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### THE MATERIALS SCIENCE DEPARTMENT

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

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Director	Prof. Marco Martini / Prof. Alessandro Abbotto (since October)
ISI-CRUI Sectors	Chemistry, Physical Chemistry, Chemical Physics Spectroscopy, Instrumentation Engineering, Analytical Sciences, Optics and Optometry, Organic Chemistry, Polymer Science, Materials Science, Physics, Condensed Matter, Applied Physics

#### ABOUT US

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

The main research fields are:

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

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

**G**eneral 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.

**R**esearch 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).

**D**egrees 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.

#### 2

### STRATEGIC GOALS

## **SCIENTIFIC BOARD**

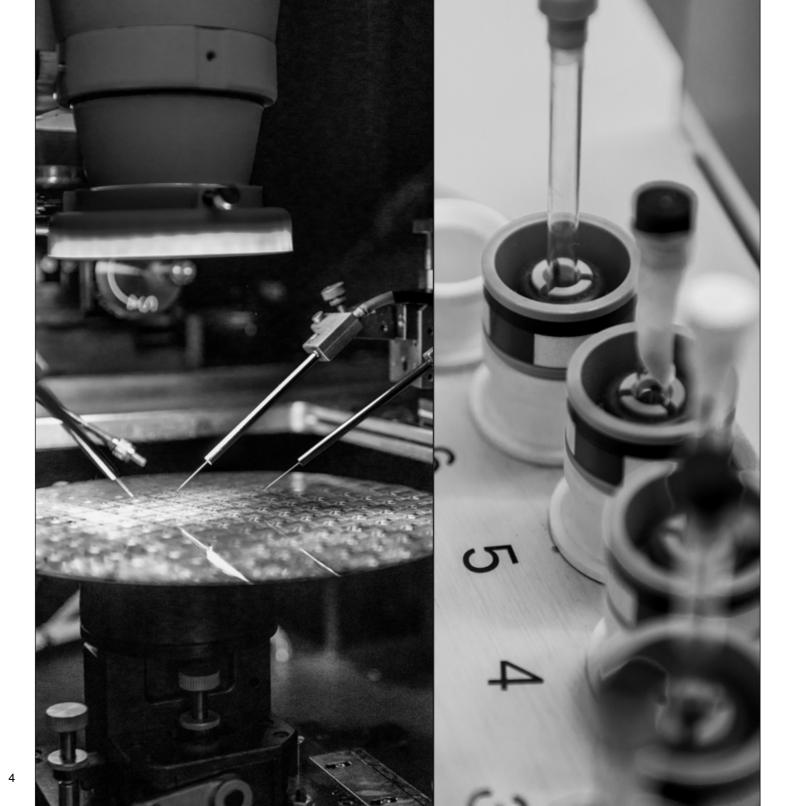
Until September / since October

**DIRECTOR** Marco Martini / *Alessandro Abbotto* 

**DEPUTY DIRECTOR** Antonio Papagni / Anna Vedda

#### COUNCIL

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



## **TEACHING BOARD**

#### CHEMICAL SCIENCE Simona Binetti

#### MATERIALS SCIENCE Alberto Paleari

**OPTICS AND OPTOMETRY** Adele Sassella

**DOCTORATE** Marco Bernasconi Francesco Montalenti (deputy)

### **DEPARTMENT OF EXCELLENCE 2018-2022**

#### FRAMEWORK

The Department of Materials Science (DMS) was one of the winners of the "Department of Excellence" call, an innovative initiative by the Italian Ministry of University and Research (MIUR). The total budget for DSM is € 10,693,820, 62% of which will be contributed by MIUR.

#### OBJECTIVES

The project aims at innovating products and processes in the chemistry and physics of materials for energetics. This embraces the entire value chain from hydrogen production, its storage under optimal conditions, the electrochemical conversion of the energy contained in hydrogen as a vector, and the subsequent accumulation in electrochemical devices.

A new laboratory (FLEXILAB) of enabling technologies, endowed with a clean room of about 1000 ft<sup>2</sup>, will be fabricated.

Based on FLEXILAB, the project aims at developing a COMPETENCES CENTER devoted to the technological transfer from the University to Regional and National industry in the field of sustainable energy.

#### TASKS

Production of solar fuels and chemicals. Focus on the solar production of hydrogen and small carbon-based molecules from sun and nature abundant and ubiquitous feedstocks ( $H_2O$ ,  $CO_2$ ) by photocatalytic and photoelectrochemical approaches using a) new organic-based materials, b) 1D and 2D semiconductors and oxides. Hydrogen storage. Focus on organic and metal-organic nanoporous materials with high surface (>4000 m²/g) to store hydrogen at more moderate pressures (100-200 bar) than those required by gas compression (700 bar). Electrochemical energy conversion (fuel cells). Focus on systems with proton or anionic conducting polymer membranes, with low-cost electrode materials (e.g. without noble metals).

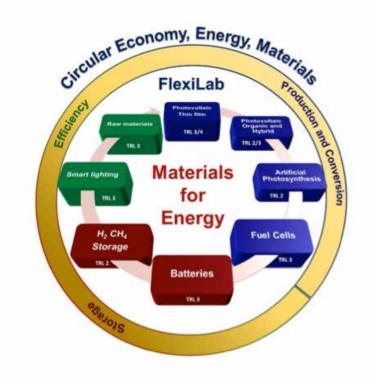
Electrochemical energy storage. Focus on lithium and post-lithium (e.g. sodium) batteries. Both electrodes (e.g. intercalation-type and conversion-type materials) and electrolytes will be investigated.

Photovoltaic cells: Focus on new inorganic and hybrid thin films (e.g. perovskites) in order to realize tandem cells to reach 30% efficiency target.

#### TECHNOLOGY TRANSFER: EXAMPLES OF ACTIVITIES AND PRODUCTS

Development of photovoltaic cells integrated in buildings for a more functional use of the available surface. Development of electrochromic windows to optimize consumption related to heating and cooling. Development of prototypes of batteries and MEAs for fuel cells. Development of combined systems for the production of electricity and related local storage by developing the self-consumption sector, as reported in the SEN (National Energy Strategy). Demonstrators for the storage and semi-industrial scale production of solar fuels and chemicals from water and carbon dioxide, with focus on sustainable transport and chemical feedstock.







Professors Emeriti: Giorgio BENEDEK (FIS/03), Alessandro BORGHESI (FIS/01)

Full Professors: Alessandro ABBOTTO (CHIM/06), Marco BERNASCONI (FIS/03), Gian Paolo BRIVIO (FIS/03), Cristiana DI VALENTIN (CHIM/03), Marco FANCIULLI (FIS/03), Marco MARTINI (FIS/07), Leonida MIGLIO (FIS/03), Piercarlo MUSTARELLI (CHIM/02), Gianfranco PACCHIONI (CHM/03), Alberto PALEARI (FIS/01), Antonio PAPAGNI (CHMI/06), Adele SASSELLA (FIS/01), Piero SOZZANI (CHIM/04), Anna VEDDA (FIS/01)

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**Post-Docs:** Marco ALBANI, Floriana ALITE, Mani AZADMAND, Anu BABY, Irene BASSANETTI, Roberto BERGAMASCHINI, Charles BEZUIDENHOUT, Michele CACCIA, Simone CAGLIO, Valentina CANTATORE,

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**Spinoffs:** Alberto BIANCHI (Graftonica), Francesco BRUNI (G2P), Chiara CAPITANI (G2P), Silvia FER-RARIO (Graftonica), Marina GANDINI (G2P), Graziella GARIANO (G2P)



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Sergio BIETTI Enea BORIA Carmen CANEVALI Lorenzo FERRARO Claudio LAGRASTA Francesco MASPERO Giorgio PATRIARCA Luisa RAIMONDO Silvia TRABATTONI Bruno VODOPIVEC























#### **Materials Science**

#### B.Sc.

ACHILLI Stefano, ALESCI Giuseppe, BARBERIO Alessandro, BONASSI Federico, BRIGATTI Stefano, BRUTTOMESSO Alessio, CALCATERRA Alessio, CANNETTI Gianluca, CASERINI Alice, CAVALIERE Giulio Pietro, CAVENAGO Luca, CESANA Jacopo, CHECCHI Filippo, COLAZZO Luca, COLELLA Daniele, COLOMBO Camilla, DA LISCA Mattia, DANIELE Raffaele, DE MARTINI Denis, DE MICHELI Davide, DELLA FONTANA Matilde, DI GIUSEPPE Simone, DRAGONI Lara, ERROI Andrea, FORMENTI Gianluca, GHIRARDI Alessandro, GNOATTO Lorenzo, LOMBARDI Gioele Maria, MAXENTI Veronica, MESSINA Davide, MEZZOMO Lorenzo, MOIA Valentina, MORI Nino, RIVA Tommaso, ROVERA Davide, SUSANA Laura, TALONI Marcello, TAMBONE Riccardo, TAMBURINI Giulia, TARRICONE Giulia, TRIZIO Enrico, VENTURA Michael, VOLONTÈ Francesco

#### M.Sc.

ALICINO Davide Antonio, BOCHICCHIO Emanuele Antonio, BONALDO Camilla, BONZI Maura, BOZZETTI Michele, CALIGIORE Federica Elvira, CRAPANZANO Roberta, KACANI Ledia, MAHAJNEH Amal Eleonora, MARZO Andrea, ORSITTO Debora, ROC-CO Alice, ROSSI Marco, SIPALA Roberta, ZAFFALON Matteo Luca, ZANENGA Fabio, ZUCCA Gaia

### **Optics and Optometry**

#### B.Sc.

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### Chemistry

#### B.Sc.

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Research

(in alphabetic order)

m

m

## Materials for energy and environment

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

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

Carlo Antonini. Surface Engineering and Fluid Interfaces – SEFI

Gian Paolo Brivio. Theory and computations of adsorbate interfaces

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

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

Cristiana Di Valentin, Daniele Selli. Theory of 2D and 0D materials: bidimensional layers and nanoparticles

Massimo Moret. Crystal growth and characterization: study of polymorphism

Piercarlo Mustarelli. Materials for electrochemical energy conversion: synthesis, ex-situ and operando characterization

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

Riccardo Ruffo. Electrochemical activities



Emiliano Bonera, Fabio Pezzoli. Optical spectroscopy of semiconductors

functional nanomaterials

and spintronics

materials for optical technology

conductor heteroepitaxy

tures

Adele Sassella. Organic molecular films and heterostructures

## Materials for microelectronics

- Marco Bernasconi. First principles simulations of materials for microelectronics
- Sergio Brovelli, Francesco Meinardi, Angelo Monguzzi. Advanced spectroscopy of
- Marco Fanciulli, Fabrizio Moro. Materials and spectroscopies for nanoelectronics
- Mauro Fasoli, Alberto Paleari, Anna Vedda. Oxide nanostructures and silica-based
- Leo Miglio, Francesco Montalenti, Emilio Scalise. Modeling and simulations of semi-
- Stefano Sanguinetti. Fabrication and study of semiconductor guantum nanostruc-



## Materials in cultural heritage

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



## **Mathematics**

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

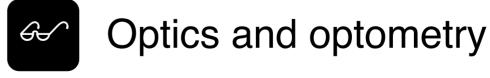


Luca Beverina. Functional dyes and pigments for photonics, electronics and optoelectronics

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

Antonio Papagni. Organic functionalized materials for optoelectronic applications and thermally and photochemically activate organic systems with cross-linking potentials

Roberto Simonutti. Synthesis and characterization of novel polymeric nanostructures



Silvia Tavazzi. Optics and optometry

## Organic and polymeric materials

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



#### ALESSANDRO ABBOTTO, NORBERTO MANFREDI

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

## ARTIFICIAL PHOTOSYNTHESIS: CLEAN AND RENEWABLE SOLAR FUELS

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

#### ORGANIC AND HYBRID 3RD GENERATION PHOTOVOLTAICS

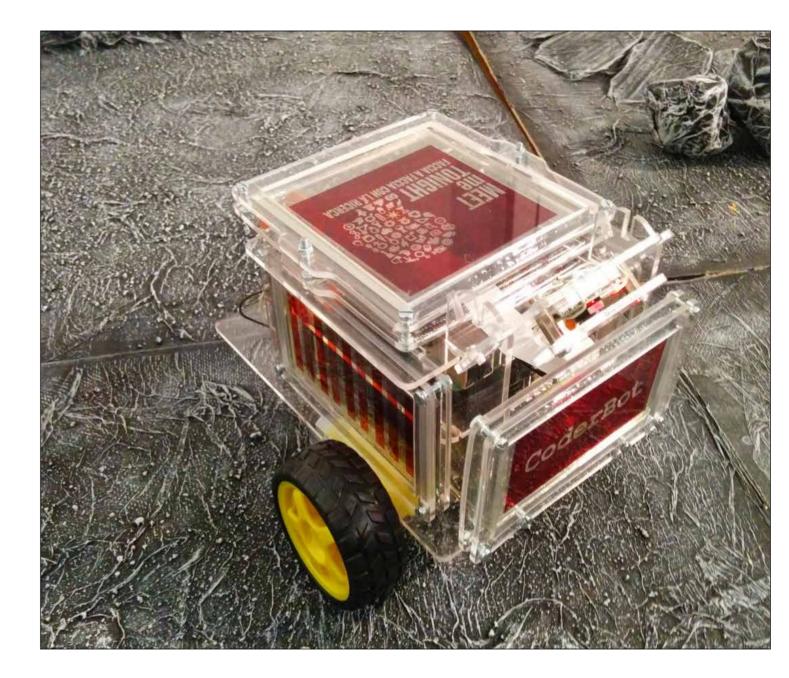
We investigate last generation organic and hybrid photovoltaics, namely: -dye-sensitized solar cells (DSSC) -perovskite solar cells (PSC) -tandem multijunction cells. Focus is on last generation devices such as graphene-based sensitizers and eco-friendly drinkable media.We also investigate tandem multijunction cells in combination with silicon and thin film inorganic

media. We also investigate tandem multijunction cells in combination with silicon and thin film inorganic technologies, in order to access higher performances. A large variety of materials (organic and organometallic dyes, electron and hole transporting materials, electrolytes, semiconductor oxides, electrodes) are investigated as well as lab-scale and pre-industrial photovoltaic panels.

#### MAIN FACILITIES

Fully equipped organic synthesis and characterization laboratory. Spectroscopic (absorption, emission, NMR) characterization. Glove boxes. Clean room for preparation and characterization of photovoltaic cells and modules.

Facilities for preparation and measurement of photocatalytic hydrogen/oxygen production and PEC water splitting





## 1

## Photovoltaics, thermoelectrics and carbon dioxide capture





#### 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<sub>2</sub>ZnSnS<sub>4</sub> (CZTS), was considered, too. Two main growth methods are under investigation and testing: sputtering process and chemical methods (i.e. dip coating, spray pyrolysis).



#### 

### Surface Engineering and Fluid Interfaces – SEFI Lab.



#### CARLO ANTONINI

The Laboratory of Surface Engineering and Fluid Interfaces (SEFI Lab) brings about research and innovation for the development of new technologies towards clean water and energy-efficient processes, two corner stones for sustainable development.

**R**esearch activities focus on understanding interfacial transport phenomena, for the design of innovative smart interfaces. SEFI Lab is characterized by an interdisciplinary approach, at the interface between thermofluidics, material science and surface micro- and nano-engineering.

#### SMART INTERFACES FOR ENERGY APPLICATIONS

Smart interfaces with tailored wetting properties to control liquid behavior at interfaces, e.g. on solid surfaces, have a tremendous potential of high in a variety of engineering and energy related applications. Non-wetting superhydrophobic surfaces are developed at SEFI Lab for their extreme potential against ice nucleation and accretion on solid substrates, a severe issue in aeronautics, for structures in cold climates and for low-temperature heat exchangers, and for efficient condensation processes. To control phase change processes, materials and surfaces are rationally designed and fabricated, with complex patterning down to the micro- and nanoscale.

#### SMART INTERFACES FOR WATER

**S**mart interfaces with controlled wetting and nano-structuring play a major role in the development of efficient processes for clean water, including both drinking water and polluted sea water cleaning, e.g. after large oil spill. Within the framework of green material fabrication, cellulose nanofibrils from natural resources were used to fabricate extremely porous light-weight materials, with selective liquid sorption, due to tailored hydrophobic-oleophilic interfacial wetting properties.



# Theory and computations of adsorbate interfaces



#### GIAN PAOLO BRIVIO

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

## ULTRAFAST PROCESSES OF ELECTRON TRANSFER RATES OF A CORE EXCITON

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

## FEMTOMAGNETISM OF CORE EXCITED FUNCTIONALIZED GRAPHENE

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

#### SPECTROSCOPIC AND OPTICAL PROPERTIES OF POTASSI-UM DOPED PTCDA ON METALS

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



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



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

A challenging issue is the dynamics of nanoporous solids. The research activity is focused on the insertion of molecular rotors in the building blocks of the porous materials, giving access to the control of rotary motion by chemical and physical stimuli. The combination of porosity with ultra-fast rotor dynamics is investigated in molecular crystals, covalent organic frameworks and MOFs by complementary techniques, which were proved to be sensitive to motion at regimes ranging from 104 to 1011 Hz. Remarkably, the rotor dynamics can be switched on and off by guest absorption/desorption, showing a change of material dynamics, which, in turn, produces modulated physical responses. Novel fluorinated dipole-bearing molecular rotors can be inserted on porous architectures, realizing ordered arrays of fast dipolar molecular rotors. The extremely rapid re-orientation in solids is challenging and enables the fabrication of ferroelectric switches, as revealed by dielectric measurements. The combination of pore-structure and dipolar rotors can be exploited for stimulated guest release.

A series of flexible molecular crystals made by azobenzene tetramers, that form porous molecular crystals in their trans configuration is pursued. The efficient trans  $\rightarrow$  cis photo-isomerization of the azobenzene units converts the crystals into a non-porous phase but crystallinity and porosity are restored upon Z  $\rightarrow$  E isomerization promoted by visible light irradiation or heating. The photo-isomerization enables reversible on/off switching of optical properties as well as the capture of CO<sub>2</sub> from the gas phase.



## Chemistry of inorganic and hybrid materials - NanoMat@Lab



m





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

#### NANOSTRUCTURED MATERIALS FOR CATALYSIS, PHOTOCATALYSIS AND ENERGY STORAGE

The research aims at the synthesis by soft-chemistry methods of morphology-controlled oxide nanoparticles (e.g.  $TiO_2$ , ZnO, MoO\_3) and tuneable porous systems (macro/mesoporous silica or Metal Organic Frameworks, MOF), and at the study of their (photo)catalytic mechanism (formation and interfacial reactivity of paramagnetic defects) by spectroscopic and spectromagnetic techniques. In particular, the possibility of tailoring size, anisotropy and surface functionalities of these systems by employing catalysts (acid or bases), soft templates (e.g. amphiphilic surfactants), capping molecules or particular solvents, has been exploited for the modulation of the inorganic-organic interfaces. This play a crucial role in determining their properties and implementation for the development of advanced hybrid materials commonly utilized for water/air depollution,  $CO_2$  photoconversion in renewable fuels and Na-ion batteries.

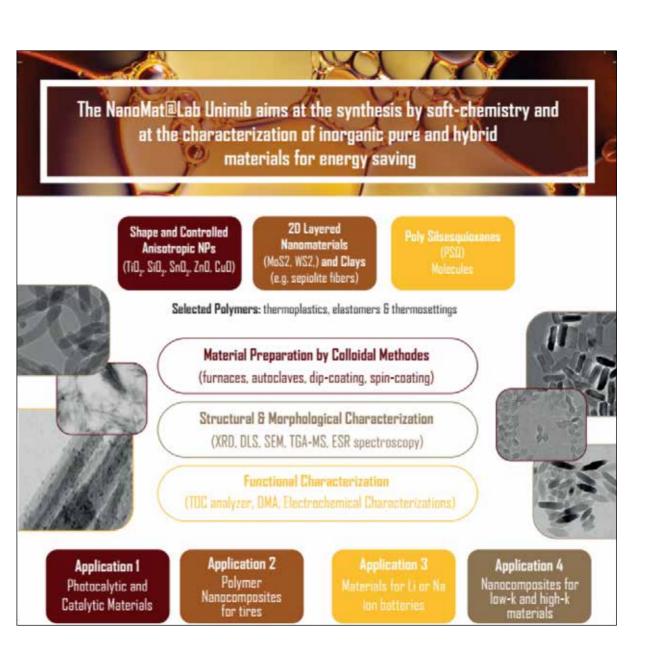
## INORGANIC NANOFILLERS FOR MULTIFUNCTIONAL POLYMER NANO-COMPOSITES

The research focus on the preparation by bottom-up approaches of oxides (mainly ZnO and SiO<sub>2</sub>) nanoparticles and polysilsesquioxanes (PSQ) with controlled morphological and surface features, employed in a wide range of applications (i.e. automotive, high performance dielectrics, gas-barrier). In particular, since 2008, these materials have been exploited by our group, in collaboration with other academic and industrial partners (i.e Pirelli Tyres, SAES Getters), for the preparation of novel polymer nanocomposites mainly utilized in tires application. In this context, the results of the activity have provided a relevant scientific and technological impact, leading to the production and implementation of a material developed in the NanoMat@Lab in the industrial plant. Currently, the group is working on the application of these designed fillers in other multifunctional nanocomposites (conductive composites for low-k or high-k materials, O<sub>2</sub> barrier coatings) where, besides a peculiar functionality, remarkable mechanical strength, low deformability and high thermal stability are required.

#### FACILITIES

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

Bruker ESR spectrometer equipped with liquid N<sub>2</sub>/He Cryostat.



### m

### Theory of 2D and 0D materials: bidimensional layers and nanoparticles NanoQlab



#### CRISTIANA DI VALENTIN, DANIELE SELLI

#### COMPUTATIONAL NANOMEDICINE

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

#### COMPUTATIONAL ELECTROCHEMISTRY AND FUEL CELLS



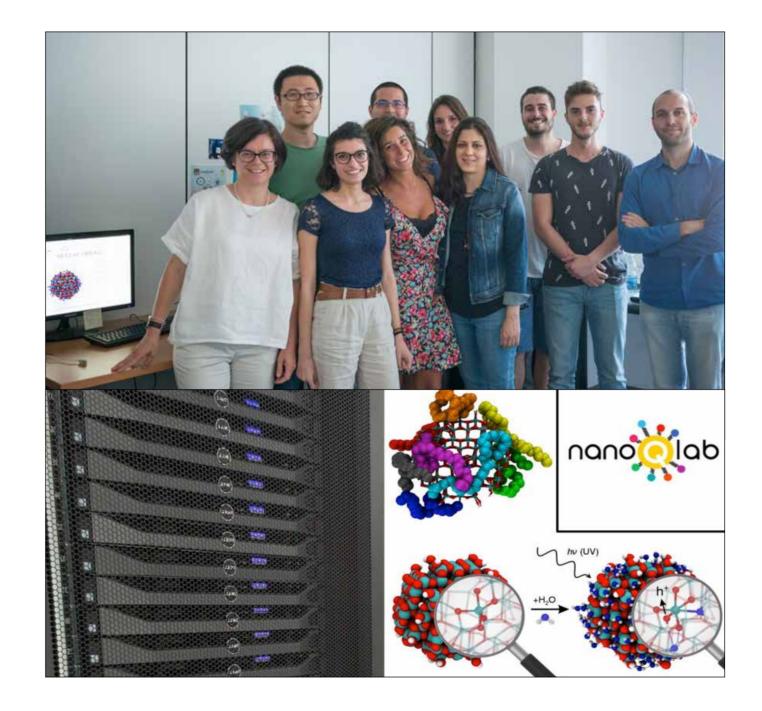
We use electronic structure calculations to design novel electrode materials for electrochemical devices and fuel cells, which are as efficient as or even more capable than precious and environmental unfriendly metal electrodes. Gibbs free energies of reaction in an aqueous environment for the all the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

#### CATALYSIS UNDER COVER (2D LAYERS)

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

#### GRAPHENIC NANOSTRUCTURES FROM MOLECULAR PRE-CURSORS

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



## m

# Crystal growth and characterization: study of polymorphism



#### MASSIMO MORET

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

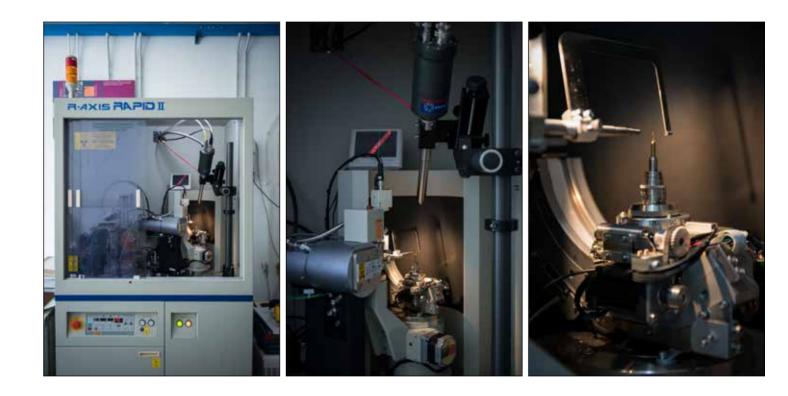
The research activities are mainly devoted to crystal growth from solution (flexible coordination polymers, MOFs, inorganic solids for catalysis, composite crystalline systems, amino acids), study of sorption processes at the crystal/solution interface in natural and artificial environments (e.g. doping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

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

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

#### FACILITIES

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



## Materials for electrochemical energy conversion: synthesis, ex-situ and operando characterization



#### PIEBCARI O MUSTARELLI

The research activity chiefly deals with the fabrication of innovative materials for electrochemical energy conversion (e.g. polymer fuel cells), and with their structure, thermal and functional characterization. A relevant part of the research is also devoted to the development on NMR/MRI methods for operando investigation of interfaces and devices for electrochemical conversion and storage. Main topics:

#### MEMBRANES AND MEMBRANE-TO-FLECTRODE ASSEM-BLIES (MEAS) FOR POLYMER FUEL CELLS

Polymer fuel cells operating al low temperature (< 100°C) are the systems-of-choice for energy conversion for automotive (buses, trucks, shuttles) and for grid applications. At present, the state of the art is represented by proton-conducting devices operating with NafionTM membranes. These fuel cells suffer of several problems, e.g. need of precious metal catalysts (e.g. platinum and platinum-group metals (PGM)), catalyst poisoning by CO at low temperature, membrane high cost. Alternative routes are offered by proton-conducting devices operating in the range 100-200°C, which based on membranes made by polybenzimidazole and related composite materials. This allows to reduce the membrane cost. Another intriguing possibility is to move towards anion (OH) conducting membranes, which allow substituting the PGM catalysts with other based on cheap elements (e.g. Fe). The research line aims at developing and characterizing both proton- and OH-conducting materials.

#### SOLID POLYMER AND COMPOSITE ELECTROLYTES FOR EN-**ERGY STORAGE**

At present, the market of electrochemical energy storage is dominated by lithium-ion rechargeable batteries. These batteries, however, have not enough energy density to support the demanding requirements of automotive, and are not really safe because of the high volatility and flammability of the organic liquid electrolyte. The quest for higher energy density can be solved by substituting the graphite anode with a lithium metal one, originating the so-called lithium metal batteries (LMB). These batteries require a solid electrolyte able to block the formation of lithium dendrites which can cause short circuits and battery faults. The availability of solid electrolytes will also help to solve the present safety problems. This research line aims at developing solid electrolytes based on functional polymers. e.g. poly(ethylene oxide) (PEO), or on polymer-ceramic nanoarchitectures.

#### NMR/MRI OPERANDO CHARACTERIZATION

The functional characterization of materials involved in electrochemical interfaces, or even in complete devices, cannot prescind from their study under conditions as near as possible to real operation (operando conditions). This indeed requires the use of non-destructive characterization techniques,

e.g. X-rays, electron microscopies, of spectroscopies like RAMAN or NMR. This research line aims at developing and applying advanced methodologies of NMR spectroscopy and micro-imaging (MRI) to the operando investigation of materials for batteries, supercapacitors and fuel cells.

#### MAIN FACILITIES

- Solid-state 400 MHz NMR spectrometer with microimaging accessory
- Test station for fuel cells
- High-pressure/high-temperature autoclave for polymer synthesis



Test systems for batteries, frequency response analyzers, potentiostats/galvanostats (in cooperation with Riccardo Ruffo)

## Theory of oxide surfaces, interfaces, supported clusters

#### MAIN FACILITIES

- Total computing power of 960 AMD Opteron cores in local facilities. scientific proposals.



#### GIANFRANCO PACCHIONI, SERGIO TOSONI

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

#### OXIDE SURFACE AND THIN OXIDE FILMS

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

#### SUPPORTED CLUSTERS

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

#### DEFECTS AND DOPANTS IN OXIDES



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

#### OXIDE SEMICONDUCTORS AND HETEROJUNCTIONS

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



- Access to CINECA supercomputing centre facilities via an institutional account financed by the University as well as via peer-reviewed



### **Electrochemical activities**



#### **R**ICCARDO **R**UFFO

**S**ince the birth of the Department, the group is active in fields of Energy Storage and Production, Gas Sensing, and characterization of Organic Molecular or Polymeric Materials. Group facilities comprise a fully equipped electrochemical lab with several potentiostats-galvanostats, two multichannel systems for long time testing, two semi-automatic glove boxes at N<sub>2</sub> 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

**P**otentiometric 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.



## First principles simulations of materials for microelectronics



 $\mathbf{Q}$ 

#### MARCO BERNASCONI

#### PHASE CHANGE MATERIALS FOR DATA STORAGE

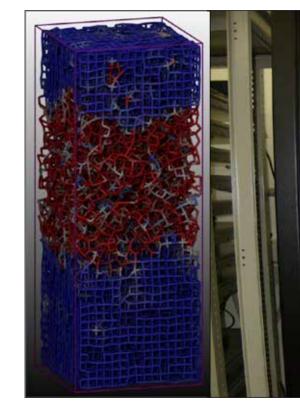
**P**hase change materials ( $Ge_2Sb_2Te_5$  and related telluride alloys) are attracting an increasing interest worldwide for applications in optical disks (DVDs) and in a novel non volatile electronic memory, the phase change memory cell. Both applications rely on a fast (10-100 ns) and reversible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

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

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

#### SURFACE PHONONS AND TOPOLOGICAL INSULATORS

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







# Optical spectroscopy and fabrication of semiconductors and semiconductor quantum structures





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

**S**iGe 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;

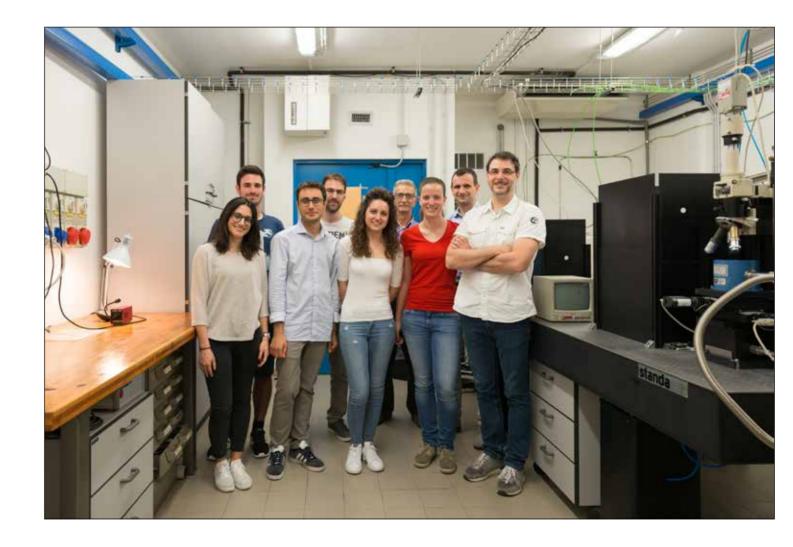
2. We study the nanostructure properties via spectroscopic measurements addressing electronic structure and carrier relaxation mechanisms;

3. We study the transfer of the III-As QD devices on Si for integration with standard electronics.

#### FACILITIES

**S**pectroscopic 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.



### Advanced spectroscopy of functional nanomaterials







#### SERGIO BROVELLI, FRANCO MEINARDI, ANGELO MONGUZZI

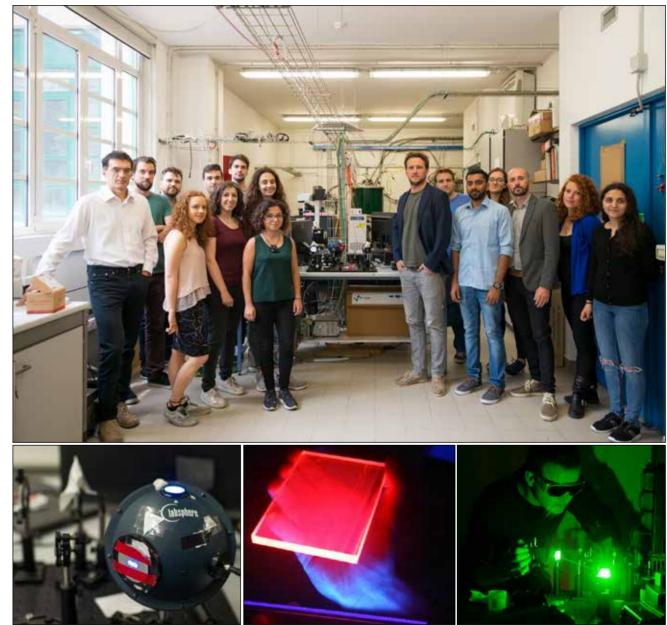
Non-Coherent Photons Up-conversion. The generation of photons of higher energy with respect to the excitation (up-conversion) through the non linear optical response of a material is a phenomenon useful to reach spectral regions otherwise not accessible. However, is appreciable only for coherent light sources delivering light intensity in the order of MW/cm<sup>2</sup>. We are working on new routes to lower down to µW/cm<sup>2</sup> 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.

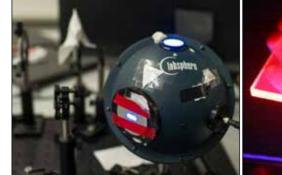
One Dimensional Photonic Crystals DFB Lasers. The avant-garde development of smart structures to provide optical feedback paves the way to the realization of novel laser emitters. An interesting approach is the distributed feedback (DFB) based on photonic crystals. In these systems a periodicity of the 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 channel-forming 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. 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.







## Materials and spectroscopies for nanoelectronics and spintronics (MSNS Laboratory)



#### MARCO FANCIULLI, FABRIZIO MORO

**O**ur research is mainly devoted to the experimental investigation of semiconductors, oxides, semiconductor/oxide interfaces, silicon and germanium nanostructures, MoS<sub>2</sub> growth, for advanced and innovative nanoelectronic, spintronic, and neuroelectronic devices. The research activity is carried out in strong collaboration with the CNR-IMM, MDM Laboratory and leading semiconductor industries, Micron and STMicroelectronics

#### POINT DEFECTS IN SEMICONDUCTORS AND OXIDES

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



#### SEMICONDUCTOR/OXIDE INTERFACES

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

#### Si AND Ge NANOSTRUCTURES

The electronic and spintronic properties of the following nanostructures

- Silicon nanowires produced by e-beam lithography and oxidation.
- Silicon nanowires produced by metal-assisted chemical etching (MACE)

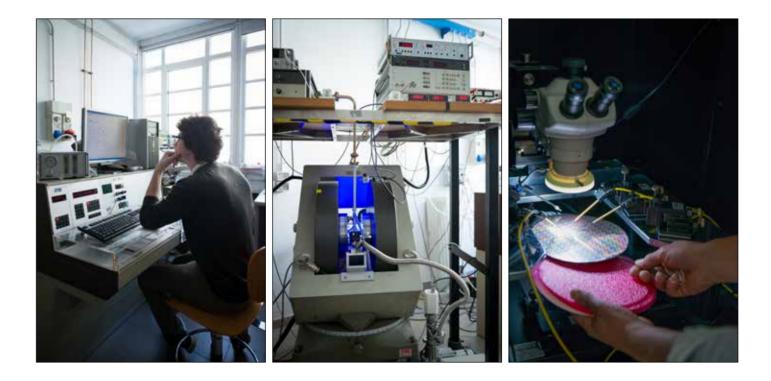
Silicon and germanium nanowires and nanoclusters produced by CVD and MBE are investigated using mainly spin dependent transport techniques aiming at the characterization of shallow donors, electro-statically confined electrons, Coulomb blockade.

#### GROWTH AND CHARACTERIZATION OF TMDC (MoS<sub>2</sub>, WS<sub>2</sub>)

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

#### **EXPERIMENTAL FACILITIES**

Growth and processing Atomic Layer Deposition (ALD) mini-chamber with O<sub>3</sub> line for in-situ characterization. Horizontal and vertical furnaces for annealing and diffusion Q-switched Ruby laser for laser annealing Characterization Two CW X-band systems for electron spin resonance (ESR) spectroscopy, electrically detected spin resonance spectroscopy (EDMR) and electron nuclear double resonance spectroscopy (ENDOR). Variable temperature measurements (4-600 K). Multi-frequency (0.1-40 GHz) EDMR Set-up for inelastic electron tunnelling spectroscopy (IETS) working in the temperature range 4-300 K



# Oxide nanostructures and silica-based materials for optical technology



#### MAURO FASOLI, ALBERTO PALEARI, ANNA VEDDA

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

#### **RESEARCH LINES**

**O**ptical 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<sub>2</sub>O<sub>3</sub> and SnO<sub>2</sub> nanocrystals in silicates, analyzing the applicability as light-emitting systems, photo-sensitive optical materials, cubic non-linear components, and transparent conductors.

#### FACILITIES

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



# Modeling and simulations of semiconductor heteroepitaxy



#### LEO MIGLIO, FRANCESCO MONTALENTI, EMILIO SCALISE

**D**eposition 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.

**P**articular attention is also dedicated to understanding the onset of plastic relaxation (injection of misfit dislocations) both in flat SiGe/Si films and in SiGe 3D islands, and its competition with elastic relaxation. To this goal, we developed a suitable methodology to treat extended defects within a continuum approach.

Lately most of our attention has been focused on exploiting suitable patterning of a Si(001) substrate to obtain ordered arrays of islands and/or to influence dislocation nucleation, confining defects in desired positions. We have discovered that on a suitably pit-patterned substrate, very peculiar processes take place, leading to an extra-relaxation (with respect to the flat substrate case) of nanoislands, with important consequences also on the onset of plastic relaxation.

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







## Fabrication and study of semiconductor quantum nanostructures (EpiLab)



#### STEFANO SANGUINETTI

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

#### QUANTUM DOT EMITTERS FOR QUANTUM PHOTONICS APPLICATIONS

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

#### NANOSTRUCTURED SEMICONDUCTORS FOR OPTOELECTRONICS

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

#### QUANTUM FUNCTIONAL MATERIALS FOR PHOTO-ELECTRO-CHEMICAL APPLICATIONS

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

## FUNDAMENTAL STUDY OF EPITAXIAL GROWTH OF SEMICONDUCTORS

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

#### FACILITIES

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





## Organic molecular films and heterostructures

#### ADELE SASSELLA

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

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

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

#### FACILITIES

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

carried out as a function of temperature, down to few K, under polarized light and at different incidence angles. Atomic force microscopy is used ex-situ for the morphology characterization of all the samples and for the study of the film growth process; morphology is usually checked over sereval  $\mu m^2$  wide regions, while on crystalline samples molecular resolution is also achievable.





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



#### ANNA GALLI, MARCO MARTINI, EMANUELA SIBILIA

#### THE ARCHAEOMETRY LAB

**S**ince 1980 our activity focused on the application of scientific techniques to archaeology, geology and cultural heritage, in particular in the field of absolute dating and characterization of archaeological materials.

Thermoluminescence (TL) and optically stimulated luminescence (OSL) are used to determine the event of ceramics firing and sediment deposition respectively. Other available techniques are dendrochronology and radiocarbon. Recently, we started investigating the new Rehydroxylation (RHX) dating technique, based on the water gain of pottery after firing in kiln.

Our research also deals with non-invasive spectroscopic methods, mainly performed using portable instruments, to study polychrome artefacts of various kind (paintings on boards, enamels, decorated ceramics, metal artifacts ...).

The laboratory is member of CUDaM (Centro Universitario Datazioni Università di Milano Bicocca amd of BIPAC, Centro Ricerche per il Patrimonio Storico, Artistico e Culturale.

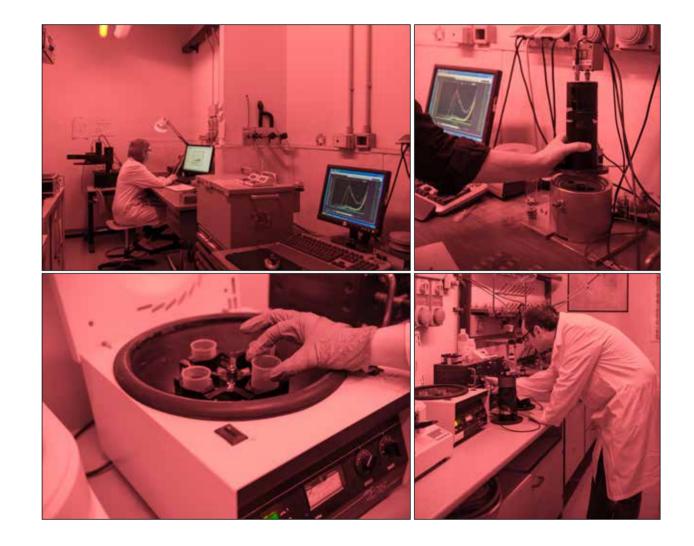
The laboratory is associate member of EURADOS (European Radiation Dosimetry Group, Working Group 10), of MODIS (Mortar Dating Intercomparison Study) and of the RHX International Research group to validate and study the rehydroxylation dating technique.

Since 2012 the laboratory is a first level hub in the CH\_NET E-RIHS Italian cultural heritage network.

#### **RESEARCH LINES**

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

Development of portable systems for in situ XRF analysis



## Singular elliptic equations: asymptotic analysis, unique continuation, spectral stability for singularly perturbed problems



#### VERONICA FELLI

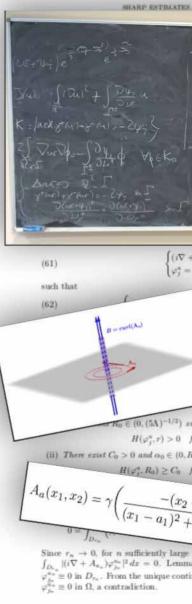
The following problem are investigated:

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

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

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

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



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# Functional dyes and pigments for photonics, electronics and optoelectronics



#### LUCA BEVERINA

**O**rganic-conjugated compounds have experienced over the last decades a tremendous interest as versatile and highly performing active components in a large variety of devices and applications including, among the others, OLEDs, OFETs, solar cells, sensors, photodetectors, electrochromic devices, anti static coatings and actuators. The vast majority of the above mentioned applications rely on the peculiar nature of the charged states in organic semicondutors, namely: a strong electron-phonon coupling and a major dependence of optical properties on the doping process.We are currently exploring the ability of carefully designed organic materials to:

-change colour upon multiple oxidation and reduction processes (electrochromic devices); -convert incident Vis-NIR light in electric power (solar cells);

-show efficient photoconductivity in NIR window (photodetectors);

-absorb light all over the visible spectrum and convert it to efficient and concentrated NIR emission (luminescent solar concentrators).

#### LUMINESCENT SOLAR CONCENTRATORS

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

#### CONJUGATED ORGANIC MATERILAS FOR OPTELECTRONIC-SUMINESCENT SOLAR CONCENTRATORS

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

#### **OTHER ACTIVITIES**

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



# Spinning NMR



#### SILVIA BRACCO, PIERO SOZZANI

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

#### CURRENT RESEARCH PROJECTS

**C**omposite materials based on ceramics and polymers and characterization of heterogeneous interfaces (elastomeric materials reinforced with silica, in-situ formation of silica by gelification in polymer matrices). Confinement of molecules and macromolecules to cylindrical nano- and mesotubes (cross section of 0.5, 1 and over 30 nm). Some matrices, showing extended interactive areas (>1200 m<sup>2</sup>/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 (<sup>129</sup>Xe) diffusing into solids, for microphases determination and nanoporosity by NMR.

#### FACILITIES

**N**MR 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<sup>-9</sup> torr) pump and equipment for hyperpolarized Xenon spectroscopy -laser excited NMR). Dynamic Mechanical Analyzer, Differential Scanning Calorimetry Gel Permeation Cromatography and access to large NMR facilities.



## Organic functionalized materials for optoelectronic applications and thermally and photochemically activate organic systems with cross-linking potentials



#### **A**NTONIO **P**APAGNI

The current research interests are focused both in the field of functional organic materials and in developing thermally and photochemically generated reactive species with a potential application in cross-linking of polymers and biomacromolecules.

#### ORGANIC SEMICONDUCTORS

The first line involves the planning and synthesis of new organic molecular and or polymeric organic semiconductors as active components in different type of devices such as, for example, Field Effect Transistors (OFETs), Light Emitting Diodes (OLEDs) Photovoltaics cells (OPVs) and organic-based water photosplitting systems. Within this field,

recently the interest has been focused on organic heterocycle-based n-semiconductors as tetracene based p-type ones.

#### P-TYPE SEMICONDUCTORS

Strategies for the preparation of p-type semiconductors such as oligothiophenes and tetracenes, starting from the suitable commercially available or on purpose prepared precursors, are planned and realized. Polymeric semiconductors, including Donor-Acceptor ones, are prepared by cross-coupling reaction using transition metal catalysts (Still and Suzuki protocols) from suitable electron-rich and electro-deficient monomers.

#### **N-TYPE SEMICONDUCTORS**

The introduction of fluorine atoms into aromatic and heteroaromatic systems is the strategy used for preparing n-type semiconductors such as polyfluoroacridine and polyfluorophenazines and polymers containing these units. The starting polyfluorinated-acridines and phenazine are accessible from commercially available polyfluorinated anilines and ketones. It is noteworthy that perfluorinated phenazines show very low HOMOs and LUMOs and, for these properties, proposed in photooxidation processes of water.

Parallel to these research activities, the synthesis of bromo containing polycyclic aromatic are prepared for conducting thermally activated Ullmann-like cross coupling reaction onto the surface of Cu, Ag and Au crystals. These processes will allow to realize graphenic structures on the surface of these crystals.

#### **CROSS-LINKING SYSTEMS**

The second research line is addressed to synthesize molecules or to develop new organic systems able to produce, thermally and photochemically, highly reactive species (carbenes and nitrilimines). These species are involved in cross-linking processes of protein-base biomolecules or polymeric materials



# Synthesis and characterization of novel polymeric nanostructures



#### **R**OBERTO **S**IMONUTTI

**N**anostructured 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).

**R**ecently, 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.

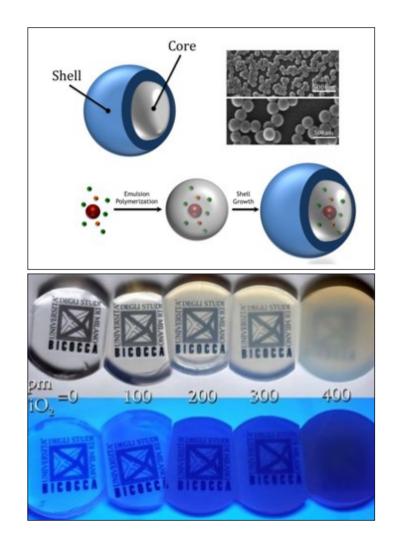
#### NANOPARTICLE POLYMER NANOCOMPOSITES

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.

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

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

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





## **Optics and Optometry**



#### SILVIA TAVAZZI

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

#### MATERIALS FOR CONTACT LENSES

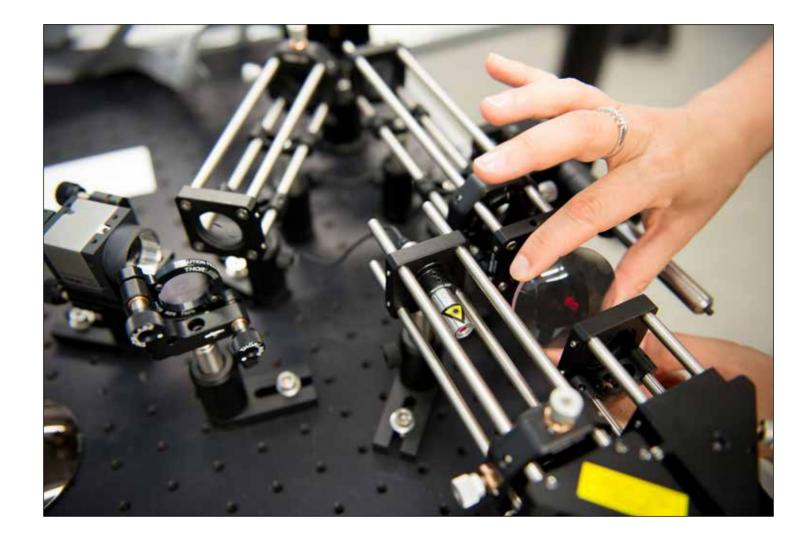
**R**ecent studies were focused on the properties of materials for soft contact lenses in terms of microscopic structure and uptake/release of hyaluronan, lactoferrin, and drugs. Different materials were investigated. The uptake was studied in terms of loading capability, penetration depth in the lens,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

#### **OPTICAL SYSTEMS**

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

#### FACILITIES

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





Project/Research Contract Title	Funded by	Principal Investigator
Ab initio simulation of chalcogenide materials	MICRON SEMICONDUCTOR ITALIA	M. Bernasconi
Exploitation of self-assembly and photochemistry for the straight- forward, low cost production of nanostructured organic photovoltaic devices	FONDAZIONE CARIPLO	L. Beverina
Nuovi materiali coniugati per celle solari organiche	ENI	
CHEETAH-Cost-reduction throughmaterial optimisation and Highrt EnErgy outpuT of solAr pHotovoltaic modules-joining Europe's re- search and Development efforts in support of its PV industry	EU	
Caratterizzazione di silicio multicristallino cresciuto in condizione di microgravità, a partire da silicio metallurgico	AGENZIA SPAZIALE ITALIANA (ASI)	S.Binetti
PLS - PN - Scienza dei Materiali	MIUR	
Sviluppo di strati buffer per celle a base di CZTS	ENEA	
Caratterizzazione e la relativa analisi di celle solari ad alta efficienza tramite misure di risposta spettrale	CESI	
Crescita e caratterizzazione di film sottili di calcogenuri per applicazioni FV	RSE	
KiC- Raw Materials @schools 3.0	EU	
Misure di spettroscopia Raman per la caratterizzazione dello stress indotto nel silicio	CNR	E. Bonera
THINFACE-Thin-film Hybrid Interfaces: a training initiative for the design of next-generation energy devices	EU	G. Brivio
Electronic Doped Colloidal Nanocrystal Heterostructures for transformational Breakthrought in solid-state lighting	FONDAZIONE CARIPLO	S. Brovelli
Realizzazione di preforme e caratterizzazione di fibre scintillanti da impiegare come elementi di sensori di radiazione ionizzante	PRYSMIAN	N. Chiodini
Nanoporous materials with tailored structure for high performance methane storage and purification	MIUR	A. Comotti

## FUNDED PROJECTS

Project/Research Contract Title	Funded by	Principal Investigator
Biomethane low impact production and carbon dioxide bio-capture for circular economy BALANCE	FONDAZIONE CARIPLO	
KiC- LIGHTBODY- Infrastructure and expertise network for Light- weight mobility: body and chassis	EIT RAW MATERIALS GMBH	
Meccanismi di attivazione della CO2 per la progettazione di nuovi materiali per l'efficienza dell'energia e delle risorse	MIUR	
BIOINOHYB-Smart Bioinorganic Hybrids for Nanomedicine	EU	
DECORE-Direct ElectroChemical Oxidation Reaction of Ethanol: optimization of the catalyst/support assembly for high temperature operation	EU	C. Di Valentin
Nuovi materiali fotocatalitici per la conversione di energia solare basa- ti su eterogiunzioni	FONDAZIONE CARIPLO	
Oltre il grafene: strati di carbonio nanostrutturati disegnati su misura per ottenere nuovi materiali per la catalisi e la chimica sostenibile	MIUR	
A new course on the Physics and technology of semiconductor devic- es with hand-on activity in a characterization and simulation lab	MICRON TECHNOLOGY FOUNDA- TION INC	M. Fanciulli
Variational methods, with applications to problems in mathematical physics and geometry	MIUR	V. Felli
Nanostructured oxide-in-oxide glasses for solar-blind UV-monitoring of work-safety and energy-saving in electric power distribution	FONDAZIONE CARIPLO	R. Lorenzi
MOBARTECH: una piattaforma mobile tecnologica, interattiva e partecipata per lo studio, la conservazione e la valorizzazione di beni storico-artistici	REGIONE LOMBARDIA	M. Martini

## Project/Research Contract Title

Multimodal nanotracking for exosome-based therapy in dmd ryenhancing)
Luminescent solar concentration windows for next generation gintegrated photovoltaics
CHALLENGE: 3C-SiCHetero-epitaxiALLy grown on silicon c ancE substrates and new 3C-SiC substrates for sustaiNable band-Gap powEr devices
Materiali per Up-conversion a bassa potenza con applicazio Solare e nella Bio-teranostica Multimodale
Theoretical analysis of the dislocation distribution in SILTRON Si (001) graded layers
Advanced Simulation Design of Nanostructured Thermoelectric rials with Enhanced Power Factors
NANOTHERMA
Solar driven chemistry: new materials for photo- and electro-c (SMARTNESS)
Cascade deoxygenation process using tailored nanocatalyst production of biofuels from lignocellulosic biomass
CATSENSE
Ossidi Nanostrutturati: multi-funzionalità e applicazioni
KiC- IMAGINE- Development and implementation of EIT KIC Materials Master Program(s) in Sustainable Materials
Spin optoElectronics ARCHitectures based on group IV composed on group I
Sviluppo di materiali elettrodici per batterie ricaricabili a sodi
Give Sodium a Chance! Investigation of nanostructured mix oxides as electrode materials for energy storage
Preparazione e caratterizzazione elettrochimica di materiali e per batterie a ioni sodio (NIB)
4PHOTON-Novel Quantum Emitters monolithically grown on and III-V substrates
COSMITO - COmpressive Sampling Multispectral Imaging car remoTe Observation
COSMOS

	Funded by	Principal Investigator
(theo-	MINISTERO DELLA SALUTE	F. Meinardi
buildin-	UNIMIB-INNOVATION GRANT	
compli- e wide-	EU	L. Miglio
ne nel	REGIONE LOMBARDIA	A. Monguzzi
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mera for	REGIONE LOMBARDIA	S. Sanguinetti
	FONDAZIONE CARIPLO	

Project/Research Contract Title	Funded by	Principal Investigator
FemToTera- Plasmon-enhanced Tera-Hertz emission by Femtosecond laser pulses of nanostructuredsemiconductor/metal surfaces	EU	
TEcnologie INnovative per i VEicoli Intelligenti	REGIONE LOMBARDIA/EU	
Micro-crystals Single Photon InfraREd detectors – $\mu$ SPIRE – Horizon 2020 FET project	EU	
Studio di specchi piani a multistrato attraverso misure di riflettanza ed ellissometria spettroscopica	MEDIA LARIO	A. Sassella
Rational design of hybrid organic-inorganic interfaces: the next step towards advanced functional materials – Action MP1202	EU	R. Scotti
Augmented Environment for Control in amyotrophic lateral sclerosis	ARISLA - AGENZIA DI RICERCA PER LA SCLEROSI LATERALE AMIOTRO- FICA	
Influence of cylindrical power on visual functions and performance	HOYA HOLDING	S. Tavazzi
Contratto di licenza per la distribuzione e la vendita dell"apparato ENDOKER	FRASTEMA OPHTHALMICS	
Analisi optometriche in soggetti non abbienti	FONDAZIONE ONESIGHT	

Project/Research Contract Title
AIDA 2020-Advanced European Infrastructures for Detectors a erators
INTELUM-International and intersectoral mobility to develop ad scintillating fibres and Cerenkov fibres for new hadron and jet eters for future colliders
KiC-OPTNEWOPT - Materials substitution in optoelectronic d
IDS-FunMat-Inno-2. International Doctoral School in Functiona rials & Innovation
ASCIMAT- Increasing the scientific excellence and innovation of in Advanced Scintillation Materials of the Institute of Physics for Czech Academy of Sciences
EIT-RM SPARK - Substitution and recycling of critical eleme materials for ionizing radiation detection
PLS - Scienza dei Materiali - 2015-2018

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## PUBLICATIONS PHD THESES

## Articles 2018 by impact factor (IF) 30 25 20 15 10 5 0 2-3 3-4 4-6 6-10 10-20 >20 <2 IF

# INTERNATIONAL JOURNALS

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1	Abatangelo, L; Felli, V; Noris, B; Nys, M, <i>Estimates for eigenvalues of Aharonov-Bohm operators with varying poles and non-half-integer circulation</i> , ANALYSIS & PDE 11, 1741	1,75
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3	Acciarri, M; Le Donne, A; Marchionna, S; Meschia, M; Parravicini, J; Gasparotto, A; Binetti, S, <i>CIGS thin films grown by hybrid sputtering-evaporation method: Properties and PV performance</i> , SOLAR ENERGY 175, 16	4,374
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5	Albani, M; Assali, S; Verheijen, M; Koelling, S; Bergamaschini, R; Pezzoli, F; Bakkers, E; Miglio, L, <i>Critical strain for Sn incorporation into spontaneously graded Ge/GeSn core/shell nanowires</i> , NANOSCALE 10, 7250	7,233
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128	Villa, I; Villa, C; Monguzzi, A; Babin, V; Tervoort, E; Nikl, M; Niederberger, M; Torrente, Y; Vedda, A; Lauria, A, <i>Demonstration of cellular imaging by using luminescent and anti-cytotoxic europium-doped hafnia nanocrystals</i> , NANOSCALE 10, 7933	7,233
129	Villa, P; Pollarolo, L; Conforti, J; Marra, F; Biagioni, C; Degano, I; Lucejko, J; Tozzi, C; Pennacchioni, M; Zanchetta, G; Nicosia, C; Martini, M; Sibilia, E; Panzeri, L, <i>From Neandertals to modern humans: New data on the Uluzzian</i> , PLOS ONE 13, 1	2,766
130	Xing, G; Bassanetti, I; Ben, T; Bracco, S; Sozzani, P; Marchiò, L; Comotti, A, <i>Multifunc-</i> <i>tional Organosulfonate Anions Self-Assembled with Organic Cations by Charge-Assist-</i> <i>ed Hydrogen Bonds and the Cooperation of Water</i> , CRYSTAL GROWTH & DESIGN 18, 2082	3,972
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132	Zeri, F; Naroo, S; Zoccolotti, P; De Luca, M, Pattern of reading eye movements during monovision contact lens wear in presbyopes, SCIENTIFIC REPORTS 8, 15574	4,122





## CONFERENCES AND SEMINARS

#	Authors and Title (by first author's name)	Conference/Workshop
1	Albani, M; Ghisalberti, L; Bergamaschini, R; Friedl, M; Salvalaglio, M; Voigt, A; Montalenti, F; Fontcu- berta i Morral, A; Miglio, L, <i>Modelling the kinetic</i> <i>growth mode of GaAs nanomembranes</i>	NANO-structures and nanomaterials SEIf-Assembly (NANOSEA), Carquei- ranne, French Riviera
2	Bernasconi, M, Atomistic Simulation of Crystal- lization Kinetics and Aging of amorphous GeTe Nanowires. INVITED	Glass & Optical Division Annual Meeting of the American Ceramical Society, San Antonio (USA)
3	Bernasconi, M, <i>Atomistic Simulations of Crystalli-</i> <i>zation and Aging of Amorphous GeTe Nanowires</i> . INVITED	"Symposium FM - Emerging Materi- als, Technologies and Applications for Non-volatile Memory Devices" of the CIM- TEC 2018 Conference, Perugia
4	Bernasconi, M, <i>Large Scale Atomistic Simulations</i> <i>of Phase Change Materials</i> . INVITED	European Phase Change and Ovonics Symposium 2018, Catania
5	Beverina, L, Efficient Suzuki-Miyaura micellar Cross-Coupling in water, at room temperature and under aerobic atmosphere. Organic materials go green. INVITED	Nuovi Orientamenti nella sintesi organi- ca, Università degli Studi di Milano XXXII Convegno 27 Novembre 2017, Milan, Italy
6	Beverina, L, Organic Materials for Solid state re- chargeable batteries and electrochromic devices. INVITED	First Enerchem School, Firenze

7	Bietti, S; Basso Basset, F; Reindl, M; Esposito, L; Fedorov, A; Huber, D; Rastelli, A; Bonera, E; Trotta, R; Sanguinetti, S, <i>High-Yield Fabrication of Entan- gled Photon Emitters for Hybrid Quantum Network-</i> <i>ing Using High-Temperature Droplet Epitaxy.</i> INVITED	ICPS International Conference of Physics of Semiconductors, Montpellier, France
8	Binetti, S, Photoluminescence and infrared spec- troscopy for impurities identification in silicon for photovoltaic applications. INVITED	The 8th Forum on the Science and Tech- nology of Silicon Materials 2018, Okaya- ma JAPAN
9	Binetti, S, The current status and future prospects of chalcogenide thin film solar cells. INVITED	GEI 2018 Giornate dell'Elettrochimica Italiana, Sestriere (TO) , Italy
10	Bracco, S; Comotti, A; Negroni, M; Castiglioni, F; Pedrini, A; Sozzani, P, Ultra-fast <i>Molecular Rotor</i> <i>Dynamics and their Regulation in Nanoporous</i> <i>Architectures</i>	Euromar Nantes 2018, European Magnet- ic Resonance Meeting, (1 - 5 July 2018), Nantes, France
11	Campione, M; Villa, C; Santiago-González, B; Bon- aldo, C; Villa, I; Vedda, A; Alessandrini, F; Erratico, S; Zucca, I; Bruzzone, M; Forzenigo, L; Malatesta, P; Mauri, M; Trombetta, E; Brovelli, S; Torrente, Y; Meinardi, F; Monguzzi, A, <i>Composite functional</i> <i>nanomaterials for multimodal imaging and pho-</i> <i>to-dynamic therapy of sick tissues.</i>	Nanoscience & Nanotechnology 2018 - Laboratori Nazionali di Frascati, Frascati (RM)
12	Chin, R; Zhu, Y; Coletti, G; Binetti, S; Le Donne, A; Pollard, M; Hameiri, Z, <i>Insights into Striations</i> <i>in N-type Czochralsky wafers investigated via</i> <i>low-temperature hyperspectral and tempera-</i> <i>ture-dependent spectral photoluminescence.</i>	10th International Workshop on Crystal- line Silicon for Solar Cells, Sendai (Japan)
13	Comotti, A, Innovative methods for CO <sub>2</sub> recovery: nanoporous materials. INVITED	International Autumn school "From waste to microalgae: an example of circular economy" (22nd – 23rd October 2018), Gargnano, Brescia

14	<i>Comotti, A, Structure, dynamics and gas detection in porous solids: the crystallographic and NMR perspectives. INVITED</i>	CHANCES: CrystallograpHy And NMR in ComplEmentary Structural investigations - University of Florence, Firenze, Italy		21	Di Valentin, C; Fazio, G; Selli, D; Seifert, G, ling Realistic TiO <sub>2</sub> Nanoparticles, Their Phot vation and Interaction with Water. INVITED
15	Comotti, A, Switchable Rotor Dynamics in Crystal- line Porous Architectures. INVITED	Crystal Engineering - Gordon Research Conference "Progress in Crystal Engi- neering - Design, Properties, and Func- tion", Newry, ME, USA	-	22	Di Valentin, C; Liu, H, From bulk to (001) su $Fe_3O_4$ : electronic properties and water adso INVITED
16	Comotti, A; Bracco, S; Castiglioni, F; Negroni, M; Alite, F; Sozzani, P, Ultra-fast Molecular Rotors in Porous Supramolecular Architectures and Dynam- ics Control by Chemical Stimuli. INVITED	7th EuCheMS Chemistry Congress (Liver- pool, UK, 26–30 August 2018), Liverpool, UK		23	Di Valentin, C; Selli, D; KAVIANI BAGHBAD ANI, M; Liu, H; Datteo, M; Ronchi, C, Mode Realistic TiO <sub>2</sub> Nanoparticles, Their Photoact and Interaction with Water. INVITED
17	Comotti, A; Bracco, S; Castiglioni, F; Pedrini, A; Sozzani, P, Dynamics and Flexibility in Gas-ab- sorptive Porous Materials. INVITED	ISMS III - International Symposium for Materials Scientists III (Osaka, Japan, 3-4 dicembre 2018), Osaka, Japan		24	Di Valentin, C; Selli, D; Kaviani, M, Quantur ical simulations of stimuli-responsive nanon for biomedical applications. INVITED
18	Comotti, A; Bracco, S; Sozzani, P; Pedrini, A; Cas- tiglioni, F, Porous Supramolecular Architectures: Ultra-fast Molecular Rotors and Dynamics Control by Chemical Stimuli.	PoMoS, Meeting on Porous Molecular Solids, Vietri sul Mare, Italy		25	Facchinetti, I; Ruffo, R; Beverina, L; Sassi, I Fontanesi, C; Vanossi, D, <i>The role of electro</i> <i>ions on the electrochemical properties of the</i> <i>based conducting polymers.</i>
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19	Comotti, A; Catiglioni, F; Bracco, S; Pedrini, A; Per- ego, J, Porous Crystalline Architectures: Ultrafast	ECM31 2018 European Crystallographic Meeting, Oviedo, Spain	]		INVITED
	Molecular Rotors and Dynamics Control by Gas Stimuli. Keynote			27	Fasoli, M, Optically stimulated luminescenc defects energy levels in RE-doped LuAG cr INVITED
20	Cova, F; Lucchini, M; Pauwels, K; Auffray, E; Chio- dini, N; Fasoli, M; Moretti, F; Mares, J; Jary, V; Nikl, M; Vedda, A, Dual response of RE-doped sol-gel silica fibers to high energy electrons.	International Conference on Luminescent Detectors and Transformers of Ionizing Radiation, LumDetr 2018, Prague, Czech Republic			

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ntum chem- nomaterials	Workshop on Electronic Excitations ETSF, Milano
si, M; ctrolyte f thiophene	The Annual Meeting of the International Society of Electrochemistry, Bologna, Italy
and	TO-BE COST Action "Towards Ox- ide-Based Electronics" Sping Meeting 2018, Sant Feliu de Guíxols, Catalonia, Spain
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28	Fiore, M; Longoni, G; Santangelo, S; Pantò, F; Stelliano, S; Frontera, P; Antonucci, P; Ruffo, R, Improving the electrochemical behaviour of highly abundant, low cost iron oxide as anode material for sodium-ion rechargeable batteries.	GEI 2018 Giornate dell'Elettrochimica Italiana, Sestriere (To)
29	Fiore, M; Santangelo, S; Pantò, F; Frontera, P; Antonucci, P; Ruffo, R, <i>Iron based materials for</i> <i>electrochemical energy storage.</i>	The Annual Meeting of the International Soci- ety of Electrochemistry, Bologna, Italy
30	Gabardi, S; Sosso, G; Behler, J; Bernasconi, M, Priming effects in the crystallization of the phase change compound GeTe from atomistic simula- tions. INVITED	Faraday Discussion: "New memory para- digms: memristive phenomena and neuromor- phic applications", Aachen (D)
31	Galli A., L. Panzeri, M. Martini, F. Maspero, E. Sibil- ia, L. Kakani, P. Rondini, R. Poggiani Keller, <i>Rock</i> <i>surface luminescence dating of monoliths from the</i> <i>megalithic sanctuary of Ossimo-Pat</i> (Valle Camon- ica, Italy)	42nd International Symposium on Archaeom- etry, Merida; Mexico
32	Galli A., M. Martini, F. Maspero, L. Panzeri, E. Sibil- ia, <i>Latest results in OSL mortar dating</i> at Milano Bicocca Laboratory	42nd International Symposium on Archaeom- etry, Merida; Mexico
33	Ismaeel, R; Masoudi, A; Wang, Y; Talataisong, W; Chiodini, N; Lee, T; Beresna, M; Brambilla, G, <i>Giant Faraday rotation in gadolinium doped silica</i> <i>optical fibers for high performance optical isolators</i> .	Optical Fiber Communication Conference, OFC 2018, San Diego, USA
34	Lee Chin, R; Zhu, Y; Coletti, G; Binetti, S; Pollard, M; Hameiri, Z, Insights into Bulk Defects in n-type Monocrystalline Silicon Wafers via Tempera- ture-Dependent Micro-Photoluminescence Spec- troscopy.	IEEE World Conference on Photovoltaic Energy Conversion, WCPEC 2018 10-15 June, Waikoloa Village; United States
35	Lorenzi, R, Identification of a new defect in dia- monds: application of Raman spectrometers be- yond Raman scattering. INVITED	Raman Workshop, Zurich, Swiss

36	Lorenzi, R; Remondina, J; Golubev, N; Ig E; Sigaev, V; Sassella, A; Trabattoni, A; A
	M; Paleari, A, Charge transport in oxide-in nanostructured silica-based dielectrics. INVITED
37	Lorenzi, R; Ziaytdinova, M; Jarý, V; Palea Sigaev, V; Nikl, M; Fasoli, M; Golubev, N, <i>luminescence of yttria-aluminoborate glas</i> <i>huntite-like composition.</i>
38	Lorenzi, R; Ziaytdinova, M; Paleari, A; Sig Nikl, M; Golubev, N, <i>Radioluminescence</i> earth doped yttria-aluminoborate glasses tite-like composition.
39	Maspero F., A. Galli, M. Martini, L. Panze cia, E. Sibilia, Thermoluminescence (TL) the clay-cores of the Colosso di Barletta: fusion phases
40	Meinardi, F, Advances and Challenges in cent Solar Concentration for Building Inte Photovoltaics. INVITED
41	Montalenti, F , <i>Theoretical interpretation of ing-angle maps in heteroepitaxial films</i> . INVITED
42	Mostoni, S; Susanna, A; D'Arienzo, M; Di co, B; Hanel, T; Morazzoni, F; Scotti, R, T the up-scaled production of highly disper- nanoparticles on silica as novel catalyst f industrial rubber vulcanization process.
43	Narducci, D, Enhancing solar energy con by hybrid photovoltaic thermoelectric cell INVITED

Acciarri, in-oxidevanced Dielectrics and related Devices, Bariari, A; , Radio- sses withLUMDETR 2018 - International Con- ference on Luminescent Detectors and Transformers of Ionizing Radiation, Prague, Czech Republicgaev, V; of rare s with hun-CCC 2018 - 70th Crystal Clear Confer- ence general meeting, CERN - Genevarri, M. Cac- study of dating itsX Congresso nazionale dell'Associazione Italiana di Archeometria, Torino, Italiaof tilt-ISTDM/ICSI 2018, Potsdam (Germany)of tilt-Advanced Inorganic Material, AIM 2018, Padova, ItalyoversionCIMTEC 2018, Perugia, Italy		
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	nversion ls.	CIMTEC 2018, Perugia, Italy

44	Negroni, M; Bracco, S; Comotti, A; Bezuidenhout, C; Bassanetti, I; Marchiò, L; Sozzani, P, <i>Reorienta-</i> <i>tion jumps and energy profile for Xe diffusing from</i> <i>site to site along the channels of porous molecular</i> <i>crystals.</i>	Xemat 2018_International Xenon Sym- posium (Philadelphia, USA, 5 – 8 May 2018), Philadelphia, USA
45	Pacchioni, G, <i>Characterization of catalysts: theo-</i> <i>retical view.</i> INVITED	EFCATS School on Catalysis, Liblice Castle (Czech Republic)
46	Pacchioni, G, <i>Computer driven materials discovery.</i> INVITED	KIC Raw Materials, CLC South Partners Meeting, Milano
47	Pacchioni, G, <i>Design of active catalysts from first principles: concepts, examples, and perspectives.</i> INVITED	Rideal Conference 2018 – Designing new catalytic processes to address global chal- lenges, Abington (UK)
48	Pacchioni, G, <i>Direct versus inverse catalysts: the role of metal/oxide interface.</i> INVITED	5th Cluster surface interaction workshop 2018, Trondheim (Norvegia)
49	Pacchioni, G, <i>Mixing CeO</i> <sup>2</sup> with ZrO <sup>2</sup> or ZnO for photo-catalysis: doping versus hetero-structures. INVITED	International Symposium on Energy and Enviornmental Photcatalytic Materials, Cracovia, Poland
50	Pacchioni, G, <i>New frontiers in nanotechnology.</i> INVITED	CRUI Meeting - Italy and Japan. Partners in research and education, Pavia
51	Pacchioni, G, <i>Role of electronic structure theory in catalysis: concepts, examples, and perspectives.</i> INVITED	Congresso Nazionale della Divisione di Chimica Industriale, Milano, Italy
52	Pacchioni, G, T <i>he crucial role of metal-oxide inter- faces in catalysis.</i> INVITED	VI San Luis Conference on Surface, Inter- faces, and Catalysis, Santa Fe (Argentina)

53	Pacchioni, G, <i>Tuning metal cluster properties: the important role of the support.</i> INVITED	Nano and sub-nano Clusters as the Smallest and Highly Tunable Interfaces – APS March Meeting, Los Angeles
54	Panzeri L., F. Maspero, A. Galli, M. Martini, E. Sibil- ia, <i>Rehydroxilation: researches and results from</i> <i>Milano-Bicocca lab</i>	42nd International Symposium on Archae- ometry, Merida; Mexico
55	Panzeri L., G. A. Galli, M. Martini, F. Maspero, E. Sibilia. <i>Luminescence and Radiocarbon dating of mortars</i>	MODIM 2018 (Mortar Dating International Meeting), Bordeaux, France
56	Pedrini, J; Perego, J; Bezuidenhout, C; Ronchi, A; Sozzani, P; Meinardi, F; Comotti, A; Monguzzi, A, <i>Triplet-Triplet Annihilation Based Photon Up-Con-</i> <i>version in Covalent Porous Aromatic Frameworks.</i>	MRS Spring Meeting 2018, Phoenix, Ari- zona (USA)
57	Perego, J, Highly <i>Porous Organic 3D Polymers for</i> <i>carbon dioxide capture and high-pressure methane</i> <i>storage.</i>	International Autumn school 22nd – 23rd October 2018 "From waste to microalgae: an example of circular economy", Gargna- no (Brescia), Italy
58	Perego, J; Piga, D; Bassanetti, I; Bracco, S; Co- motti, A; Sozzani, P, <i>Porous Organic Polymers for</i> <i>high pressure methane uptake and storage.</i>	mc2 Workshop "Materials, Characteriza- tion, and Catalysis" (ETH Zurich, Switzer- land, 15-17 January 2018), Zurich, Swit- zerland
59	Pezzoli, F, Challenges and perspectives of optical spin orientation applied to group IV heterostruc- tures. INVITED	50 years of optical orientation in semicon- ductors: From the original discovery to new horizons, Parigi, France
60	Pezzoli, F; De Cesari, S; Balocchi, A; Vitiello, E; Jahandar, P; Grilli, E; Amand, T; Marie, X; My- ronov, M, <i>Carrier and Spin Coherent Dynamics in</i> <i>Strained Germanium-Tin Semiconductor on Sili-</i> <i>con.</i>	International conference on the physics of semiconductors - ICPS, Montpellier, France
61	Pezzoli., F, <i>Spin-dependent phenomena in group</i> <i>IV semiconductors.</i> INVITED	International conference on supercon- ductivity and magnetism - ICSM, Antalya, Turkey

62	Rovaris, F; Gatti, R, <i>Multi-Scale Modeling of Plas-</i> <i>ticity: a Coupling between Dislocation Dynamics</i> <i>and FEniCS.</i>	FENICS'18 21-23 March, Oxford Universi- ty, United Kingdom
63	Rovaris, F; Isa, F; Gatti, R; Jung, A; Isella, G; Montalenti, F; von Kaenl, H, <i>SiGe/Si Vertical Het-</i> <i>erostructures: Switching the Dislocation Sign by</i> <i>Substrate Under-Etching.</i>	Joint ISTDM / ICSI 2018 Conference, Postdam, Germany
64	Rovaris, F; Zoellner, M; Zaumseil, P; Schubert, M; Di Gaspare, L; De Seta, M; Capellini, G; Schroed- er, T; Storck, P; Haeberlen, M; Schwalb, G; Richter, C; Schülli, T; Marzegalli, A; Montalenti, F, <i>Dynamics</i> <i>of cross-hatch evolution in heteroepitaxy.</i>	EMRS 2018 Fall meeting, Warsaw, Po- land
65	Ruffo, R; Fiore, M, <i>Reaction mechanisms and</i> structure properties correlations in carbonaceous anode materials for sodium ion batteries.	The Annual Meeting of the International Society of Electrochemistry, Bologna
66	Scotti, R; D'Arienzo, M; Di Credico, B; Mostoni, S; Susanna, A, <i>Double function filler for rubber rein-</i> <i>forcing and vulcanization.</i> INVITED	Plast 2018, Fiera Milano Rho
67	Sozzani, P; Bracco, S; Comotti, A; Bassanetti, I; Castiglioni, F; Negroni, M; Pedrini, A; Perego, J, <i>Switchable Dynamics and Flexibility in Gas-absorp-</i> <i>tive Porous Materials.</i> INVITED	Materials.it 2018 - Italian National Con- ference on Materials Science and Tech- nology (Bologna, October 22 - 26, 2018), Bologna, Italy
68	Sozzani, P; Comotti, A; Bracco, S; Perego, J; Piga, D, <i>Porous Materials: the Interplay with Linear Poly-</i> <i>mers.</i> INVITED	2nd PoMoS, Meeting on Porous Molecu- lar Solids (Vietri sul Mare, Italy, 6 - 8 June 2018)., Vietri sul Mare, Italy
69	Tavazzi, S, Proprietà ottiche di filtri vari. Come i filtri partecipano alla visione binoculare. INVITED	Congresso nazionale dell'albo degli ottici optometristi, Perugia, Italy

70	Tavazzi, S, Un'esperienza di ricerca inter are in contattologia in Italia. INVITED
71	Tawfilas, M; Mauri, M; Simonutti, R, <i>Com</i> tion of inorganic nanoparticles in polymer novel nanocomposite materials.
72	2 Tawfilas, M; Mauri, M; Simonutti, R, Fabri titanium dioxide nanocomposite materials matrix.
73	Thoraval, M; Blanken, N; Saleem, M; Ante Impact of a compound drop on a solid su
74	Trifiletti, V; Mostoni, S; Butrichi, F; Colom Bochicchio, E; Scotti, R; Binetti, S, <i>In situ</i> <i>mation of high quality kesterite thin films.</i>
75	5 Trifiletti, V; Mostoni, S; Scotti, R; Binetti, S SnS₄ precursor ink for spin coating depositechnique.
76	5 Trifiletti, V; Mostoni, S; Scotti, R; Binetti, S gel formation of high quality earth abunda cogenide thin film for PV application.
77	<sup>7</sup> Ugolotti, A; Brivio, G; Fratesi, G, Electron optical properties of hydrogenated Silicer Ag(111): a computational study.
78	B Ugolotti, A; Brivio, G; Gratesi, G, Hydroge Silicene on Ag(111): a theoretical investig through optical excitations.
79	Vedda, A, Characterization of defects in s and phosphors. INVITED
80	Vedda, A, Rare-earth doped silica-based ing fibers for ionizing radiation sensing. INVITED

rdisciplin-	V congresso Ailac, Roma, Italy
npatibiliza- r matrix for	Macrogiovani 2018: giornata di discus- sione su progetti di ricerca macromole- colare, Dipartimento di Ingegneria In- dustriale/DIIN dell'Università di Salerno, Fisciano (SA)
rication of Is with TPU	II XXIII Convegno Nazionale dell'AIM, l'Associazione Italiana di Scienza e Tec- nologia delle Macromolecole., Catania
tonini, C, <i>ırface</i> .	American Physical Society - Division Fluid Dynamics, Atlanta, Georgia, USA
nbo, M; <i>u gel for-</i>	1st ENERCHEM School, Firenze
S, Cu₂Zn- sition	E-MRS Spring Meeting and Exhibit, Stras- bourg, Francia
S, In situ lant chal-	E-MRS Spring Meeting and Exhibit, Stras- bourg (France)
nic and ne on	Materials.it, Bologna, Italy
enated gation	ETSF Workshop on Electronic Excitations (Interdisciplinary Views on Quantum Ma- ny-Body Theory), Milan, Italy
scintillators	Summer school on scintillation, dosimetric and phosphor materials, Prague, Czech Republic
l scintillat-	SPSSM 2018 – International Symposium on Structure-Property Relationships in Solid State Materials, Pescara, Italy
	A

81	Vedda, A, Thermally stimulated luminescence as a tool for the investigation of point defects in lumi- nescent materials. INVITED	Seminario presso ETH - Swiss Federal Institute of Technology Zurich,
82	Vedda, A; Villa, I, <i>The ESQUIRE project: Experi-</i> <i>ment with Scintillating QUantum dots for Ionizing</i> <i>Radiation Events.</i>	LUMDETR 2018 - Luminescent Detectors and Transformers of Ionizing Radiation, Prague, Czech Republic



## BOOKS AND CONTRIBUTIONS

1	Houssa, M., Scalise, E., Afanas'Ev, V., & Synthesis of silicene on alternative subs In "NanoScience and Technology" (pp. 1
2	Morazzoni, F. (2018). <i>Physical Methods in Inorganic Chemistry</i> Universitas Studiorum S.r.I Casa Editri
3	Narducci, D., Bermel, P., Lorenzi, B., Wa Hybrid and Fully Thermoelectric Solar H Springer International Publishing.
4	Pacchioni, G. (2018). <i>The Overproduction of Truth - Passion, o</i> Oxford University Press.
	3

& Stesmans, A. (2018). strates. 197-209). Springer Verlag.

ry. rice.

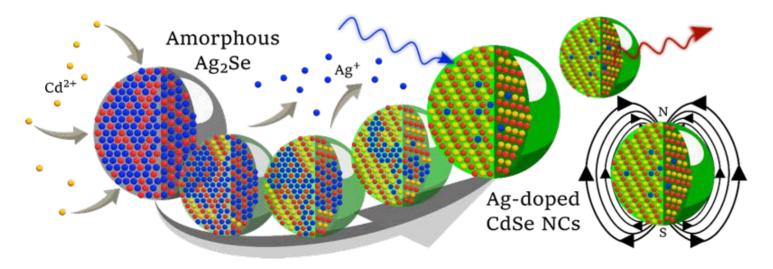
/ang, N., & Yazawa, K. (2018). *Harvesting.* 

competition, and integrity in modern science.

# HIGHLIGHTS

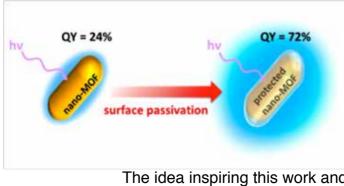
Pinchetti, V.; Di, Q; Lorenzon, M.; Camellini, A.; **Fasoli, M.**; Zavelani-Rossi, M.; **Meinardi, F**.; Zhang, J.; Crooker, S.A.; **Brovelli, S.**, *Excitonic pathway to photoinduced magnetism in colloidal nanocrystals with nonmagnetic dopants.* NATURE NANOTECHNOLOGY 13, 145 (2018)

Electronic doping of colloidal semiconductor nanostructures holds promise for future device concepts in optoelectronic and spin-based technologies. In this work, we combine optical, spectro-electrochemical and magnetic spectroscopies to show that the exciton recombination process in nanocrystals doped with nonmagnetic silver atoms is inextricably tied to photoinduced magnetism. As a result, Ag-doped nanocrystals exhibit optically-activated paramagnetic properties and concomitant sp–d exchange interactions between excitons and Ag dopants. These results represent the first demonstration that optically switchable diluted magnetic semiconductor nanomaterials can be obtained by exploiting the excitonic processes involving nominally nonmagnetic impurities.

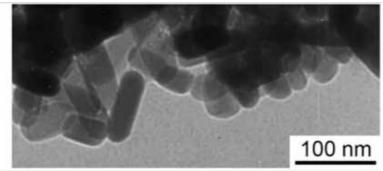


#### **Monguzzi, A**; Ballabio, M; Yanai, N; Kimizuka, N; Fazzi, D; Campione, M; **Meinardi, F**. *Highly Fluorescent Metal–Organic-Framework Nanocomposites for Photonic Applications*. NANO LETTERS, 18, 528 (2018)

Metal-organic frameworks (MOFs) are porous hybrid materials built up from organic ligands coordinated to metal ions or clusters by means of self-assembly strategies which allow to manipulate both the composition and ligands arrangement in order to control their optical and energy-transport properties. Therefore, optimized MOFs nanocrystals (nanoMOFs) potentially represent the next generation of luminescent materials with features like those of their inorganic predecessors, that is, the colloidal semiconductor guantum dots. The peculiarity of the nanoMOFs is the possibility to pack the ligand chromophores close enough to allow a fast exciton diffusion but sufficiently far from each other preventing the aggregation-induced effects of the organic crystals. In particular, the formation of strongly coupled dimers or excimers is avoided, thus preserving the optical features of the isolated molecule. However, nano-MOFs have a very small fluorescence quantum yield (QY). In order to overcome this limitation and achieve highly emitting systems, we analyzed the fluorescence process in blue emitting nano-MOFs and modeled the diffusion and quenching mechanism of photogenerated singlet excitons. Our results demonstrate that the excitons guenching in nano-MOFs is mainly due to the presence of surface-located, nonradiative recombination centers. In analogy with their inorganic counterparts, we found that the passivation of the nano-MOF surfaces is a straightforward method to enhance the emission efficiency. By embedding the nanocrystals in an inert polymeric host, we observed a +200% increment of the fluorescence QY, thus recovering the emission properties of the isolated ligand in solution.



# HIGHLIGHTS

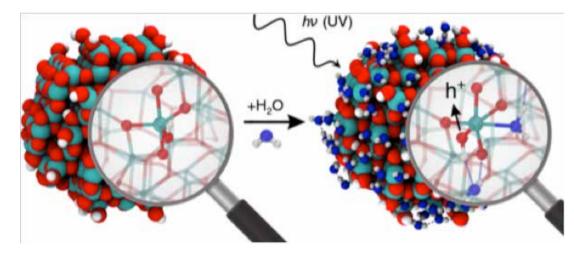


The idea inspiring this work and a TEM image of the studied nanoMOFs

# HIGHLIGHTS

Shirai, K.; Fazio, G.; Sugimoto, T.; Selli, D.; Ferraro, L.; Watanabe, K.; Haruta, M.; Ohtani, B.; Kurata, H.; Di Valentin, C.; Matsumoto, Y. Water-Assisted Hole Trapping at Highly Curved Surface of Nano-TiO, Photocatalyst. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 140, 1415 (2018).

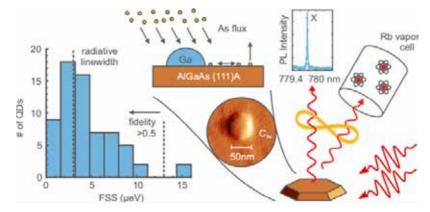
Heterogeneous photocatalysis is vital in solving energy and environmental issues that this society is confronted with. Although photocatalysts are often operated in the presence of water, it has not been yet clarified how the interaction with water itself affects charge dynamics in photocatalysts. Using water-coverage-controlled steady and transient infrared absorption spectroscopy and large-model (~800 atoms) ab initio calculations, we clarify that water enhances hole trapping at the surface of TiO<sub>2</sub> nanospheres but not of well-faceted nanoparticles. This water-assisted effect unique to the nanospheres originates from water adsorption as a ligand at a low-coordinated Ti–OH site or through robust hydrogen bonding directly to the terminal OH at the highly curved nanosphere surface. Thus, the interaction with water at the surface of nanospheres can promote photocatalytic reactions of both oxidation and reduction by elongating photogenerated carrier lifetimes. This morphology-dependent water-assisted effect provides a novel and rational basis for designing and engineering nanophotocatalyst morphology to improve photocatalytic performances.



Adsorbed water enhances hole trapping ability of superficial -OH groups on TiO<sub>2</sub> spherical nanoparticles.

Basso Basset, F; Bietti, S; Reindl, M; Esposito, L; Fedorov, A; Huber, D; Rastelli, A; Bonera, E; Trotta, R: Sanguinetti, S. High-Yield Fabrication of Entangled Photon Emitters for Hybrid Quantum Networking Using High-Temperature Droplet Epitaxy. NANO LETTERS 18, 505-512 (2018).

Metal-organic frameworks (MOFs) are porous hybrid materials built up from organic ligands coordinated to metal ions or clusters by means of self-assembly strategies which allow to manipulate both the composition and ligands arrangement in order to control their optical and energy-transport properties. Therefore. optimized MOFs nanocrystals (nanoMOFs) potentially represent the next generation of luminescent materials with features like those of their inorganic predecessors, that is, the colloidal semiconductor guantum dots. The peculiarity of the nanoMOFs is the possibility to pack the ligand chromophores close enough to allow a fast exciton diffusion but sufficiently far from each other preventing the aggregation-induced effects of the organic crystals. In particular, the formation of strongly coupled dimers or excimers is avoided, thus preserving the optical features of the isolated molecule. However, nano-MOFs have a very small fluorescence quantum yield (QY). In order to overcome this limitation and achieve highly emitting systems, we analyzed the fluorescence process in blue emitting nano-MOFs and modeled the diffusion and quenching mechanism of photogenerated singlet excitons. Our results demonstrate that the excitons quenching in nano-MOFs is mainly due to the presence of surface-located, nonradiative recombination centers. In analogy with their inorganic counterparts, we found that the passivation of the nano-MOF surfaces is a straightforward method to enhance the emission efficiency. By embedding the nanocrystals in an inert polymeric host, we observed a +200% increment of the fluorescence QY, thus recovering the emission properties of the isolated ligand in solution.



# HIGHLIGHTS

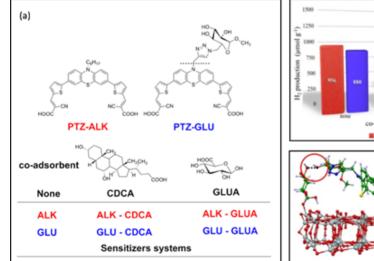
Quantum dots grown by droplet-epitaxy with a low fine structure splitting (FSS) can be used as a source of entangled photon pairs energy-matched with Rb-vapor cells for quantum information technology.

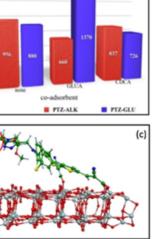
# HIGHLIGHTS

Manfredi, N., Monai, M., Montini, T., Peri, F., De Angelis, F., Fornasiero, P. & Abbotto, A. Dye-Sensitized Photocatalytic Hydrogen Generation: Efficiency Enhancement by Organic Photosensitizer-Coadsorbent Intermolecular Interaction. ACS ENERGY LETTERS 3, 85 (2018).

In dye-sensitized photocatalytic (PC) hydrogen generation the role of molecular antennas to optimize light harvesting is strategic. In this work we have organized self-assembled layers on the catalyst surface to control the efficiency of the electron injection from the dye excited state and minimize self-guenching. We have achieved this result by modifying the molecular structure of the dye with a sugar terminal, able to afford strong intermolecular bonds with a sugar-based spacer.

Dye-sensitized photocatalytic H2 generation has been investigated using a metal-free phenothiazine-based donor-acceptor sensitizer (PTZ-GLU) in combination with coadsorbents. The coadsorption of the PTZ-GLU dye, functionalized with a glucose end-group, in combination with a glucose-based coadsorbent, aff orded improved photocatalytic activity compared to the absence of coadsorbents, to the use of a conventional (chenodeoxycholic acid) coadsorbent, or by replacing the dye glucose functionality with an alkyl chain. The results suggest the strategic role of directional intermolecular dye- coadsorbent interactions on the semiconductor surface, as confirmed by first principles computational modeling, which likely suppressed detrimental recombination processes.





Structure of the sensitizers and coadsorbents (a); hydrogen production (b); theoretical

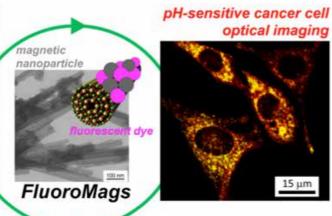
Villa, C; Campione, M; Santiago-González, B; Alessandrini, F; Erratico, S; Zucca, I; Bruzzone, M. G; Forzenigo, L; Malatesta, P; Mauri, M; Trombetta, E; Brovelli, S; Torrente, Y; Meinardi, F; Monguzzi A. Self-Assembled pH-Sensitive Fluoromagnetic Nanotubes as Archetype System for Multimodal Imaging of Brain Cancer.

#### ADVANCED FUNCTIONAL MATERIALS 1707582. (2018).

Fluoromagnetic systems are recognized as an emerging class of materials with great potential in the biomedical field. Here, it is shown how to fabricate fluoromagnetic nanotubes that can serve as multimodal probes for the imaging and targeting of brain cancer. An ionic self-assembly strategy is used to functionalize the surface of synthetic chrysotile nanotubes with pH-sensitive fluorescent chromophores and ferromagnetic nanoparticles. The acquired magnetic properties permit their use as contrast agent for magnetic resonance imaging, and enable the tracking of tumor cell migration and infiltration responsible for metastatic growth and disease recurrence. Their organic component, changing its fluorescence attitude as a function of local pH, targets the cancer distinctive acidity, and allows localizing and monitoring the tumor occurrence and progression by mapping the acidic spatial distribution within biopsy tissues. The fluoromagnetic properties of nanotubes are preserved from the in vitro to the in vivo condition and they show the ability to migrate across the blood brain barrier, thus spontaneously reaching the brain tumor after injection. The simplicity of the synthesis route of these geomimetic nanomaterials combined with their demonstrated affinity with the in vivo condition strongly highlights their potential for developing effective functional materials for multimodal theranostics of brain cancer.

# magnetic resonance in vivo imaging

tumor core



# HIGHLIGHTS

Magnetic resonance and optical imaging of tumor tissues and cells using multifunctional fluoromagnetic nanotubes (Fluoromags).

## **PHD THESES**

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

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

D. Asnaghi	Supramolecular porous crystals: anesthetic vapors uptake and enantioselective recognition properties
F. Basso Basset	GaAs nanostructures for the generation of entangled photons: design, development, and spectroscopy
D. Bertani	Synthesis and self-assembly of biocompatible amphiphilic block copolymers
P. Brazzo	New strategies for the controlled release of vulcanization curatives in rubber blends
F. Carulli	Novel materials for solar energy conversion devices: Towards industrial scaling-up
E. Cobani	Novel approach to rubber reinforcement by silica based nanofiller
G. Fazio	Ab initio modeling of the physical and (photo)chemical properties of realistic TiO2 nanoparticles in vacuum and in aqueous environment
D. Galliani	Poly(3,4-ethylendioxythiophene) based materials for thermoelectric applications
M. Lorenzon	Role of nonradiative surface defects on exciton recombination processes in semiconductor colloidal nanostructures
S. Mattiello	Variations on self-assembly of surfactant-based confined systems
V. Pinchetti	Advanced Spectroscopy of Interface Engineered, Doped and "Electronically" Doped Colloidal Semiconductor Nanocrystals
A. Ruiz Puigdollers	Catalytic Properties of Zirconia: Role of Nanostructuring and Metal-Oxide Interface
M. Rooney	Self-assembled, nanostructured organic materials for applications in electronics and optoelec- tronic devices.
E. Vitiello	Strain-dependent spin phenomena in Ge-based low dimensional structures

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1	Acciarri, M; Vodopivec, B; Binetti, S; Maurilio, Nuovi composti per la cattura di anidride carb ed impianto (l'invenzione tutela i composti dei #102015000086665
2	Acciarri, M; Vodopivec, B; Binetti, S; Maurilio, Nuovi composti per la cattura di anidride carb ed impianto (l'invenzione tutela l'impianto); #102015000086727
3	Acciarri, M; Vodopivec, B; Binetti, S; Maurilio, Novel compounds for the capture of carbon of cess and plant; #10,143,969
4	Antonini, C; Nylen, O; Geiger, T <i>Method of preparing a nano- and/or microsca</i> #EP18210076
5	Giannini, L; Tadiello, L; Hanel, T; Cobani, E; D Julve Sebastian, D Elastomeric materials for components of tyres #WO 2018078500
6	Tadiello, L; Cipolletti, V; Giannini, L; Hanel, T; Tagliaro, I Elastomeric compositions comprising silicate vehicles that comprise them; #WO 2018116125
7	Tadiello, L; Giannini, L; Hanel, T; Redaelli, M; New reinforcement materials, elastomeric cor #WO 2018078480

## TENTS

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bonica da miscele gassose e successivo rilascio, relativo procedimento

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dioxide from gaseous mixtures and subsequent release, related pro-

ale cellulose foam:

Di Credico, B; D'Arienzo, M; Scotti, R; Morazzoni, F; Perez Cacho, J;

es and tyres comprising modified silicate fibres;

F; Galimberti, M; Scotti, R; Di Credico, B; Morazzoni, F; D'Arienzo, M;

e fibres with needle-shaped morphology of nanometric size and tyres for

; D'Arienzo, M; Di Credico, B; Scotti, R; Morazzoni, F ompositions and tyres for vehicles wheels comprising the same;

# Facilities Centres

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## Consultancy

http://www.mater.unimib.it/servizi-imprese/prestazioni-conto-terzi

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

- Materials characterization
- Research projects
- Consultancy
- Training

Materials Characterization - Investigating the properties of materials such as:

- Structure/microstructure
- Composition
- Thermal behavior
- Morphology

- Optical, electric, electro-optical, magnetic properties
- Dating and characterization of ancient materials

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

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





CUDAM, CENTRO UNIVERSITARIO DATAZIONI E ARCHEOMETRIA MILANO BICOCCA www.cudam.mater.unimib.it

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. DEPART-MENT OF EARTH AND ENVIRONMENTAL SCIENCES. DEPARTMENT OF PHYSICS "G. OCCHIALINI", DEPART-MENT OF COMPUTER SCIENCES

Dating techniques: Thermoluminescence, Optically Stimulated Luminescence, Dendrochronology, Radiocarbon, RHX





**BIPAC**, CENTRO INTERDIPARTIMENTALE DI RICERCA SUL PATRIMONIO STORICO ARTISTICO E CULTURALE centrobeniculturali@unimib.it



BIPAC encourages the Third Mission of the University System and the University Social Responsibility. Promotes infotainment, public engagement programs as well as cultural and educational activities on Cutural Heritage in the wider possible contexts. Members of BIPAC are 12 over 14 departments of UNIMIB:

DIPARTIMENTO DI SCIENZA DEI MATERIALI, DIPARTIMENTO DI SCIENZE DELL'AMBIENTE E DEL TERRITORIO; DIPARTIMENTO DI FISICA, DIPAR-TIMENTO DI INFORMATICA, SISTEMISTICA E COMUNICAZIONE; DIPAR-TIMENTO DI SCIENZE UMANE PER LA FORMAZIONE RICCARDO MASSA: DIPARTIMENTO DI SOCIOLOGIA E RICERCA SOCIALE; DIPARTIMENTO DI GIURISPRUDENZA; DIPARTIMENTO DI PSICOLOGIA; DIPARTIMENTO DI BIOTECNOLOGIE E BIOSCIENZE; DIPARTIMENTO DI ECONOMIA, METO-DI QUANTITATIVI E STRATEGIE DI IMPRESA: DIPARTIMENTO DI SCIENZE ECONOMICO-AZIENDALI E DIRITTO PER L'ECONOMIA: DIPARTIMENTO DI STATISTICA E METODI QUANTITATIVI



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

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

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



Laboratory of Scanning Electron Microscopy and Microanalysis www.mater.unimib.it/utenti/sem/SEMWEB/

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

#### Instrument

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

## INTER-UNIVERSITY CENTER FOR NANOMETRIC EPITAXIAI STRUCTURES ON SILICON AND SPINTRONICS



## 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<sup>™</sup> 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 jons), milling (precision down to 10 nm) and deposition (with the insertion of a small needle delivering special gases).

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

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

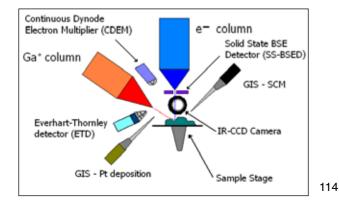
· on-line operations in which the SEM is used 'to film' the cross-section face while FIB mills normal to the surface:

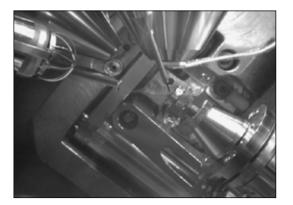
· the electron imaging of charging specimen in absence of metallization can take place before or after the FIB operations in the same chamber;

Charge neutralization of the sample with electron beam during FIB milling:

• Two gas injector systems (GIS) for selective carbon milling (SCM) and Pt deposition;

 Alternative use of the electron beam induce deposition instead of the ion beam induced deposition in order to deposit films and growth nanostructures in a milder way.







**MIB-SOLAR SOLAR ENERGY RESEARCH CENTER** www.mibsolar.mater.unimib.it

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

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

Main objectives of MIB-SOLAR are:

- Study and research of new materials and devices related to solar energy in its various forms;
- The aggregation and coordination of researchers in the field of solar energy:
- Training of young researchers in the field of materials science and technology for solar energy;
- The development of intellectual property of the University of Milano-Bicocca in the field of solar energy:
- Cooperation with institutions, public and private research centers, and Fondazioni in the field of solar energy; - Support and technology transfer to companies operating in the field of solar energy:

knowledge in the field of solar energy.

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

- a) and organic thin films;
- preparation and full characterization of materials and devices for solar fuels (artificial photosynthesis); 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 devices (sputtering system, nitrogen and argon filled glove boxes, e) laser scribing machine, titanium hotplates, screen printers, UV-ozone cleaners, etc.)
- f) main facilities for the full characterization of solar devices (solar simulators up to 6 x 6 inches, I/V char acterization, internal and external quantum efficiency, light soaking chamber for cell ageing, stability studies, electrochemical impedance spectrometer, mesurements of hydrogen and oxygen via water split ting under irradiation).

- Promotion of seminars, conferences, meetings and discussions for the study and exchange of information and

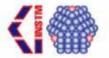
preparation and full characterization of materials and devices for photovoltaics, from silicon, to inorganic



**CNISM - CONSORZIO NAZIONALE INTERUNIVERSITARIO PER LE** SCIENZE FISICHE DELLA MATERIA www.cnism.it

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

- Growth and optical spectroscopy of semiconductor guantum 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 applica tions
- Theory of low dimensional materials
- Ab-initio simulations of materials for data storage



**INSTM - CONSORZIO INTERUNIVERSITARIO NAZIONALE PER LA** SCIENZA E LA TECNOLOGIA DEI MATERIALI www.instm.it

Our University participates in INSTM, the National Interuniversity Consortium of Materials Science and Technology; its local Research Units is hosted by the Materials Science Department. The INSTM Consortium was founded in order to provide organisational, technical and financial support to disseminate knowledge in the field of materials science and technology within its affiliate universities. Its efficiency in bringing together and managing their considerable talents creates an effective critical mass that renders them highly competitive in taking on innovative research projects.

General Fields of Research are: Advanced mechanics, construction and transport, Energy and environment, Systems for the preparation, transmission and storage of information, Health and Nutrition.

The success of INSTM is underlined by the sheer number and quality of the domestic and international projects involving INSTM's research groups that have been financed to date.



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



ETSF-European Theoretical Spectroscopy Facility www.etsf.eu

The University of Mllano 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.



## CORIMAV - CONSORZIO PER LA RICERCA SUI MATERIALI AVANZATI



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

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

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

### PLEGROWTH PILEGROWTH TECH S.R.L. TECH

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

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



www.galateabiotech.com

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



GRAFTONICA. TECNOLOGIE D'INNESTO, **INNESTO DI TECNOLOGIE** www.graftonica.it

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

#### GALATEA BIOTECH- THE WHITE BIOTECH COMPANY



GLASS TO POWER www.glasstopower.com

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

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

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





## CREDITS

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