2-D layers	International Conference on Synthetic Metals (ICSM 2014). Turku (Finland).
74	Sozzani, P.	Peptide-based Porous Architectures and Covalent Frameworks for Guest Manipulation	Supra Nanomed - From Supramolecular Architectures to Nanomedicine 'Beyond the Molecule' . Università degli Studi di Milano - Bicocca, Milano.

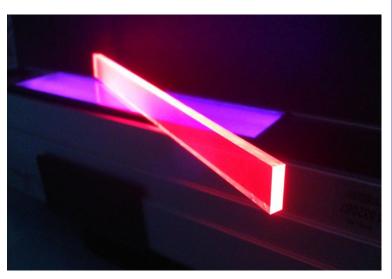
75	Sozzani, P; Comotti, A; Bracco, S; Beretta, M.	High surface area porous hyper- crosslinked polymers and hybrid materials: in-situ polymerization and guest-modulated rotor dynamics	POLYSOLVAT- International IUPAC Conference in Polymer-Solvent Complexes & Intercalates. Salerno.
76	Tombolato, S; Colombo, A; Acciarri, MF ; Boshta, M; Binetti, S.O.	Cu2ZnSnS4 Thin Film Solar Cells Produced by Thiourea Complexes Suspension	European PV Solar Energy Conference and Exhibition. Amsterdam (The Nederlands)
77	Trabattoni, S; Raimondo, L; Campione, M; Braga, D; Holmberg, VC; Norris, DJ; Moret, M ; Ciavatti, A; Fraboni, B; Sassella, A.	Growth and device integration of millimeter-sized rubrene films with single crystals quality	ICOE International Conference on Organic Electronics. Modena.
78	Vedda, A.	Influence of defects and traps in the scintillation process	QUANTARM 2014 - International Conference and Workshop Quanta and Matter: Yerevan–Tsaghkadzor (Armenia).
79	Vedda, A.	Governing the incorporation of rare earth ions in sol-gel silica: from microscopic mechanisms of nano-cluster formation to the realization of scintillating optical fibres. (invited)	QUANTARM 2014 - International Conference and Workshop Quanta and Matter: Yerevan–Tsaghkadzor (Armenia).
80	Vedda, A.	Multifunctional role of rare-earth doping in nanosized Hf-based phosphors	Workshop on complex luminescence phenomena in inorganic materials. Erice (Trapani).
81	Vedda, A ; Dell'Orto, E; Fasoli, M; Moretti, F; Shen,Y; Liu,S; Wu, L;Shi, Y; Feng, X; Pan,Y.	Detection and control of local structural disorder indello rare-earth doped Lu3Al5O12 optical ceramics	EURODIM 2014. University of Kent - Canterbury (UK)
82	Villa, I; Lauria, A; Fasoli, M; Niederberger, M; Vedda, A.	Investigation of HfO2 nanoparticles intrinsic luminescence	Eurodim 2014. University of Kent - Canterbury (UK).

PHD THESIS

V. KUMAR	Few layer graphene reinforced rubber compounds for tires	
S. PRADA	Enhancing oxide surface reactivity by doping or nano-structuring	
A. GIORGIONI	Spin physics of Ge-based heterostructures	
S. PALEARI	Characterization of defects at the interface between germanium and oxides by electrically detected magnetic resonance and admittance spectroscopy	
S. BERGANTIN	Organic semiconductor rubrene: crystal chemistry of derivatives and high-pressure polymorphism	
C. GRAZIANETTI	Scanning tunneling microscopy investigation of III-V compound semiconductors and novel 2D nanolattices	
V. LEANDRI	Organic materials for dye-sensitized solar cells	
M. REZA GHAANI	Study of new materials and their functionality for hydrogen storage and other energy applications	
F. CARONE FABIANI Adsorbption and scattering phenomena in materials science		

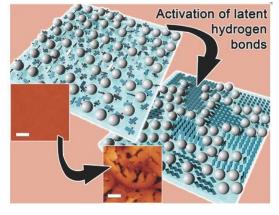
Meinardi, F; Colombo, A; Velizhanin, KA; **Simonutti, R**; Lorenzon, M; **Beverina, L**; Viswanatha, R; Klimov, VI; **Brovelli, S**, *Large-area luminescent solar concentrators based on* '*Stokes-shift-engineered' nanocrystals in a mass-polymerized PMMA matrix*, NATURE PHOTONICS 8, 392 (2014).

Luminescent solar concentrators (LSCs) cost-effective are complements to semiconductor photovoltaic (PV) systems that can both boost the power output of standalone solar cells and allow for integration of PV-active architectural elements into buildings in the form of, for example, semi-transparent PV windows. In this work, scientists of our Department (Meinardi, Colombo, Simonutti, Lorenzon, Beverina, and Brovelli) in collaboration with the Los Alamos National Laboratory in New Mexico (USA) used "Stokes-shiftengineered" CdSe/CdS core/shell colloidal quantum dots (QDs) with especially thick shells to realize the first LSCs without any losses to re-absorption for optical paths as long as tens of centimeters.



These novel devices (see picture) were obtained using high-optical-quality QD polymethylmethacrylate (PMMA) composites fabricated by a modified version of a common industrial cell-casting synthesis adjusted in such a way as to minimize harmful interactions of the QDs with radical polymerization initiators. The use of this new fairly gentle procedure together with the robustness of thick-shell QDs, in which emitting core-localized excitons are isolated from the environment, preserved the QD light emitting properties completely intact upon incorporation into PMMA. The studies of these prototype LSC devices yield optical quantum efficiencies of more than 10% per absorbed photon. Following its publication in Nature Photonics, this study was highlighted by over 200 newspapers and web-magazines worldwide, as well as in dedicated TV and radio interviews.

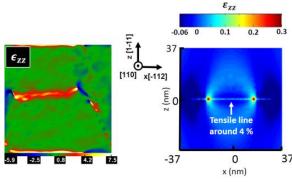
Bruni, F; Sassi, M; Campione, M; Giovanella, U; **Ruffo, R;** Luzzati, S; **Meinardi, F; Beverina, L; Brovelli, S**, *Post-deposition Activation of Latent Hydrogen-Bonding: A New Paradigm for Enhancing the Performances of Bulk Heterojunction Solar Cells,* ADVANCED FUNCTIONAL MATERIALS 24, 7410 (2014).



This study, published as cover article in *Advanced Functional Materials*, demonstrated a new paradigm for fine tuning of the nanoscale connectivity of organic bulk heterojunction solar cells based on the post-deposition exploitation of latent hydrogen bonding. Through this approach, scientists of our Department (Bruni, Sassi, Ruffo, Meinardi, Beverina, and Brovelli), in collaboration with the ISMac-CNR Institute in Milano, achieved over 20 fold enhancement of the device power conversion efficiency. The strategy can be readily extended to many conjugated organic systems for achieving highly efficient small-molecule solar cells.

Conesa-Boj, S; Boioli, F; Russo-Averchi, E; Dunand, S; Heiss, M; Ruffer, D; Wyrsch, N; Ballif, C; **Miglio, L;** Morral, AF, *Plastic and Elastic Strain Fields in GaAs/Si Core-Shell Nanowires,* NANO LETTERS 14, 1859 (2014).

Thanks to their unique morphology, nanowires have enabled integration of materials in a way that was not possible before with thin film technology. In turn, this opens new avenues for applications in the areas of energy harvesting, electronics, and optoelectronics. This is particularly true for axial heterostructures, while core-shell systems are limited by the



appearance of strain-induced dislocations.

Even more challenging is the detection and understanding of these defects. We combine geometrical phase analysis with finite element strain simulations to quantify and determine the origin of the lattice distortion in core-shell nanowire structures. Such combination provides a powerful insight in the origin and characteristics of edge dislocations in such systems and quantifies their impact with the strain field map. We apply the method to heterostructures presenting single and mixed crystalline phase. Mixing crystalline phases

along a nanowire turns out to be beneficial for reducing strain in mismatched core-shell structures.

Vanacore, G; Hu, J; Liang, W; Bietti, S; **Sanguinetti, S**; Zewail, A, *Diffraction of quantum dots reveals nanoscale ultrafast energy localization,* NANO LETTERS 14, 6148 (2014).

Unlike in bulk materials, energy transport in low-dimensional and nanoscale systems may be governed by a coherent 'ballistic' behavior of lattice vibrations, the phonons. If dominant, such behavior would determine the mechanism for transport and relaxation in various energy-conversion applications. In the study published in Nano Letters by the Nobel Prize in Chemistry Ahmed H. Zewail (CalTech) in collaboration with the group of Prof. Stefano Sanguinetti (our department), who developed the materials used in this study, the lattice dynamics in nano-scale quantum dots of gallium arsenide was studied in time and space using ultrafast electron diffraction. When the dot size is smaller than the inelastic phonon meanfree path, the energy remains localized in high-energy acoustic modes which travel coherently within the dot. As the dot size increases, an



energy dissipation toward low-energy phonons takes place, and the transport becomes diffusive. These results are fundamental for the understanding of energy conversion in nano-scale materials, and for the control of properties involving thermal conductivity and optical design. See also: "Quantum-dot per la generazione elettrica del futuro", Smart City, Voci e luoghi dell'innovazione (http://www.radio24.ilsole24ore.com/programma/smart-city/mercoledidicembre-101014-gSLAxOVsp)

Comotti, A; Bracco, S;Ben, T; Qiu, S; **Sozzani, P**, *Molecular Rotors in Porous Organic Frameworks*. ANGEWANDTE CHEMIE 53, 1043 (2014).



Porous organic frameworks exhibit ultra-fast molecular rotors (10^8 Hz at RT) in their architectures, resulting in a dynamic material whose motion can be frozen or released at will. In fact, the rotational motion can be actively regulated in response to guests. As the temperature is increased, the rotors spin ever faster, approaching free-rotational diffusion at 550 K. The unusual combination of remarkable nanoporosity with fast dynamics is intriguing for engineering oscillating dipoles and producing responsive materials with switchable ferroelectricity, and for applications spanning from sensors to actuators, which capture and release chemicals on command.

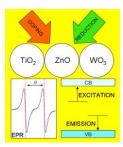
Para-phenylene rings ...

De Angelis, F; **Di Valentin, C**; Fantacci, S; Vittadini, A; Selloni, A, *Theoretical studies on anatase and less common TiO2 phases: Bulk, surfaces, and nanomaterials,* CHEMICAL REVIEWS 114, 9708 (2014).



Titanium dioxide is a very popular semiconducting oxides which is applied in a wide variety of technological fields. In this review we present a survey of the theoretical studies on the stability, reactivity, electronic and structural properties of anatase and other less common TiO_2 phases. Since sensitization and nanostructuring play a crucial role in most of the application, the review spans from bulk to surfaces, to two-dimensional systems, to nanoparticles. The evolution of modern computing has largely expanded the scope of first-principles calculations which now provide an accurate description of systems of few nanometers size.

Di Valentin, C; **Pacchioni, G**, Spectroscopic properties of doped and defective semiconducting oxides from hybrid density functional calculations, ACCOUNTS OF CHEMICAL RESEARCH 47, 3233 (2014).



Very rarely metal oxides are used in their pure and fully stoichiometric form. On the contrary, in most of the applications, ranging from catalysis to electronic devices, they are either doped or made defective (e.g. oxygen deficient) because interesting chemical, electronic, optical and magnetic properties arise only when foreign components or defects are introduced in the lattice. For this reason an enormous effort is devoted to the understanding of the physical and chemical properties of doped oxides. This review shows how the direct comparison between spectroscopic experimental and computational data allow one to acquire a deep understanding and control of these complex systems.

Beverina, L; Pagani, G, *π*-conjugated zwitterions as paradigm of donor-acceptor building blocks in organic-based materials, ACCOUNTS OF CHEMICAL RESEARCH 47, 319 (2014).

The very peculiar characteristics of zwitterions, as well as a clear and unambiguous definition, have been overlooked in past literature. However, these compounds are particularly important in view of the impact they have had in the recent past and will likely continue to have in the future as components of performing functional organic and hybrid materials. In this Account, authors primarily aim to define critically important organic concepts of zwitterions regarding both their design and nomenclature.



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COORDINATOR	PROJECT	FUNDED BY
A. ABBOTTO	A. ABBOTTO Dispositivi Solari a Coloranti di Nuova Generazione: Sensibilizzatori e Conduttori Nano-Ingegnerizzati (DSSCX)	
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	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-generation energy devices		EU
S. BROVELLI Electronic Doped Colloidal Nanocrystal Heterostructures for transformational Breakthrought in solid-state lighting		EU
A. COMOTTI Meccanismi di attivazione della CO2 per la progettazione di nuovi materiali per l'efficienza dell'energia e delle risorse		MIUR
	Nuovi materiali fotocatalitici per la conversione di energia solare basati su eterogiunzioni	Cariplo
C. DI VALENTIN	Oltre il grafene: strati di carbonio nanostrutturati disegnati su misura per ottenere nuovi materiali per la catalisi e la chimica sostenibile	MIUR
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S. SANGUINETTI	FemToTera- Plasmon-enhanced Tera-Hertz emission by Femtosecond laser pulses of nanostructured semiconductor/metal surfaces	Regione Lombardia
	COSMOS	Cariplo
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Indagini strutturali: Misure di diffrazione di raggi X da cristallo singolo

Research Facilities



CUDAM, CENTRO UNIVERSITARIO DATAZIONI 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 ($\sim 5 \text{ nm}$) 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 nonconductive 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 description: VEGA TS 5136XM variable pressure $(5 \times 10^{-3} - 500 \text{ Pa})$. 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).

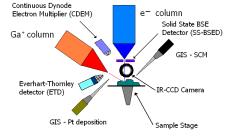
The FIB/SEM Quanta 3-D provides further options, e.g.:

• 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.







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 candidate offers the national business community support in research and development of new materials and technologies for PV application. The Centre presently counts about 25 members.

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 PV small and medium devices with full investigation of PV and stability properties.

Lab facilities:

a) preparation and full characterization of materials for DSC and CIGS solar cells;

b) fully equipped laboratories for organic and organometallic synthesis and characterization;

c) fully equipped laboratories for optical and electrochemical investigation;

d) main facilities for the preparation of DSC and CIGS cells and panels (sputtering system, nitrogen and argon filled glove box, laser scribing machine, titanium hotplates, screen printers, UV-ozone cleaners

e) main facilities for the full characterization of DSC and CIGS devices (solar simulators up to 6×6 inches, I/V characterization, internal and external quantum efficiency, light soaking chamber for cell ageing, stability studies, electrochemical impedance spectrometer)

DELTATI RESEARCH



In 2011 the University of Milano-Bicocca and ERG SpA gave birth to DeltaTi Research, a consortium entirely funded by ERG and aimed at the

development of nanostructured silicon-based thermoelectric generators. Thermoelectric conversion, although known since 1821, has found limited industrial exploitations because of the relatively low conversion yield it enables and of the high material costs. In spite of the technological limitations, recovering low-enthalpy heat would disclose unpaired opportunities to generate electric power out of thermal waste available both at civil and industrial facilities – further to improve the efficiency of thermal engines.

Based upon a new technological approach developed at the Department of Materials Science and protected by seven international patents, silicon nanostructures might be considered for industrial-scale production of low-cost, high-efficiency generators that will be used both for bulk electric generation and for power microgeneration.

The Consortium R&D activity currently involves, along with the University of Milano-Bicocca as research leader, two CNR institutes, the Universities of Modena, Naples, and Vienna, the Fondazione Bruno Kessler, the Demokritos Research Center, and Altran as a technological consultant.



The company, established in September 2012 and spin-off of the University of Milano Bicocca from the very beginning, originates from one technological breakthrough for semiconductor integration in silicon obtained by Prof. Leo Miglio (CEO) and Prof. Hans von Känel (ETH Zürich, CTO), within the L-NESS inter-university center. It aims at developing, licensing, or selling innovative technologies manufacturing semiconductor structures and devices, with specific application to thick-film systems, such as high-efficiency photovoltaic cells, imaging detectors and power electronics devices. The company received Seed Money financing from Italian venture capital investors and one industrial partner. The targets of the first year are to provide one demonstrator of Ge/GaAs-, or Ge/GaAs/InGaP-based PV cells for satellite applications, and the proof of concept that SiC-based power devices can be integrated in silicon. PileGrowth Tech is characterized by a strong link to international semiconductor laboratories, both in academia and in the industry. Actually, 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.



CNISM - CONSORZIO NAZIONALE INTERUNIVERSITARIO PER LE SCIENZE FISICHE DELLA MATERIA

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

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.

IRELLI

CORIMAV - CONSORZIO PER LA RICERCA SUI MATERIALI AVANZATI

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

ETSF - EUROPEAN THEORETICAL SPECTROSCOPY FACILITY



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.



GALATEA BIOTECH- THE WHITE BIOTECH COMPANY

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.

TEACHING

TEACHERS

	CHIMICA ORGANICA	SCIENZA DEI MATERIALI
A. ABBOTTO		SCIENZE E TECNOLOGIE
	CHIMICA ORGANICA II E LABORATORIO	CHIMICHE
M. ACCIARRI	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
A COMOTTI	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
L. GIORDANO	CHIMICA	OTTICA E OPTOMETRIA
E. GRILLI	LABORATORIO DI STATO SOLIDO ED ELETTRONICA I	FISICA
E. GRILLI	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
M. MARTINI	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
	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
R. SCOTTI	CHIMICA DEI MATERIALI INORGANICI	SCIENZA DEI MATERIALI

	CHIMICA INORGANICA I E LABORATORIO	SCIENZE E TECNOLOGIE CHIMICHE
E. SIBILIA	LABORATORIO DI TECNOLOGIA DEI MATERIALI I	SCIENZA DEI MATERIALI
E. SIDILIA	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



Elaborati finali e Tesi Magistrali



Lauree Triennali in Scienza dei Materiali

- 1. AMADINI: Studio del fenomeno di invecchiamento di due leghe d'oro rosa 18 ct.
- 2. ANTONELLI: Isole di Ge e leghe Si/Ge su Si(001)
- 3. ASTOLFI: I gel di Agar: caratteristiche, proprietà e applicazioni alla pulitura di superfici artistiche
- 4. BIANCA: Nuove strategie di sintesi di sistemi donatori-accettori per celle fotovoltaiche a eterogiunzione massiva
- 5. CEREDA: ciclo tecnologico e produttivo dei materiali cementizi e metodiche di controllo analitico dei flussi gassosi emessi
- 6. CIMÒ: Materiali ceramici compositi per protezioni balistiche leggere
- 7. DANEI: Concentratori solari luminescenti a base di quantum dot colloidale: strategie per la realizzazione di dispositivi ad ampia area
- 8. DI GIROLAMO: Metodo di elettroluminescenza per il controllo della qualità di moduli fotovoltaici
- 9. FRIONI: studio della fisica dello spin del germanio
- 10. GHIDONI: Domini di antifase di semiconduttori composti cresciuti su Silicio o Germanio
- 11. GHISALBERTI: Nanocristalli organici colloidali per imaging di fluorescenza.
- 12. GIOVENZANA: Analisi delle proprietà microstrutturali e meccaniche di ottoni per applicazioni acustiche in ambito musicale.
- 13. GUIDORZI: Confronto tra i segnali di luminescenza superficiali e di bulk in laterizi di presunta produzione rinascimentale.
- 14. LASSI: Buche quantiche a semiconduttore
- 15. MONTI: Surface-Enhanced Raman Spectroscopy (SERS)
- 16. MURABITO: Tecniche di orientazione ottica di spin in semiconduttori
- 17. NEGRONI: La polarizzazione della luce: come descriverla, controllarla ed utilizzarla nello studio dei materiali
- 18. PALERMO: Sintesi di monostrati autoassemblati di copolimeri statistici e/o miscele di omopolimeri
- 19. PERRON: Studio delle proprietà luminescenti di quarzi naturali di diversa formazione geologica
- 20. REMONDINA: MEMS-Sensori di pressioni
- 21. SANDIONIGI: Nuovi nanomateriali ad elevata efficienza di up-conversion per bioimaging in-vivo
- 22. SANTILLAN ORELLANA: Acido croconico. Sintesi e utilizzo nella preparazione di coloranti ad alte prestazioni.
- 23. TAGLIABUE: Proprietà ottiche di germanio integrato su silicio

Lauree Triennali in Ottica e Optometria

- 1. BENCARDINO: Studio comparativo sull'efficacia di due differenti integratori lacrimali
- 2. BORELLA: Valutazione tonometrica oculare in medicina preventiva
- 3. CARLI: Lenti a contatto e lattoferrina: studi di citotossicità
- 4. CASARTELLI: Valutazione di una nuova lente a contatto per la compensazione dell'astigmatismo
- 5. CAVALLI: confronto fra diversi sistemi di manutenzione con lenti a contatto in silicone hydrogel
- 6. CERIBELLI: Analisi comparativa dello stato eteroforico e relativo rapporto AC/A tra Dark test e test convenzionali
- 7. CREMONA: Valutazione pre e post applicativa di lenti a contatto per soggetti afachici
- 8. DALL'ARMELLINA: Confronto tra le abilità visuo-motorie e visuo-posturali in bambini con disturbi specifici dell'apprendimento e bambini esenti da tali disturbi
- 9. DALLEMULLE: Evoluzione delle abilità visive e dei tempi di reazione in giocatori professionisti di badminton attraverso il training visivo
- 10. D'ANGELO: Valutazione comparativa dell'errore rifrattivo rilevato attraverso l'optometro e il test soggettivo da lontano.
- 11. DELL'AQUILA: valutazione della velocità di lettura e sensibilità al contrasto in soggetti con occhio secco marginale
- 12. FERRERA: Valutazione dell'equilibrio binoculare nella visione stereoscopica
- 13. FORTUNATI: Realizzazione di materiali biopolimerici funzionalizzati per lenti a contatto
- 14. GARATTI: Abilità binoculari e accomodative valutate con target cartaceo e su tablet
- 15. GHENO: Variazioni della percezione stereoscopica mediante l'uso degli aspetti del colore nella scena visiva
- 16. INGRASSIA: Ricerca della migliore compensazione oftalmica in soggetti affetti da cheratocono: follow up
- 17. LONGONI: Analisi della superficie anteriore e posteriore della cornea
- 18. MALIKIOSI: Acquisizione al biomicroscopio, elaborazione e valutazione clinica di immagini delle cellule endoteliali della cornea
- 19. PAPA: Capacità visuomotorie prima e dopo lo sforzo fisico:il caso di un gruppo di arbitri di calcio.
- 20. PAPARO: Potere ossidante di soluzioni per lenti a contatto morbide: messa a punto del metodo di analisi, analisi di soluzioni commerciali al perossido di idrogeno, effetti della sollecitazione meccanica sulle lenti
- 21. PASTORELLI: Confronto clinico tra due materiali per lenti a contatto di ultima generazione.
- 22. PEZZOTTI: Confronto tra differenti metodi di rilevazione dei parametri di centratura delle lenti oftalmiche
- 23. PIVA: Soluzioni al perossido di idrogeno e lenti a contatto in silicone hydrogel: valutazioni clinico-contattologiche sul portatore e morfologiche sulle lenti
- 24. RIPAMONTI: Indagine delle abilità visive in normolettori e dislessici e rinforzo delle capacità visuopercettive tramite trattamento di rieducazione visiva
- 25. RIVA: Valutazione della stabilità lacrimale e dell'integrità corneale in seguito all'instillazione di un sostituto lacrimale contenente acido ialuronico e amminoacidi

- 26. SPEZZANI: Valutazione dell'allineamento binoculare in giocatori professionisti di badminton
- 27. TAKHIM: studio di cambiamenti strutturali morfologici dei lenti oftamiche a seguito di trattamenti e confronto su lenti di diversi qualità.
- 28. UGGERI: Variazioni della disparità di fissazione in diverse posizioni di sguardo inerenti l'uso del computer"
- 29. VITALI: Assorbimento e rilascio di lattoferrina in lenti a contatto morbide
- 30. ZOGLIO: Ipovisione: valutazione della velocità di lettura, dell'acuità visiva e della sensibilità al contrasto dopo un percorso di riabilitazione visiva.

Lauree Magistrali in Scienza dei Materiali

- 1. ALBERINI: Preparazione di materiali nanoporosi per polimerizzazione allo stato solido
- 2. ANDREOSSO: Sintesi e caratterizzazione di nanostrutture polimeriche ottenute attraverso polimerizzazione radicalica in emulsione.
- 3. ASNAGHI: Synthesis and characterization of microporous polymer frameworks for gas and anesthetic adsorption
- 4. BALLABIO: Crescita e studio di eterostrutture GaAs/Ge su substrati di silicio patterned
- 5. BARBAROSSA: Meccanismi di Contaminazione Metallica in processi di Impiantazione Ionica
- 6. BERTANI: Self-assembly di copolimeri a blocchi per la fabbricazione di nanovettori biocompatibili per la terapia del sistema nervoso centrale
- 7. BOARO: Calibrazione di un profilometro ottico confocale ed interferometrico per la caratterizzazione ottica e morfologica di materiali per l'industria dei semicondutori
- 8. BOLDRINI: Sintesi colloidale e solvotermale di ossidi nanometrici e fabbricazione di nanocompositi trasparenti ad alto indice di rifrazione.
- 9. BORZINI: Innovazione e ricerca industriale: sviluppo di una schiuma di polietilene reticolato a celle aperte
- 10. BRAZZO: Sintesi e caratterizzazione di leganti fotoreattivi per nanoparticelle colloidali
- 11. CAMPANA: Sintesi di polimeri iperreticolati porosi e polimerizzazione confinata
- 12. CAMPANELLA: Studio e caratterizzazione di materiali poliuretanici macroporosi modificati con biopolimeri di gelatina e di pullulano.
- 13. CARULLI: High efficiency infrared luminescent solar concentrators based on heavy-metalfree colloidal quantum dots
- 14. CASTELLI: Highly efficient all-solution-processed quantum dot LEDs with polar polymer injecting layers
- 15. COBANI: Sintesi e caratterizzazione di materiali porosi per l'immagazzinamento dei gas
- 16. COLOMBO: Crescita e caratterizzazione di film sottili di Cu2ZnSnS4 per applicazioni fotovoltaiche
- 17. COLZANI: Tecnica innovativa per la preparazione di campioni per la datazione con radiocarbonio
- 18. CORSO: Influenza delle variabili di stampaggio ad iniezione nella generazione di sforzi interni nel policarbonato
- 19. DALBON: Nanoparticelle SiO2/ZnO come attivatore di vulcanizzazione e filler rinforzante per gomma isoprene

- 20. DELCASTELLO: Caratterizzazione morfologica, meccanica ed elettrica di trincee profonde d'isolamento per tecnologie di potenza SOI
- 21. GIAMMARIA: Random copolymer grafting for interface tuning
- 22. LORENZON: Electrochemical control of recombination dynamics in colloidal quantum wells: towards highly emissive reverse photoresponsive varnishes
- 23. MATTIELLO: Highly stable, latent pigment based Luminescent Solar Concetrators
- 24. MONTEFIORI: Cristallizzazione in celle di memorie a cambiamento di fase: caratterizzazione statistica.
- 25. MORETTI: Sviluppo di metodi electroless per la deposizione di pattern metallici su substrati polimerici per applicazioni in plasmonica ed elettronica.
- 26. NAVA: Sintesi di sistemi aromatici ed eteroaromatici precursori di strutture grafeniche autoassemblate sulla superficie di metalli
- 27. PILONI: Sintesi e caratterizzazione di copolimeri a blocchi per in vivo 19F Magnetic Resonance Imaging tramite polimerizzazione RAFT
- 28. PINCHETTI: Spin dynamics of co-existing core and shell negative trions in CdSe/CdS dotin-bulk nanocrystals.
- 29. PONZETTO: Sviluppo e validazione di un metodo gascromatografico per la determinazione dei solventi residui in un principio attivo farmaceutico
- 30. RONCHI: Synthesis of new polycyclic aromatic hydrocarbon systems based on fluoranthene and perylene with potential optoelectronic applications.
- 31. SORMANI: Materiali nanoporosi iperreticolati per l'adsorbimento di gas
- 32. SORRENTINO: Produzione e caratterizzazione di inchiostri di grafene per ink-jet printing.
- 33. VITALI: Studio della diffusione di fosforo in matrici di silicio nanocristallino per applicazioni termoelettriche.
- 34. VITIELLO: Orientazione ottica degli spin e fotoluminescenza polarizzata in epistrati di Germanio su Silicio



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

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

The doctorate in Materials Science and Nanotechnology of this Department is partner and headquarters of the European doctorate in Physics and Chemistry of Advanced Materials (http://www.pcam-doctorate.eu/). The aim of the doctorate is to train graduate students in investigating fundamental, applicative and industrial topics, either experimentally or theoretically and computationally in the modern materials science and the technological innovation. The doctorate, which lasts for three years, is divided into three curricula. The first one in Materials Science deals with materials basic research and technological applications. The second one in Materials Technology, funded mainly by Pirelli tyres, is devoted to applied research in order to develop new materials of industrial interest. The third curriculum in Nanoscience covers the rapidly growing area of nanometer science including nanobiology. Every year the student has to present a seminar on the advance of his research and has to pass three exams during his doctorate. Students are also required to spend a period from 6 to 18 months in a research institution abroad. Strong links are established with industrial companies (Pirelli, SAES-Getters, to cite the most active ones).

The PCAM network is formed by 15 Universities which are: the Università of Milano-Bicocca, the Universidad Autonoma de Madrid, the University of Southern Denmark, the Kaunas University of Technology (Lithuania), the Jagiellonian University of Kraków (Poland), the Università degli Studi di Milano, the Universidad del País Vasco (Spain), the Lomonosov Moscow State University, the Université Pierre et Marie Curie of Paris, the Carl von Ossietzky University of Oldenburg (Germany), the Technical University of Cluj-Napoca (Romania), the Graz University of Technology (Austria), the University of Liverpool (UK) and the University of Luxembourg, the Technical University of Dresden. The network PCAM organizes each year a school for graduate students on a specific relevant topic and grants an extra European doctorate diploma.

Seven of PCAM Universities are being awarded EC funding via the FP7-MC network THINFACE.

Coordinator of the doctorate in Materials Science and nanotechnology and Chairman of the PCAM network is Prof. Gianpaolo Brivio.

EUROPEAN DOCTORATE IN NANOSCRUCTURES AND NANOTECHNOLOGIES http://www.nano.unimib.it

The PhD School in Nanostructures & Nanotechnologies is a three-years curriculum for Master graduated students in Science or Technology. The aim of the School is the formation of scientists or science-related professionals by a research training in the synthesis, the characterisation or the modeling of nanostructures, either organic, inorganic or biologic in nature.

The educational training in the first two years consists in research and advanced formation activities (internal and external courses). The third year will be devoted to the thesis writing in English. The tutorial and research activities are held in one of the partners European universities and research centres:-Faculty of Science of the Università di Roma Tor Vergata, Ecole Normale Supérieure, Lyon, Max Planck Institut für Festkörperforschung, Stuttgart, Institut Charles Sadron (ICS/CNRS), Strasbourg, Cardiff University (School of Chemistry), Cardiff, CCLRC Rutheford Appleton Laboratory, Chilton-Oxford, Johannes Kepler Universität, Linz, STMicroelectronics, Agrate (Milano).

Chairman is prof.Gianfranco Pacchioni

ERASMUS-LIFELONG LEARNING PROGRAMME

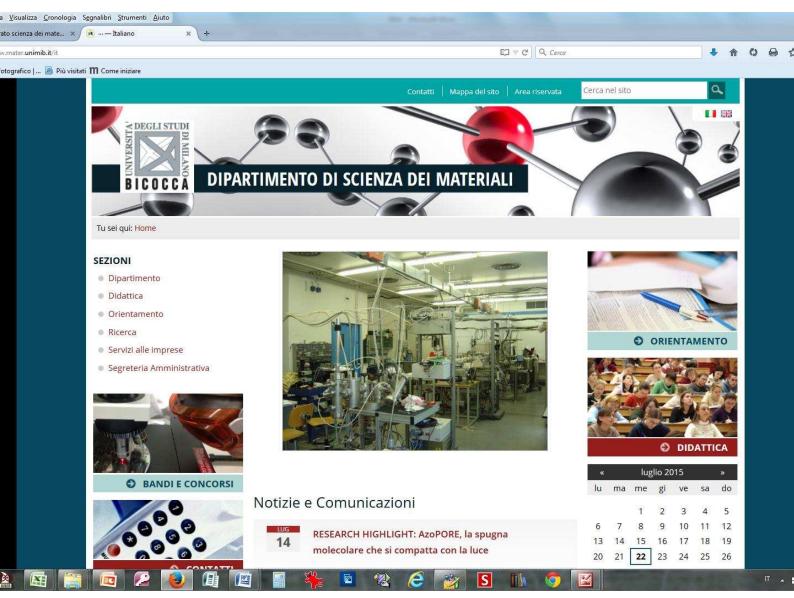
Thanks to ERASMUS, the European programme offering university students the possibility of studying or working abroad for a period of 3-12 months, several students of both Materials Science and Optics & Optometry could spend one year in selected European university.

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WEB PAGE

http://www.mater.unimib.it



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Cover: EDXRF of an Etruscan pottery for provenance analysis

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