Dipartimento di Scienza dei Materiali

Department of Materials Science

Department of excellence 2018-2022

ANNUAL REPORT 2022

UNIVERSITA' DEGLI STUDI DI MILANO BICOCCA

University of Milano - Bicocca

Front cover: SEM image of 3C-SiC nanoscale platelets grown on Silicon pillars via hot-wall low-pressure Chemical Vapour Deposition (provided by Prof. Leo Miglio)

Activity 2021

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THE DEPARTMENT OF MATERIALS SCIENCE

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

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Head: Prof. Alessandro Abbotto / *Prof.ssa Anna Vedda*

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 University of 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.

The Department was awarded Department of Excellence and granted a funding of more than 10 million euros in 2018 from the Ministry of University and Research of Italy.

STRATEGIC GOALS

General goals of the Department of Materials Science 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, solar energy, artificial photosynthesis, molecular electronics, laser, molecular modelling, insulator oxides, non-linear optics, polymers, semiconductors, sensors, organic and inorganic materials, superconductors, luminescence, glass, optical fibers. Beside the main spectroscopic and electrical characterization techniques, advanced materials analysis is achieved by means of many experimental techniques such as AFM, STM, ESR, TEM, FIB, NMR and a number of other advanced optical, magnetic, and electrical instrumentations.

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

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

The educational project aims at forming young professionals highly qualified in both physics and chemistry, able to fit their knowledge to the contemporary requirements of the related labor 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 fibers, ionic conductors, superconductors, organic and inorganic semiconductors, materials for solar energy, micro and opto-electronics, radiation detectors).

Degrees in Materials Science and in Chemical Science and Technology include a 1st cycle degree (Laurea, three years), followed by a 2nd cycle two-year specializing course (Laurea Magistrale).

The 1st cycle three-years course of Optics and Optometry gives important professional opportunities.

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

DEPARTMENT BOARD

HEAD

Alessandro Abbotto / *Anna Vedda*

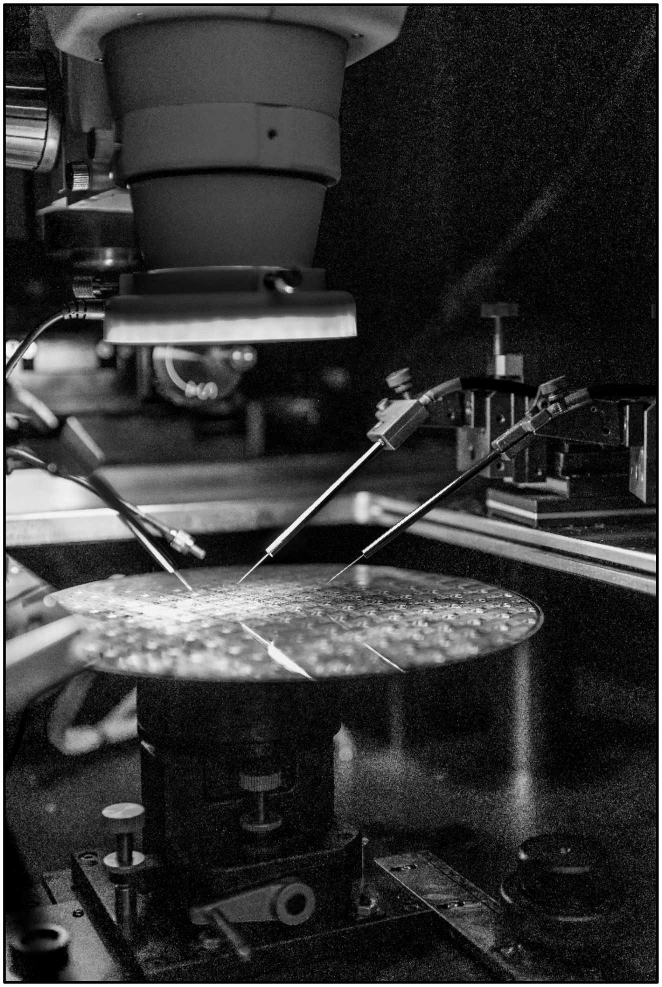
DEPUTY HEAD

Anna Vedda / *Piercarlo Mustarelli*

DEPARTMENT COUNCIL

(Head, Deputy Head, Head of Administration Office, Teaching Board, 3 elected faculty members, 1 elected representative of technical staff)

Alessandro Abbotto, Anna Vedda, Lucia Rodolfi, Simona Binetti, Angiolina Comotti, Adele Sassella, Norberto Manfredi, Antonio Papagni, Roberto Scotti, Giorgio Patriarca



TEACHING BOARD

Until October / *since November*

CHEMICAL SCIENCE

Simona Binetti / *Roberto Scotti*

MATERIALS SCIENCE

Angiolina Comotti

OPTICS AND OPTOMETRY

Adele Sassella

DOCTORATE

Marco Bernasconi

Francesco Montalenti (deputy)

DEPARTMENT OF EXCELLENCE 2018-2022

The project “Electrical Power and Energy Vectors from Renewable Sources - FLEXILAB” of the Department of Materials Science of the University of Milano – Bicocca is funded by the “*Fondo per il finanziamento dei dipartimenti universitari di eccellenza – D.L. n.232 del 11/12/2016, Vol I, Commi 314-338*”. Such competitive funding from the Italian Government was granted to the best 180 Italian Departments (807 in total) by means of a selection based on the Department productivity and the quality of a development project. The Department of Materials Science resulted among the best 11 in the area of Chemical Sciences. The total cost of FLEXILAB is 10.700.000 € with a direct funding from MIUR of 6.500.000 €. FLEXILAB has the ambition to constitute a Departmental Laboratory, open to collaboration with external stakeholders, on materials for a sustainable energy cycle.

The FLEXILAB project aims to make the Department a reference center in the development of sustainable energy materials and technologies through its value cycle. The Department can play a leading role, merging existing skills with others to be acquired. Energy supply with sustainable methods is a theme of great social impact. Recent data show that there is not a single successful technology capable of coping alone with the global energy problem, but rather a complex set of interdependent solutions aimed at both power generation and distributed networks. The project, fully in line with the priorities indicated by the European Strategic Energy Technology Plan (SET-Plan) dedicated to the development of technologies with low CO_2 emissions, will allow efficient and effective development of basic know-how and derived technologies, as well as training qualified researchers.

VISION

Five objectives will be pursued:

- Make the Department able to respond to the complex problem of sustainable energy in a structured way to the demanding tasks of the circular economy.
- Strengthen the research lines on innovative and sustainable materials for the production and efficient use of energy. Add expertise in the development of electrolyte materials, at the base of strategic technologies such as the electrochemical generation of hydrogen and its conversion (fuel cells).
- Realize a laboratory equipped with flexible and enabling infrastructures, FLEXILAB, which allows all lines of research to align on TRL ≥4, this way facilitating the transition from ideas to of devices
- Train young researchers with new skills and roles to make them able to approach the problem of sustainable energy as a whole, tackling problems ranging from the design and implementation of materials and technologies to the social, environmental and economic repercussions.
- Increase collaboration between universities and businesses.

Globally, the project aligns with the "Materials Research Science and Engineering Centers" (MRSEC) initiatives funded by the National Science Foundation for the purpose of developing interdisciplinary research programs integrated with an academic high-level training program at American universities.

WORK PACKAGES

- **WP1 - Photovoltaic cells**. Focus on new inorganic and hybrid thin films (e.g. perovskites) in order to realize tandem cells to reach 30% efficiency target. WP leader: Prof. M. Acciarri.
- **WP2 - 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. WP leader: Prof. R. Ruffo
- **WP3 - 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). WP leader: Prof. P. Mustarelli.
- **WP4 - 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. WP leader: Dr. N. Manfredi
- **WP5 - Hydrogen storage**. Focus on organic and metal-organic nanoporous materials with high surface (>4000 m^2/g) to store hydrogen at more moderate pressures (100-200 bar) than those required by gas compression (700 bar). WP leader: Prof. A. Comotti.

INTERNATIONAL ADVISORY BOARD

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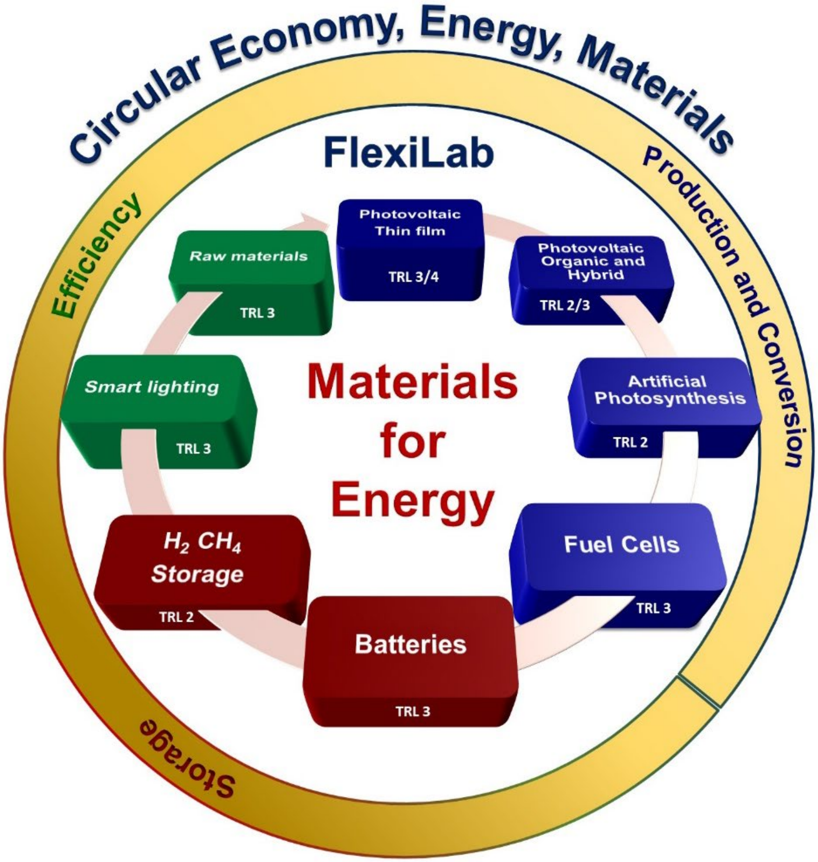
- Prof. Luca Beverina
- Prof. Simona Binetti
- Prof. Angiolina Comotti
- Prof. Piercarlo Mustarelli
- Prof. Stefano Sanguinetti (Principal Investigator)
- Prof. Anna Vedda



Circular Economy, Energy, Materials
FlexiLab
Efficiency
Production and Conversion
Storage
Materials for Energy
Photovoltaic Thin film
TRL 3/4
Photovoltaic Organic and Hybrid
TRL 2/3
Artificial Photosynthesis
TRL 2
Fuel Cells
TRL 3
Batteries
TRL 3
H_2 CH_4 Storage
TRL 2
Smart lighting
TRL 3
Raw materials
TRL 3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RESEARCH

(in alphabetic order)

Materials for energy and environment

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

Maurizio Acciarri, Simona Binetti, Dario Narducci. **Photovoltaics, thermoelectrics**

Carlo Antonini. **Surface Engineering and Fluid Interfaces (SEFI Lab)**

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 (NanoMat@Lab)**

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

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

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

Giovanni Di Liberto, Livia Giordano, Gianfranco Pacchioni, Sergio Tosoni. **Theory of inorganic materials for energy and environment**

Riccardo Ruffo. **Materials for energy storage and energy saving (EES)**

Carlo Santoro. **Electrocatalysis and Bioelectrocatalysis LAB (EBLab)**

Materials for microelectronics and photonics

Giorgio Benedek, Marco Bernasconi, Davide Campi. **First principles simulations of materials for microelectronics**

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

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

Marco Fanciulli, Fabrizio Moro. **Materials and spectroscopies for nanoelectronics and spintronics**

Mauro Fasoli, Roberto Lorenzi, Alberto Paleari, Anna Vedda. **Luminescent materials for optical technology and ionizing radiation detection**

Roberto Bergamaschini, Leo Miglio, Francesco Montalenti, Emilio Scalise. **Modeling and simulations of semiconductor heteroepitaxy**

Stefano Cecchi, Stefano Sanguinetti. **Fabrication and study of semiconductor quantum nanostructures (EpiLab)**

Alessandro Minotto, Adele Sassella. **Organic molecular films and heterostructures**

Giovanni Maria Vanacore. **Laboratory of Ultrafast Microscopy for Nanoscale Dynamics (LUMiNaD)**

Materials in cultural heritage

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

Optics and optometry

Alessandro Borghesi, Silvia Tavazzi, Fabrizio Zeri. **Optics and optometry**

Organic and polymeric materials

Luca Beverina, Mauro Sassi. **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**

Michele Mauri, Roberto Simonutti. **Synthesis and characterization of novel polymeric nanostructure**

Organic and hybrid materials and devices for solar fuels and artificial photosynthesis

Alessandro Abbotto, Norberto Manfredi

Present energy needs are classified into two main sectors: a) production of electricity; b) production of chemicals and fuels for industry, transportation, and agriculture. We focus our interest on the use of clean, no cost and abundant sources like sunlight, water, carbon dioxide, and nitrogen for photovoltaics and artificial photosynthesis. In the MIB-SOLAR and FLEXILAB labs, containing an ISO7 clean room and state-of-the-art facilities, we investigate materials and devices for artificial photosynthesis and photovoltaics.

ARTIFICIAL PHOTOSYNTHESIS: CLEAN AND RENEWABLE SOLAR FUELS AND CARBON BASED CHEMICALS

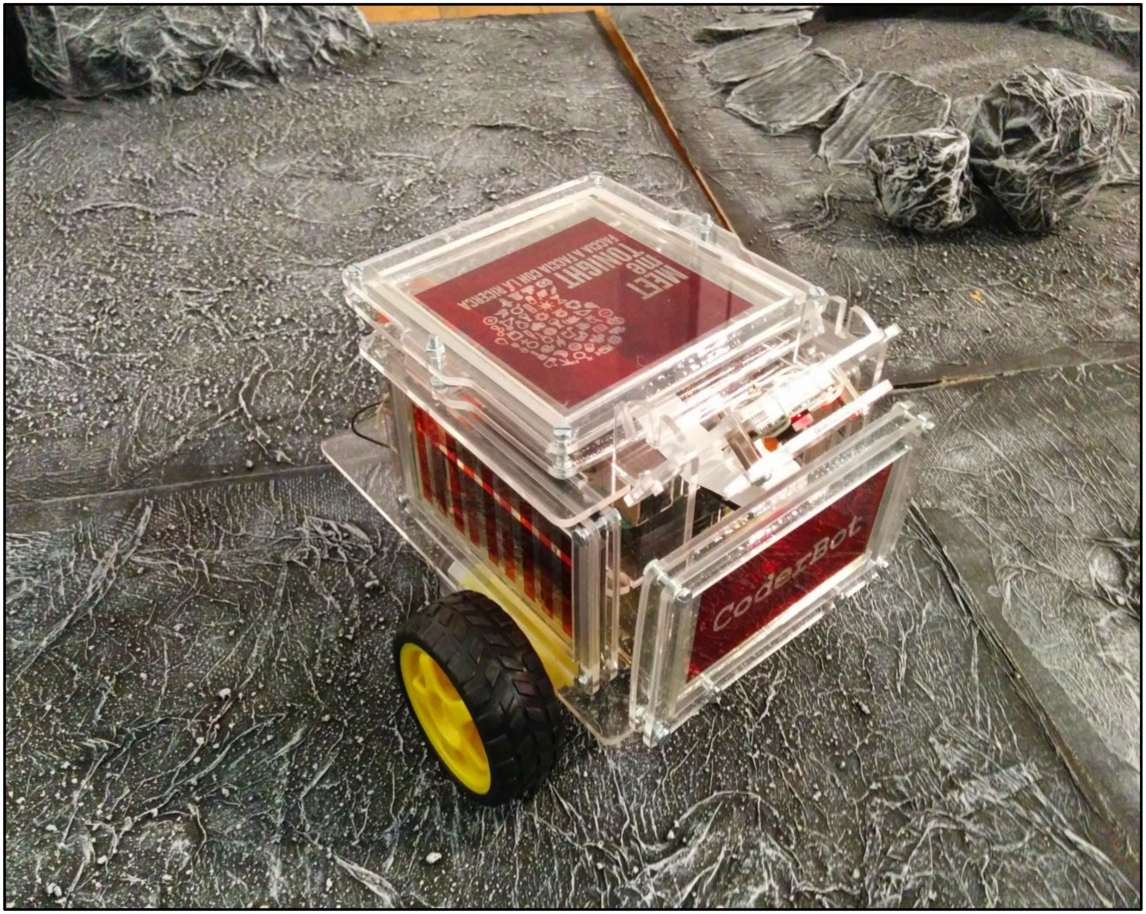
We apply the molecular approach to design and investigate dyes and catalysts for artificial photosynthetic processes, namely water splitting, reduction of carbon dioxide and artificial nitrogen fixation to ammonia. Water splitting is able to produce hydrogen, which can be used as a fuel or reactant in chemical industry. The reduction of CO_2 affords a number of 1C strategic chemicals and fuels, such as HCOOH, CO, CH_3OH and CH_4. Fixation of nitrogen is the solar-induced alternative route of the over one century old energy intensive and strongly greenhouse gas emitting polluting Haber-Bosch process to ammonia, used for fertilizers and thus highly strategic for feeding the growing population worldwide.
Two main approaches are used: a) photocatalysis; b) photoelectrochemical cells (PEC). In particular, we focus our attention on dye-sensitized photocatalysis and PEC (DS-PEC) where the key component is a molecular antenna-dye able to efficiently absorb sunlight on the surfaces of n- and p-type high band gap semiconductor oxides.
The final target is an integrated device based on low-cost earth-abundant starting materials: the artificial leaf.

ORGANIC AND HYBRID 3RD GENERATION PHOTOVOLTAICS

We investigate dye-sensitized solar cells (DSSC) in unconventional eco-friendly aqueous solvents based on Deep Eutectic Solvents (DES) in order to avoid the use of toxic and volatile components for low light and indoor application.

MAIN FACILITIES

- Fully equipped organic synthesis and characterization laboratories.
- Clean-room labs (MIB-SOLAR and FLEXILAB) for preparation and characterization of photocatalytic and photoelectrochemical devices for artificial photosynthesis and photovoltaics.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Photovoltaics and Thermoelectrics (MIB-SOLAR)



Maurizio Acciarri, Simona Binetti, Dario Narducci

INORGANIC MATERIALS FOR SOLAR ENERGY

Currently, crystalline-Si (c-Si) based devices rule the photovoltaic (PV) market, accounting for about 96% of the total annual production versus 4% for thin films based technologies (namely, CdTe, $Cu(In,Ga)Se_2$ (CIGS) and a-Si). In spite of the strong market gap between Si and thin films technologies, the development of PV absorbers proper for thin films based devices is nowadays even more crucial than in the past for future applications both in Building/Product Integrated Photovoltaics and in tandem devices. Furthermore, the availability of many raw materials used in thin film solar devices is seriously decreasing, while both energy and technology needs for the daily life are strongly increasing, which makes material saving crucial. The most studied alternatives to CdTe and CIGS in the last years were Cu_2ZnSnS_4 (CZTS) and $Cu_2ZnSnSe_4$ (CZTSe), where more abundant and less expensive elements like Zn and Sn are used in place of In and Ga. More recently, further alternatives based on earth abundant elements emerged, among them Cu_2MnSnS_4 (CMTS) and Cu_2FeSnS_4 (CFTS).

Our research activities deal with the above-mentioned PV absorbers and related solar devices. In detail:

SILICON Under the realistic assumption that c-Si based PV modules will dominate the PV market in the coming decade, our research activity has been focused on the further increase of Si solar cells efficiency (studying the effect of defects mainly by spectroscopic techniques), on the characterization of low price and high quality solar grade silicon feedstock and finally on new initiatives to build high efficiency tandem solar cells.

CIGS and $CuGaS_2$ (CGS) thin films on glass and flexible substrates (like plastic foils) are grown by an innovative hybrid sputtering-evaporation approach (combining the advantages of both techniques) and tested both in single junction and tandem devices.

CZTS, CFTS and CMTS are prepared mainly by a soft-chemical route involving the coordination of the metals into the solution thanks to the use of DMSO as solvent and thiourea as sulphur source, making it very appealing due to the absence of further organic additives and external sulphur sources. The precursors solution is directly deposited by drop-casting onto the substrate without the use of further expensive and/or industrially non-compatible instruments, making the whole procedure appealing for industrial green application.

For all these PV absorbers, a comprehensive structural and spectroscopic characterization (including scanning electron microscopy, Raman spectroscopy, X-ray diffraction and photoluminescence) is performed. All the new absorber layers are tested in prototype solar devices.

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.

Surface Engineering and Fluid Interfaces (SEFI Lab)

Carlo Antonini

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

ICEPHOBIC SURFACES

Surface icing can have many negative consequences in a broad range of fields. To avoid sever issues related to ice formation, superhydrophobic surfaces are known to be extremely efficient in terms of reducing ice nucleation and accretion on solid substrates. At SEFI Lab, we rationally design and fabricate advanced materials and surfaces, with hierarchical structuring down to the micro- and nanoscale, providing novel strategies to control phase change processes and limiting negative effects of uncontrolled icing or frosting, and developing new technological approaches for analyzing icing phenomena.

ATMOSPHERIC WATER HARVESTING

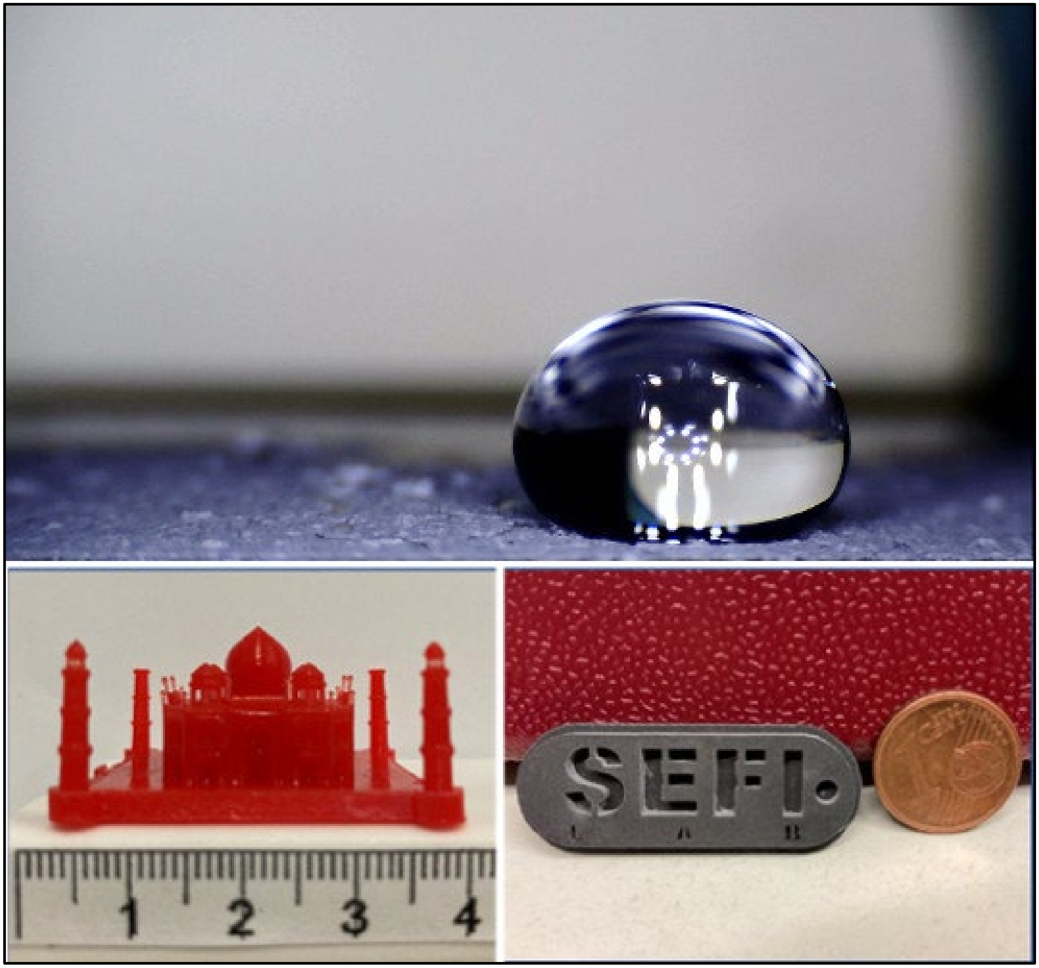
Among all water resources, fog harvesting from atmosphere is highly recommended, because it is a passive method with a considerably lower pollution and does not require high technology and costly operation and maintenance. At SEFI Lab, we are working on a new project on atmospheric water harvesting, named WaterHaB, spanning from studying the fundamental interaction of water with fibers and meshes, to engineering a windcatcher tower, modelled after a Badgir, an ancient Iranian architecture on building rooftops for enhancing fog collection.

ADDITIVE MANUFACTURING (3D PRINTING)

Among all other manufacturing technologies, we are investigating vat polymerization based Digital Light Processing (DLP) technique using liquid photopolymers (resin) as raw material. Also, we are incorporating metallic powder, few microns in diameter, to test the potential of metal printing from metal-loaded resin suspensions.

FUNCTIONAL POLYSACCHARIDE COATINGS

Polysaccharides can be used as coatings to control and reduce interaction between proteins and the capillary walls in capillary electrophoresis, with the goal of improving electrophoretic separation. We engineer polysaccharides using different chemical reactions and use them as capillary coatings.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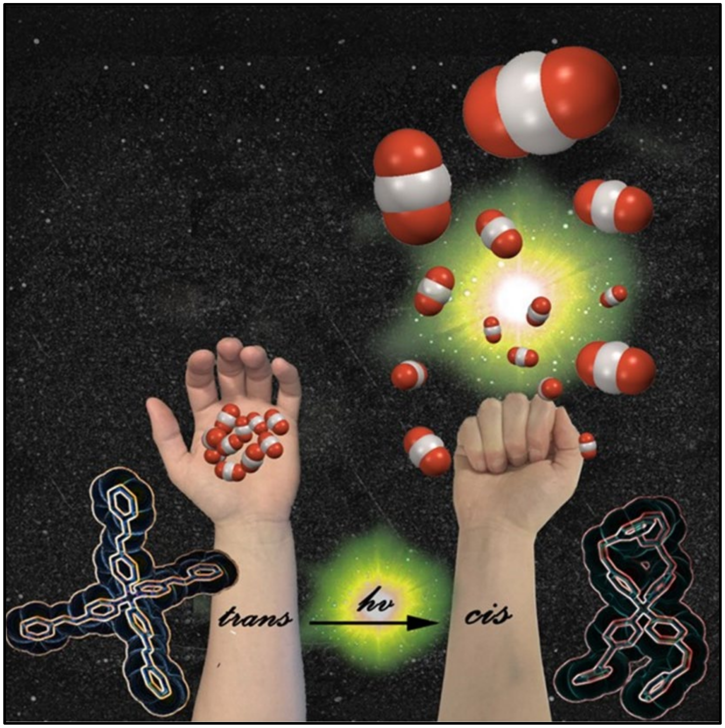
SEFI
L A B

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 10^4 to 10^{11} 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_2 from the gas phase.


trans
hv
cis

Chemistry of inorganic and hybrid materials (NanoMat@Lab)

Massimiliano D'Arienzo, Barbara Di Credico, Roberto Scotti

NANOSTRUCTURED MATERIALS FOR CATALYSIS, PHOTOCATALYSIS AND ENERGY STORAGE

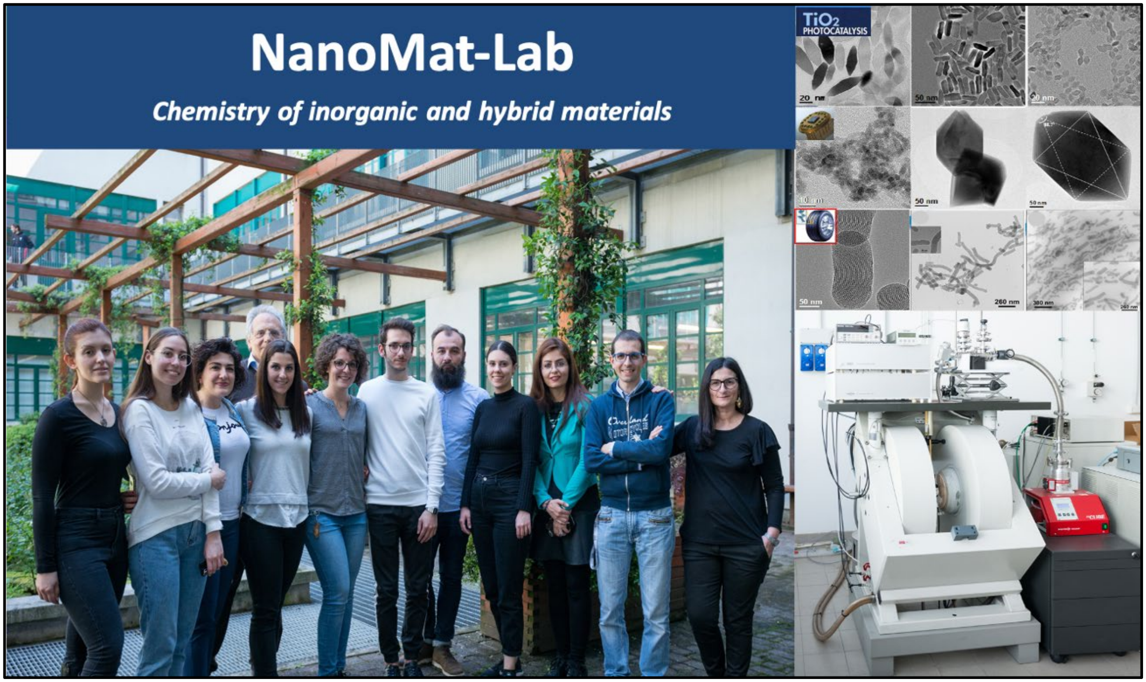
The research aims at the synthesis by soft-chemistry methods of morphology-controlled oxide nanoparticles (e.g. TiO_2, ZnO, MoO_3) and tuneable porous systems (macro/mesoporous silica or Metal Organic Frameworks, MOF), and at the study of their (photo)catalytic mechanism (formation and interfacial reactivity 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 plays 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 NANOCOMPOSITES

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

FACILITIES

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


NanoMat-Lab
Chemistry of inorganic and hybrid materials
TiO2
PHOTOCATALYSIS

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

Cristiana Di Valentin

COMPUTATIONAL NANOMEDICINE

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

COMPUTATIONAL ELECTROCHEMISTRY AND FUEL CELLS

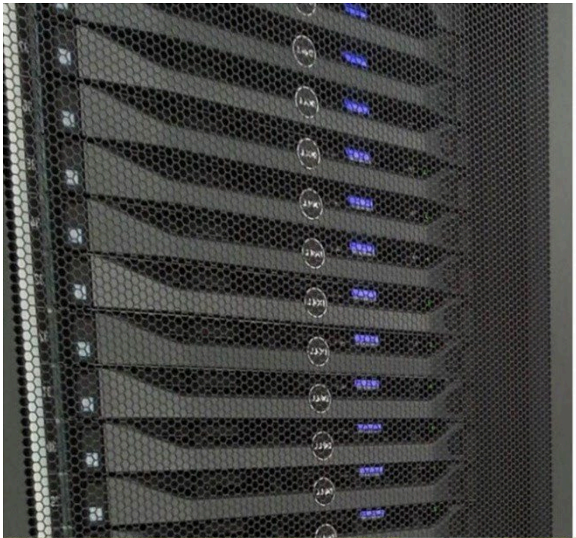
We use electronic structure calculations to design novel electrode materials for electrochemical devices and fuel cells, which are as efficient as or even more capable than precious and environmental unfriendly metal electrodes. Gibbs free energies of reaction in an aqueous environment for the all the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

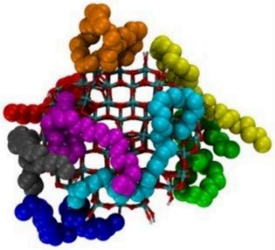
CATALYSIS UNDER COVER (2D LAYERS)

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

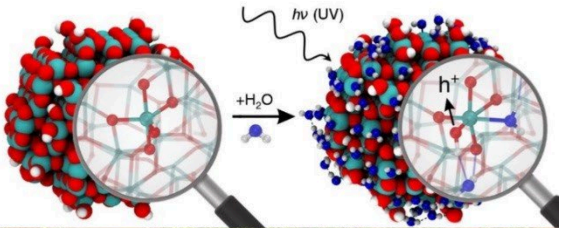
GRAPHENIC NANOSTRUCTURES FROM MOLECULAR PRECURSORS

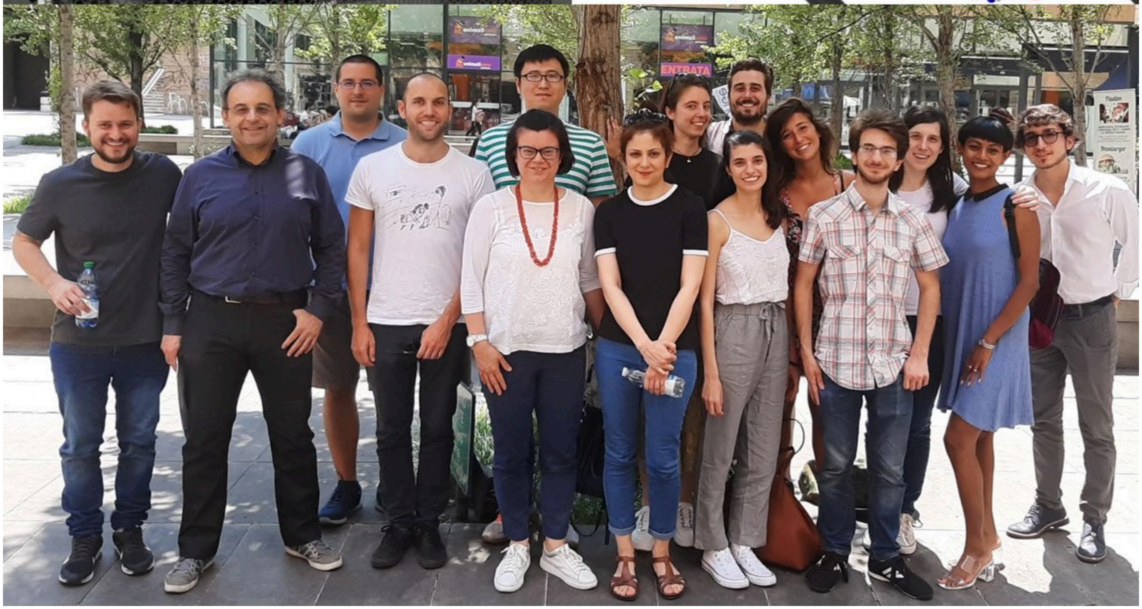
Combining density functional theory calculations with scanning tunneling microscopy and X-ray spectroscopic techniques (from our experimental partners) we investigate novel approaches for surface-assisted preparation of graphene-based nanostructures (nanoribbons, nanobowls, etc) by means of Ullmann coupling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





nanoQlab





Crystal growth and characterization: study of polymorphism

Massimo Moret

Growth of crystals and their morphological and structural characterization is a mandatory step in many fields of science and technology. Present state of the art study of crystal growth is widespread and covers both natural (geology, biomineralization) and artificial systems (semiconductors, sensors, optics, lasers, drugs, plasters).
Growth of crystals involves complex physico-chemical processes whose study allows a better control and optimization of results. Among many phenomena, genesis of polymorphic crystal structures can hamper preparation of crystalline materials. Therefore, the study of thermodynamic and kinetic factors directing growth toward a specific polymorph is of great relevance in academic and applied research. Among the parameters triggering polymorphism are temperature or ambient pressure, impurities/additives active during the nucleation stage (including preformed crystals able to select polymorphs by epitaxy), conformational flexibility, isotopic substitution. All these variables can be exploited as powerful control parameters for reaching the final goal, instead of being a source of unpredictable and irreproducible results.
Research activities involve:

CRYSTAL GROWTH

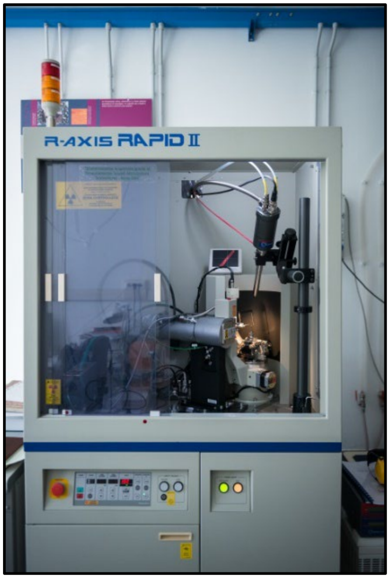
Growth of crystals with solution methods under ambient or solvothermal conditions (e.g. microporous coordination polymers exhibiting zeolite-like behavior or catalitic properties, aminoacids) allows preparation of crystals with size from centimeter to nanometer scale with control of morphology. Crystal of organic materials with medium-high vapor pressure can be grown by sublimation or physical vapor transport.

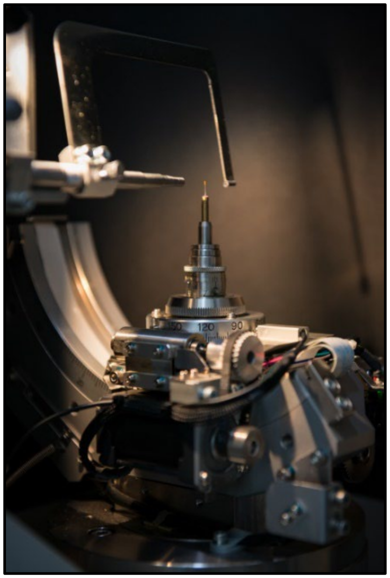
GROWTH MECHANISMS

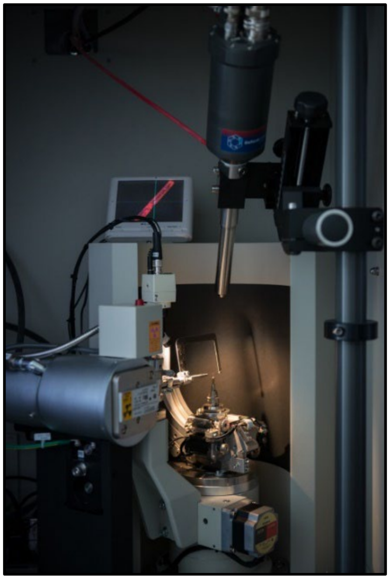
Study of surface processes during crystal growth in nature, laboratory or manifacturing plants (e.g. setting of cements/plasters in the presence of chemical additives) is directed toward aquisition of physico-chemical data ranging from the mesoscopic scale to molecular dimensions. Characterization of growing crystal surfaces is performed by means of optical microscopy or scanning probe microscopy in controlled environments. In situ visualization of growth with time evolution reveals microtopographic surface features connected to growth mechanisms. The microscopic characterization, possibly supported by single crystal X-ray diffraction analysis, can be integrated with theoretical modelling of crystal morphology through periodic bond chains analysis, where the strength of intermolecular interactions developing within the crystal structure can be exploited to estimate the theoretical equilibrium and growth crystal morphology.

MAIN FACILITIES

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


R-AXIS RAPID II





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

Chiara Ferrara, Piercarlo Mustarelli

MEMBRANES AND MEMBRANE-TO-ELECTRODE ASSEMBLIES (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 Nafion™ 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 ENERGY STORAGE

At present, the market of electrochemical energy storage is dominated by lithium-ion rechargeable batteries. These batteries, however, have not enough energy density, 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).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Ascend™ 400WB
AVANCE III 400
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Theory of inorganic materials for energy and environment




Giovanni Di Liberto, Livia Giordano, Gianfranco Pacchioni, Sergio Tosoni

The understanding of the structure-properties relationship is of fundamental importance for the design of new materials. In our group various models are employed to study the electronic structure of inorganic and ceramic materials in combination with highly accurate quantum-mechanical techniques. Particularly important is the role of theory in the study of point defects, impurities in solids, doping in semiconductors, 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 SURFACES AND 2D MATERIALS

Ultrathin oxide films and two-dimensional materials 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, regular arrays of adsorption and reactive sites, etc.

SINGLE ATOM CATALYSTS AND SUPPORTED CLUSTERS

We study the interaction of single atoms and metal clusters supported on oxides or carbon-based materals with particular attention to their activity in catalytic reactions (water splitting, CO_2 reduction, production of solar fuels).

OXIDE SEMICONDUCTORS AND HETEROJUNCTIONS

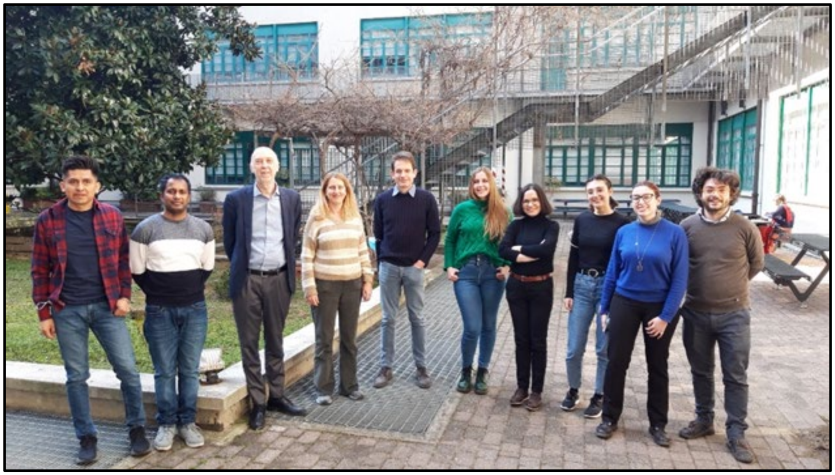
Heterojunctions between semiconductors (notably oxides) are a class of materials attracting growing attention in the field of photocatalysis. This research line aims at the accurate description of the band alignment, charge transfer phenomena, quantum confinement, and charge carrier separation at the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

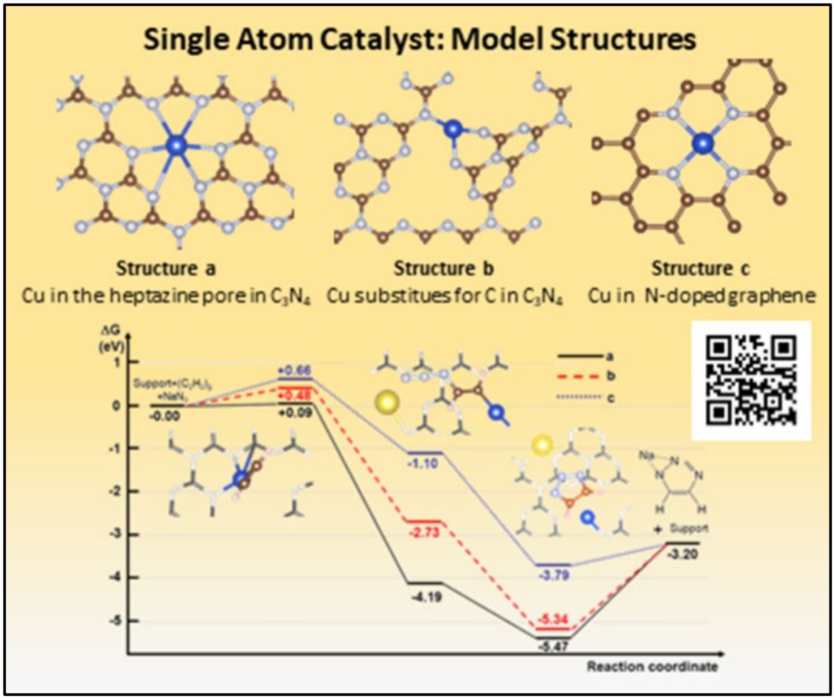
MATERIALS FOR BATTERIES

Efficient accumulators are important, among other things, to efficiently exploit renewable, but discontinous, energy sources. The simulation may assist in the design of new suitable materials, by describing the atomic and the electronic structures, and simulating the intercalation and mobility of metal cations and other charge carriers. Ongoing research lines span over various classes of layered and nanostructured materials.

MAIN FACILITIES

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





Single Atom Catalyst: Model Structures
Structure a
Cu in the heptazine pore in C_3N_4
Structure b
Cu substitues for C in C_3N_4
Structure c
Cu in N-doped graphene
ΔG (eV)
+0.66
+0.48
-0.00
+0.09
-1.10
-2.73
-3.79
-4.19
-5.34
-5.47
-3.20
a
b
c
+ Support
Reaction coordinate

Materials for energy storage and energy saving (EES)

Riccardo Ruffo

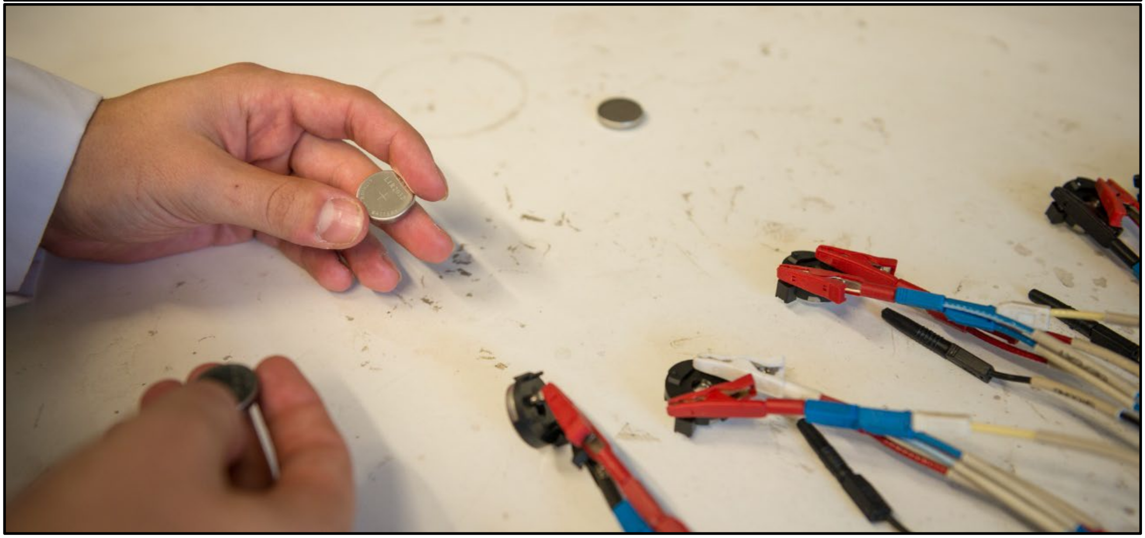
Since the birth of the Department, the electrochemical group is active in fields of Energy Storage and Production, Gas Sensing, and characterization of Organic Molecular or Polymeric Materials. Group facilities comprise a fully equipped electrochemical lab with several potentiostats-galvanostats, multichannel systems for long time testing, 3 automatic glove boxes at N_2 or Ar, a climatic chamber to control temperature and humidity, optical fibers coupled with UV-visible spectrophotometer for in-situ spectroelectrochemistry, and a quartz crystal electrochemical microbalance. Furnaces, thick/thin film applicators, and standard chemical equipments are available for chemical synthesis and electrode formulations.

MATERIALS FOR ENERGY STORAGE

This research line is devoted mainly to the investigation of electrode and electrolyte materials for Electrochemical energy storage devices, such as alkaline ion batteries, metal batteries, redox flow batteries and organic batteries. 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.
Different kinds of prototypes can be assembled, from low energy coin cells to large, single layer pouch cells, as well as three electrode cells for single interface characterization.

MATERIAL FOR ORGANIC OPTOELECTRONICS

Since 15 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.



Electrocatalysis and Bioelectrocatalysis LAB (EBLab)

Carlo Santoro

MISSION of the LAB: We want to contribute to the 2050 EU decarbonization goal with electrochemical systems. We do research and development of electrocatalysts for several electrochemical reactions based on platinum group metal-free materials pursuing biomimicking and bionspired approaches within the core of the circular economy. Research and development of bacterial and enzymatic bioelectrochemical systems from fundamental to application. Scale up of the electrochemical systems towards real-world applications. Systems of interest: fuel cells, electrolyzers, CO_2 electrolyzers, nitrogen reduction electrolyzers, microbial fuel cells, microbial electrolysis cells, etc.

ELECTROCATALYSIS

Noble-containing and/or critical raw materials-containing electrocatalysts are used in diverse electrochemical applications for fuel production and energy conversion named water electrolyzers and fuel cells. The high cost and scarcity of these materials on the Earth crust hinder or severely limit their deployment for large scale commercialization of these electrochemical devices which are generally the base of the green energy revolution. Alternatives need to be pursued. We are replacing the costly platinum group metal (PGM) electrocatalysts with more affordable Earth abundant transition metals (PGM-free) achieving similar electrocatalytic activity using biomimicking and bionspired synthesis methods and approaches and when possible also valorizing waste (e.g. waste biomass and plastic) as precursors during synthetic processes within the core of the circular economy. We are currently synthesizing PGM-free electrocatalysts for reaction such as Oxygen Reduction Reaction (ORR), Hydrogen Evolution Reaction (HER), Hydrogen Oxidation Reaction (HOR), Alcohol Oxidation Reaction (AOR), Oxygen Evolution Reaction (OER). Other reactions of interest within the decarbonization are also CO_2 electroreduction (CO_2ER) and Nitrogen Reduction Reaction (NRR).

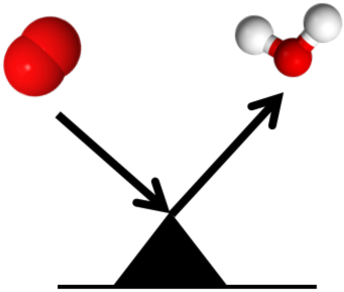
BIOELECTROCATALYSIS

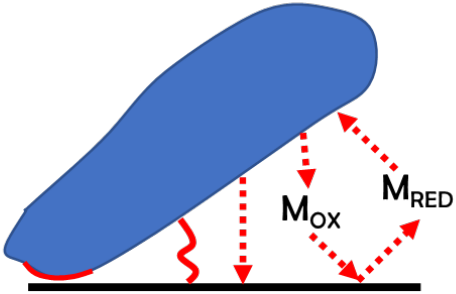
Microbial Electrochemical and Enzymatic Electrochemical technologies have captured the attention of the scientific community for the possibility of: i) Biosensing of molecules using microorganisms or enzymes; ii) degrading pollutants and organic molecules; iii) producing and storing energy using microbial or enzymatic electrochemical systems (including microbial fuel cells, enzymatic fuel cells, biosupercapacitors and bio-batteries); iii) performing electrosynthesis and transformation of waste into valuable products. In our lab, joint with Prof. Franzetti @DISAT, we synthesize carbonaceous materials (biochar) starting from waste biomass and plastics and we functionalize it as anode materials or as cathode PGM-free electrocatalysts for the oxygen reduction reaction (ORR) and the hydrogen evolution reaction (HER). The main application is microbial electrochemical technology for power production, hydrogen evolution, organic removal and soil remediation. ORR and HER occurring on the electrocatalysts based on carbonaceous, platinum-group metal and platinum-group-metal-free materials are evaluated.

MAIN FACILITIES

- Powerful and durable planetary ball mills for sample preparation of solids. Ball Milling E-max
- Rotating Ring Disk Electrode and Bipotentiostat Pine for the electrochemical characterization of electrocatalysts
- Horizontal split Furnace for performing pyrolysis processes at controlled temperature and atmosphere

ELECTROCATALYSIS
BIOELECTROCATALYSYS
LABORATORY





First principles simulations of materials for microelectronics



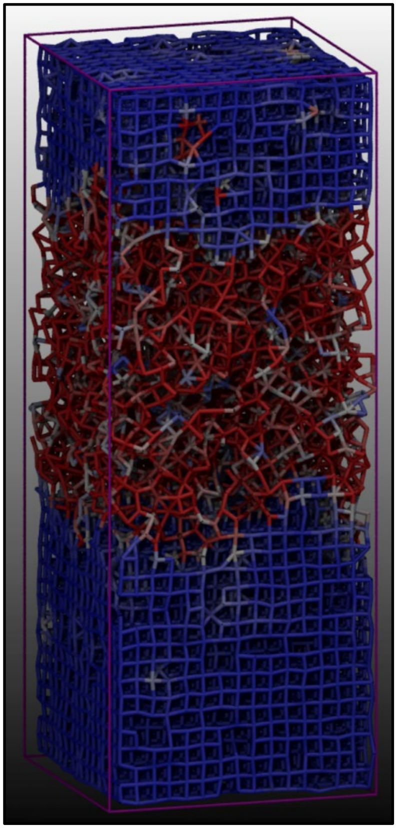
Giorgio Benedek, Marco Bernasconi, Davide Campi

PHASE CHANGE MATERIALS FOR DATA STORAGE

Phase change materials ($Ge_2Sb_2Te_5$ and related telluride alloys) are attracting an increasing interest worldwide for applications in optical disks (DVDs) and in a novel non volatile electronic memory, the phase change memory cell. Both applications rely on a fast (10-100 ns) and reversible transformation between the crystalline and amorphous phases induced by heating. The two states of the memory can be discriminated thanks to the large contrast in electronic conductivity and optical reflectivity between the two phases.
On the basis of density functional molecular dynamics simulations, we investigate the structural, dynamical and electronic properties of the amorphous and crystalline phases of materials in this class aiming at establishing correlations between the composition of the alloy and the electronic and optical functional properties exploited in the devices. The models of amorphous phases (300-500 atoms) are generated by quenching from the melt within ab-initio molecular dynamics simulations.
Large scale molecular dynamics simulations are also performed by means of interatomic potentials generated by fitting a large DFT database with Neural Network methods. The Neural Network potential allows simulating several thousand atoms for tens of ns to study thermal transport at the nanoscale, the microscopic mechanisms responsible for the fast crystallization and the properties of nanowires.

SURFACE PHONONS AND TOPOLOGICAL INSULATORS

Some chalcogenide compounds of interest for phase change applications belong to the class of topological insulators, i.e. they are bulk insulators with a non trivial topology of the electronic bands which induces the formation of topologically protected metallic electronic bands at the surface. On the basis of density functional perturbation theory, we study the surface phonons and the electron-phonon interaction of materials in this class also by comparing the theoretical results with measurements from He-atom scattering from various experimental groups in Europe we collaborate with. Acoustic surface plasmons (spin-plasmons for Ni(111)) and their interaction with surface phonons of interest for THz plasmonics are investigated as well.



Optical spectroscopy of semiconductors


Emiliano Bonera, Fabio Pezzoli

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 within the L-NESS interuniversity Centre.

SIGE HETEROSTRUCTURES

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

- 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.
- The vibrational properties of SiGe nanostructures, mainly quantum dots, are currently under study by Raman and micro-Raman measurements.
- The electronic properties of Ge/SiGe multiple quantum wells are studied by transmission and photoluminescence measurements in a wide temperature range.
- Electron spin sensitive measurements on Ge/SiGe structures are performed; the photoluminescence with light polarization control is studied.

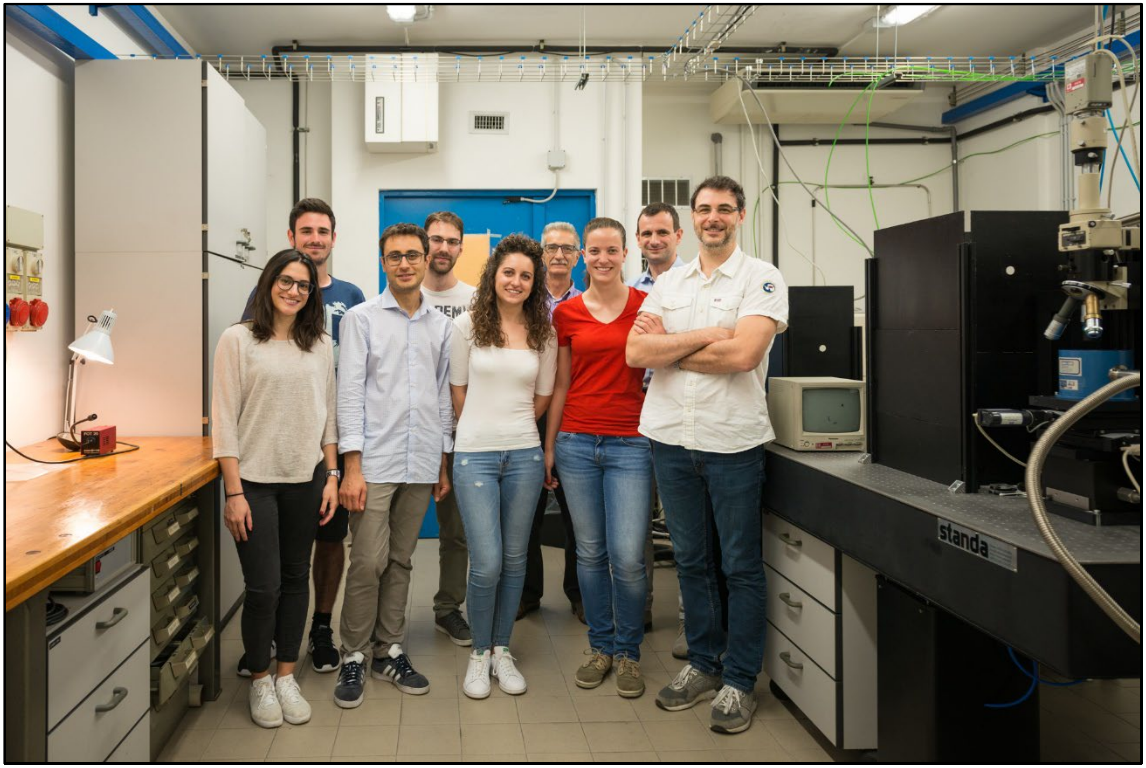
QUANTUM STRUCTURES BASED ON III-V SEMICONDUCTORS

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.

- We study the nanostructure properties via spectroscopic measurements addressing electronic structure and carrier relaxation mechanisms;
- We study the transfer of the III-As QD devices on Si for integration with standard electronics.

FACILITIES

Spectroscopic apparatuses based on dispersive and FT spectrometers are used for photoluminescence, photoluminescence excitation, transmission and Raman measurements in the 0.4 - 5.0 eV spectral range. Raman spectroscopy can be operated down to 5 cm^{-1}. Working temperatures: 2 K to 450 K. Sources: He-Ne, Ar, doubled-Ar, Ti-Sapphire, DPSS and Diode lasers, incandescent and high pressure lamps. A low temperature (4 K – 300 K) micro-photoluminescence and micro-Raman apparatus working in the 0.75 – 3.4 eV spectral range is available. Time resolved photoluminescence and photoluminescence decay down to 10^{-8} s can be measured with DPSS-QS lasers.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Advanced spectroscopy of functional nanomaterials

Sergio Brovelli, Franco Meinardi, Angelo Monguzzi

LUMINESCENT SOLAR CONCENTRATORS (LSCS)

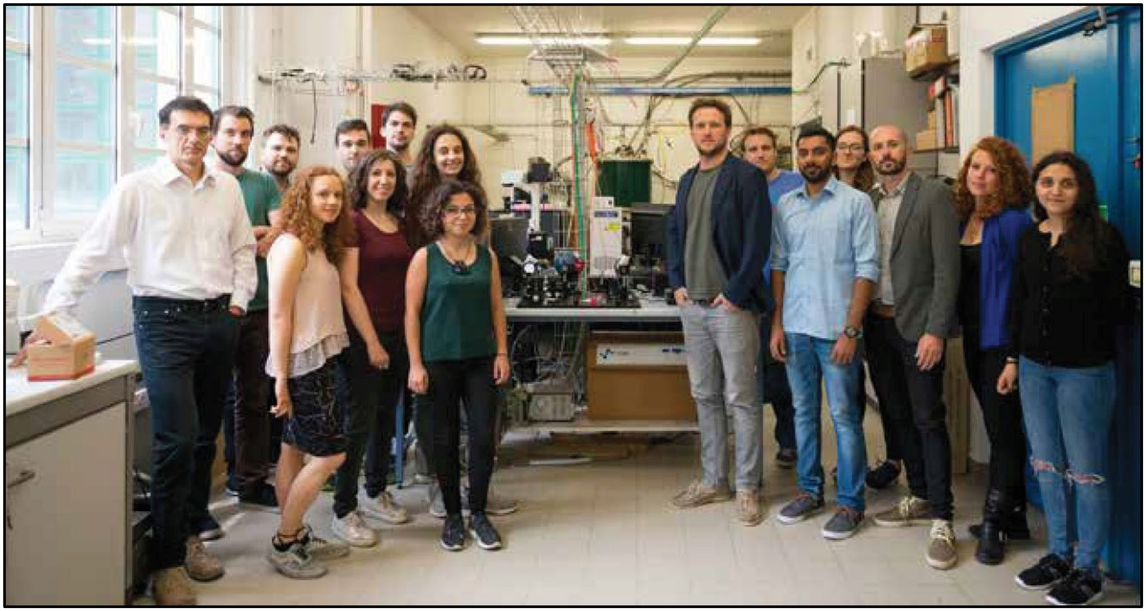
Luminescent solar concentrators (LSCs) are cost-effective complements to semiconductor photovoltaic (PV) systems that can both boost the power output of standalone solar cells and allow for integration of PV-active architectural elements into buildings in the form of, for example, semi-transparent PV windows. A typical LSC consists of a plastic optical waveguide doped with fluorophores or glass slabs coated with active layers of emissive materials. Sunlight, which penetrates the matrix, is absorbed by the fluorophores and then re-emitted at a longer wavelength. The luminescence, guided by total internal reflection, propagates towards a PV cell placed at the edge of the waveguide where it is converted into electricity. Our research team has a dedicated effort for the development of new emitters for efficient large-area LSC devices that require fluorophores with near unity emission efficiencies, broad coverage of the solar spectrum and minimized overlap between the absorption and emission spectra, so as to suppress the optical losses by re-absorption. Furthermore, an important aspect of our research is focused on advanced strategies for the incorporation of emitters into polymeric matrixes for producing polymeric nanocomposites that preserve the optical features of the fluorophore intact.

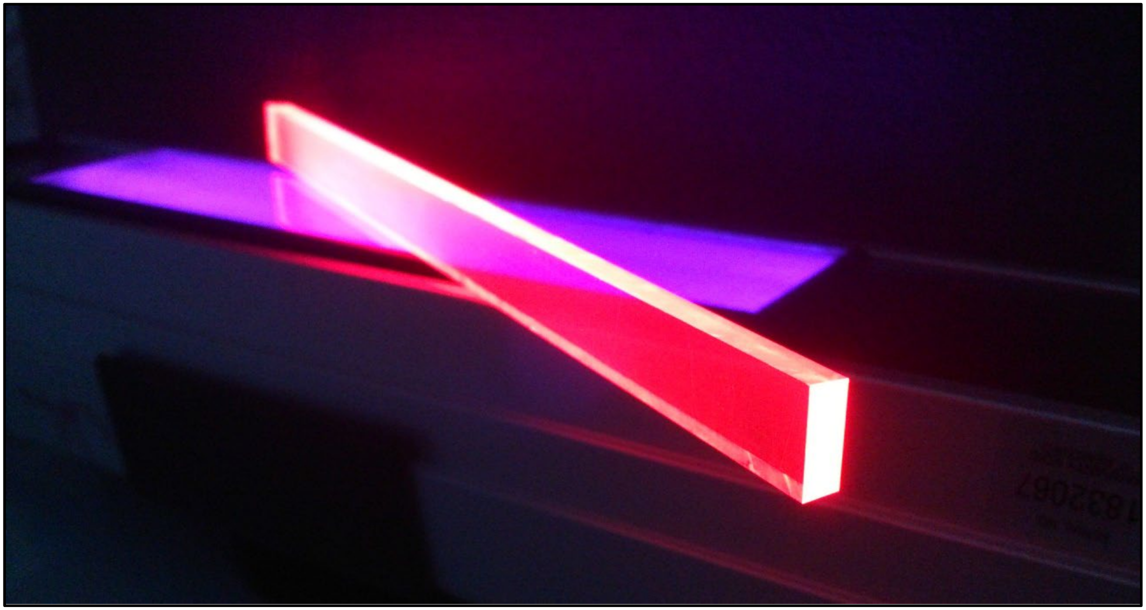
NON-COHERENT PHOTONS UP-CONVERSION

The most recent advancements in photovoltaic and hydrogen photogeneration technologies require the adaptation of the solar spectrum to the device spectral response through photon management processes, rather than the tuning of the latter to match the solar spectrum. In this framework, conventional non-linear optics approaches are not applicable as they typically require excitation densities several orders of magnitude larger than the solar radiance. Our research is focused on the development of multicomponent organic systems that exploit annihilation processes of metastable states and thereby allow for the achievement of high up-conversion efficiencies at excitation densities as low as a few µW/cm2. In our research we tackle both fundamental and applicative aspects aimed at the development of real-world devices. Our results have a significant impact both on photovoltaic technologies and on solid state lighting and imaging applications.

ADVANCED SPECTROSCOPY OF COLLOIDAL NANOCRYSTALS

Colloidal semiconductor nanocrystals (NCs) are solution-processable functional materials with growing applicative potential in strategic technological fields, such as light-emitting diodes, photovoltaic cells, lasers, luminescent markers and single photon sources. They feature high, near-unity emission efficiency, large absorption cross-sections and a tunable emission wavelength controlled by the NC size. Wavefunction engineering in NC heterostrustures and doping with transition metal ions provide additional degrees of freedom for controlling the optical and electrical properties of NCs. Our research is focused on fundamental and applied aspects of NC photophysics by means of ultrafast magneto-optics and spectroelectrochemical methods aimed at achieving advanced NC systems for application in solid-state light emitting sources, luminescent solar concentrators and NC solar cells.





Materials and spectroscopies for nanoelectronics and spintronics (MSNS Laboratory)

Marco Fanciulli, Fabrizio Moro

Our research is mainly devoted to the experimental investigation of semiconductors, oxides, and their interfaces, silicon and germanium nanostructures, MoS_2, and magnetic thin films for advanced and innovative nanoelectronic, spintronic, and neuroelectronic devices. The research activity is carried out in strong collaboration with the CNR-IMM-MDM, leading European research institutions, and semiconductor industries, Micron and ST.

POINT DEFECTS IN SEMICONDUCTORS AND OXIDES AND AT THEIR INTERFACES

Study of the electronic properties of point defects in semiconductors (Si, Ge) and in high dielectric constant materials (transition metal oxides) and at their interfaces. Applications in quantum and unconventional computing (collaboration with Wilfred G. van der Wiel, UTwente).

SI NANOWIRES

The electronic and spintronic properties of Silicon nanowires produced by metal-assisted chemical etching (MACE) (collaboration with M. Belli, CNR-IMM) are investigated using mainly spin dependent transport techniques aiming at the characterization of shallow donors.

QUANTUM DOTS

The study of QD-based devices (colloidal nanoparticles of PbS, CdSe, CdS, Au) is carried out using charge and spin transport aiming at the understanding of strongly correlated few electrons/excitons systems and their possible applications, such as reservoir computing and quantum computing.

TMDC (MOS_2, WS_2) AND MAGNETIC THIN FILMS

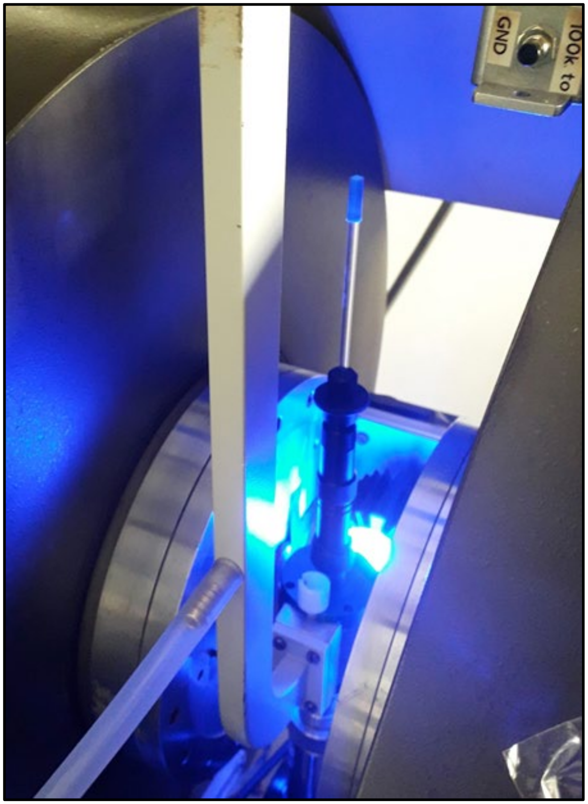
TMDC are grown with a novel patented method and their properties characterized with Raman spectroscopy (Collaboration with E. Bonera) and electrical measurements. Magnetic thin films deposited at CNR-MDM for spintronics are characterized with broad band FMR. (Collaboration with R. Mantovan and M. Belli, CNR-IMM).

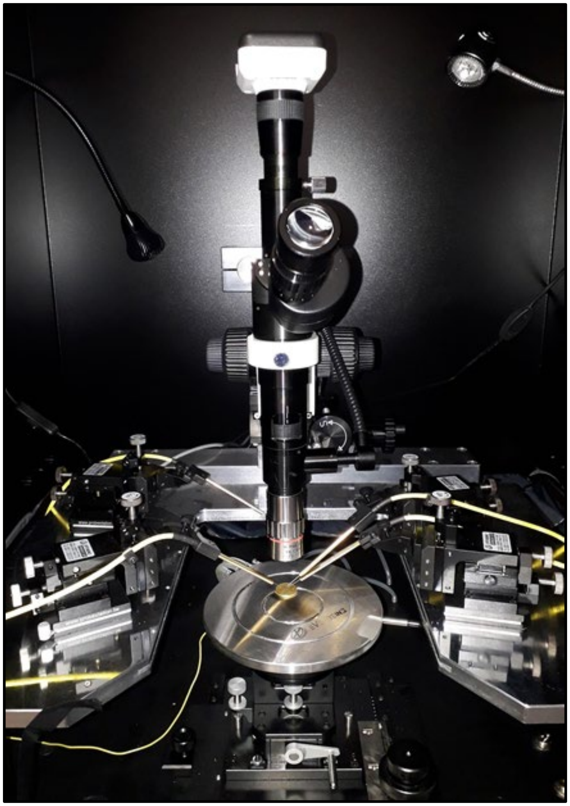
MICROELECTRODES FOR NEUROLECTRONICS

Within the Neureka EU project (www.neureka.gr) deposition by ALD and characterization by impedance spectroscopy and noise of novel materials and structures for neuron stimulation and recording.

FACILITIES

- Growth and processing: Atomic Layer Deposition (ALD) mini-chamber with O3 line for in-situ characterization; horizontal and vertical furnaces; Q-switched Ruby laser for laser annealing
- Characterization: Three CW X-band systems for electron spin resonance (ESR), electrically detected spin resonance (EDMR), and electron nuclear double resonance (ENDOR). Variable temperature measurements (4-600 K); Multi-frequency (0.1-40 GHz) EDMR and ferromagnetic resonance (FMR); Inelastic electron tunneling spectroscopy (IETS) and deep level transient spectroscopy (DLTS) working in the temperature range 4-300 K. Everbeing probe station. Keithley 4200 for I-V, C-V. Impedance Analyzer (1mHz-5MHz), Zurich Instruments MFIA. Impedance and Noise.


100k to
GND



Luminescent materials for optical technology and ionizing radiation detection




Mauro Fasoli, Roberto Lorenzi, Alberto Paleari, Anna Vedda

Our research is focused on the physical properties of luminescent materials for applications in photonics, optolectronics and ionizing radiation detection. 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. 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.

MATERIALS FOR OPTICAL TECHNOLOGY

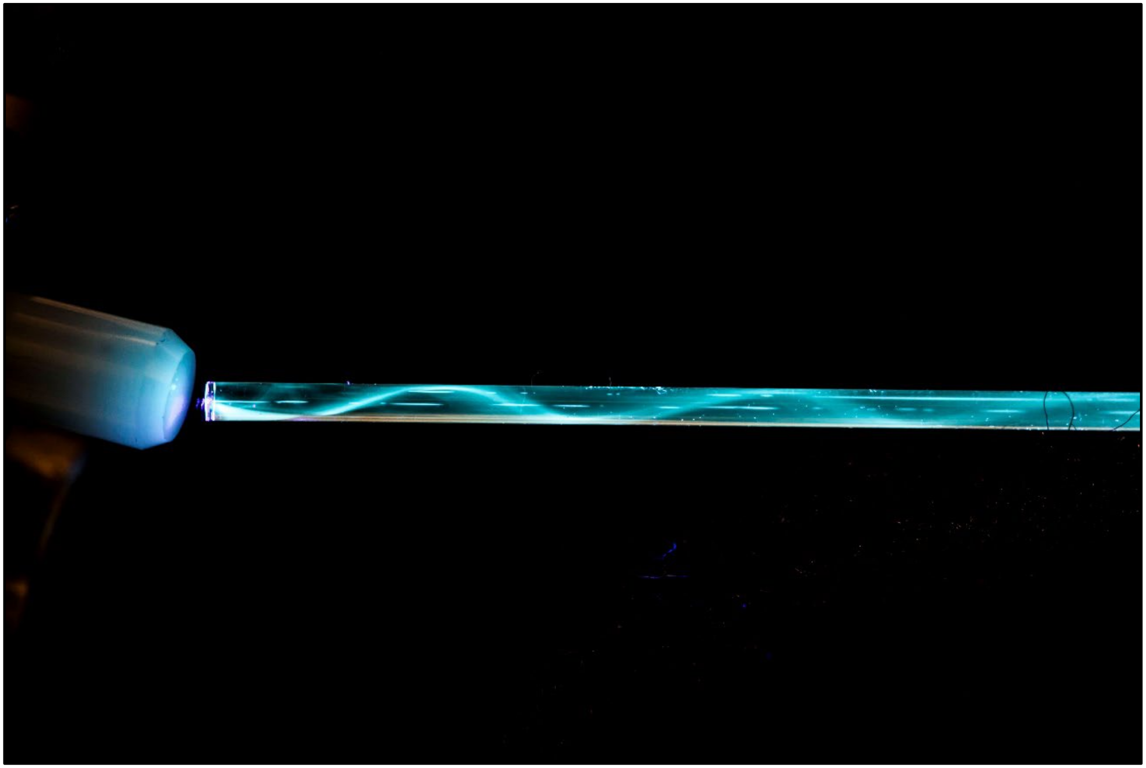
We investigate the light-emission and non-linear optical properties of wide-band-gap oxide nanostructures in glasses, such as Ga_2O_3 and SnO_2 nanocrystals in silicates, analysing the applicability as light-emitting systems, photosensitive optical materials, cubic non-linear components, and transparent conductors. 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.

LUMINESCENT MATERIALS FOR IONIZING RADIATION DETECTION

Investigation of the optical properties of a broad range of luminescent materials for ionizing radiation detection (glasses, single crystals, ceramics, nano-composites). We study the luminescence mechanisms, the interaction between the luminescence centres (e.g. rare earth ions) and the host matrix, and the role of point defects on the scintillation performances. The aim of the research is the production and optimization of materials suitable for industrial and medical applications, high-energy physics, dosimetry, etc.

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-profilometry, 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




Roberto Bergamaschini, Leo Miglio, Francesco Montalenti, Emilio Scalise

Integration of materials with superior optical and/or electronic properties on Si is extremely appealing as it leads to a wealth of new possible devices and applications while maintaining mainstream silicon technology. Examples include Ge, SiGe, GeSn, SiC, and GaAs. Heteroepitaxial growth of such materials results from the competition between several different phenomena, mostly related to lattice mismatch (causing misfit stress accumulation), to differences in thermal-expansion coefficients (leading to thermal stress), and to kinetic constraints (out-of- equilibrium growth). It is particularly critical for various applications to control the morphology of the growing material (faceting, preferential growth directions, etc.) and the distribution of defects (dislocations, stacking faults, etc.), especially when the 3D growth on patterned substrate is approached.
As the growth conditions pertain to a multi-dimensional space, too complex to be sampled by simple trial and error procedures, simulations and modelling can be extremely helpful in driving experiments. Our group provides such theoretical/computational support, aiming at suggesting to experimental colleagues ideal growth conditions for the desired application. As problems related to heteroepitaxy are often multi-scale, we use different, synergic approaches, ranging from atomistic to continuum simulations. These include ab initio calculations (exploited to evaluate surface energies, diffusion constants, defect formation energy, etc.), classical molecular dynamics (defect motion, dislocations gliding/partialization etc.), 3D dislocation dynamics, growth simulations based on phase-field methods, and elasticity theory solved by Finite Element Methods. Our attention is devoted to a wide class of qualitatively different systems such as semiconductor thin films, quantum dots, nanowires, vertical membranes, and micrometric crystals on deeply patterned substrates.
Our connection with experiments and applications is extremely tight: we work in very close collaboration with several international academic and industrial groups. Our research is financed by industrial contracts (SILTRONIC AG, Germany), EU Horizon 2020 projects (CHALLENGE Industrial Leadership project, devoted to improve the quality of heteroepitaxial SiC/Si; μ-Spire FET project, aiming at the development of a new technological platform for single-photon avalanche detectors), and regional projects (TEINVEIN - TEcnologie INnovative per i VEicoli Intelligenti, funded by Regione Lombardia, where we investigate novel infrared detectors).


SiGe hex
in NWs

Fabrication and study of semiconductor quantum nanostructures (EpiLab)

Stefano Cecchi, 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

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

QUANTUM FUNCTIONAL MATERIALS FOR PHOTO-ELECTROCHEMICAL APPLICATIONS

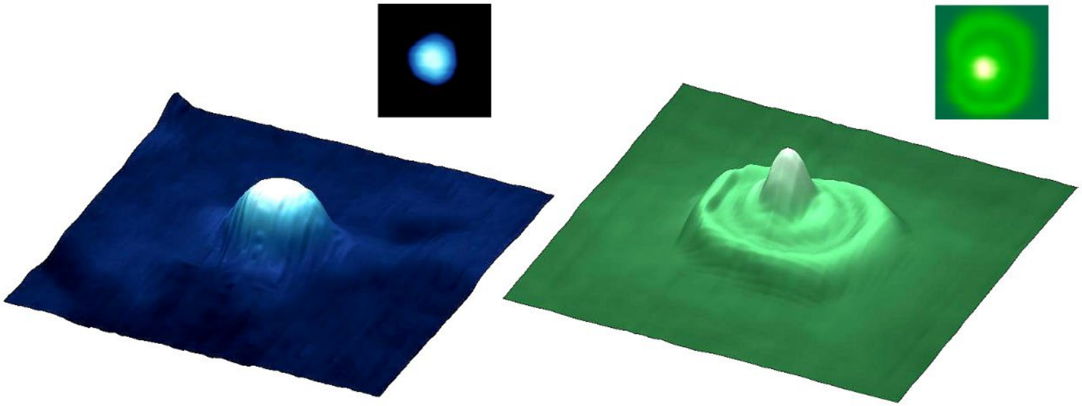
Growth and characterization of nanostructured InN/InGaN materials for photocatalytic electrodes for applications in biochemical sensors and hydrogen solar generation.

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

Alessandro Minotto, Adele Sassella

THIN FILM GROWTH

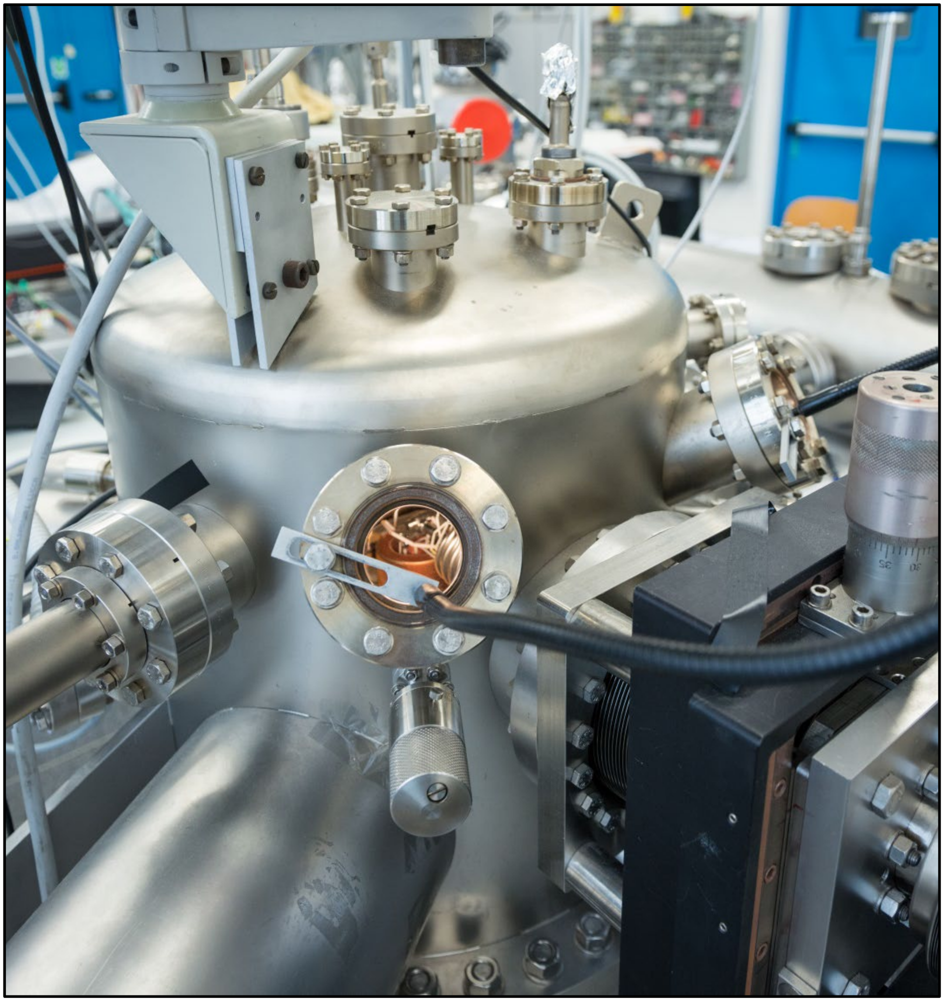
Films of organic molecular semiconductors are grown by organic molecular beam epitaxy (OMBE) under different conditions, such as pressure, substrate type and temperature, absence or presence of external fields. The study of the OMBE growth process itself is carried out by detecting in situ and in real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

HETEROSTRUCTURES

Heterostructures and nanostructures of organic molecular materials interesting for their solid state properties are also among the interests of the group. They are grown by OMBE and studied, in view of the understanding of their properties as a result of properly tuned growth protocols. Films of different molecules on high quality single crystal substrate, made of the same or similar molecular organic compounds, permit studying the conditions for epitaxy, therefore the fabrication of 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.

FACILITIES

The OMBE apparatus consists of high vacuum and 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 μm^2 wide regions, while on crystalline samples molecular resolution is also achievable.



Laboratory of Ultrafast Microscopy for Nanoscale Dynamics (LUMiNaD)

Giovanni Maria Vanacore

EXPLORING ULTRAFAST PHENOMENA IN THE NANO-WORLD

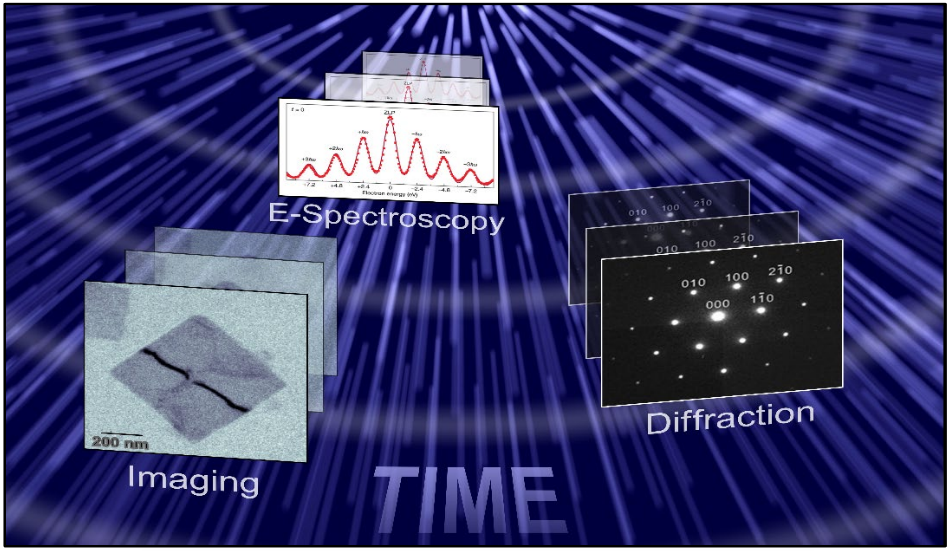
Our research activity is dedicated to the investigation of ultrafast phenomena in nanoscale low-dimensional materials. In particular, we focus on semiconductor quantum dots, nanowires, graphene and 2D van-der-Waals solids, nano-plasmonic structures, energy-related materials, topological insulators and molecular systems. Our ultimate goal is the ability to finely control their unique electronic and structural properties by optically manipulating the subtle balance and correlation between the relevant degrees of freedom (electronic, spin, orbital and lattice). Because such intricate coupling gives rise to a multi-dimensional phase space, a complete understanding of the physical behaviour of such systems can only be achieved when simultaneously capturing their coherent dynamics at the proper temporal and spatial scales.

ULTRAFAST ELECTRON MICROSCOPY

Our method consists in monitoring the spatio-temporal behaviour of a specific quantum system using ultrashort electron pulses following a spectrally- and spatially-resolved impulsive photonic excitation. This approach is based on an Ultrafast Electron Microscope, as initially pioneered by Nobel Laurate Ahmed H. Zewail, where a femtosecond laser is coupled to a transmission electron microscope (TEM). Such setup would provide unprecedented simultaneous spatial and temporal resolutions (10 orders of magnitude better than a standard TEM). It would be the first setup of its kind in Italy, and one of the few in the entire world.

CROSS-SCALE APPROACH TO MATERIALS DYNAMICS

Because of the versatility of our cross-scale approach, which combines real-space (imaging), reciprocal-space (diffraction) and spectroscopic tools with high temporal sensitivity, the Ultrafast Electron Microscope at LUMiNaD will provide the unique capability of observing many fundamental phenomena, such as: i) the coherent dynamics of both collective and quasi-particle excitations, ii) electronic/structural correlations under non-equilibrium conditions, iii) real-time motion of nano-objects and extended defects in solids, iv) the role of chirality in the dynamics of topological quantum states, and v) the electron/light/matter quantum interaction at sub-wavelength scales



LUMiNaD

Smart Electron

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

Anna Galli, Marco Martini

THE ARCHAEOMETRY LAB

Since 1980 our activity has been focusing 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 ...).

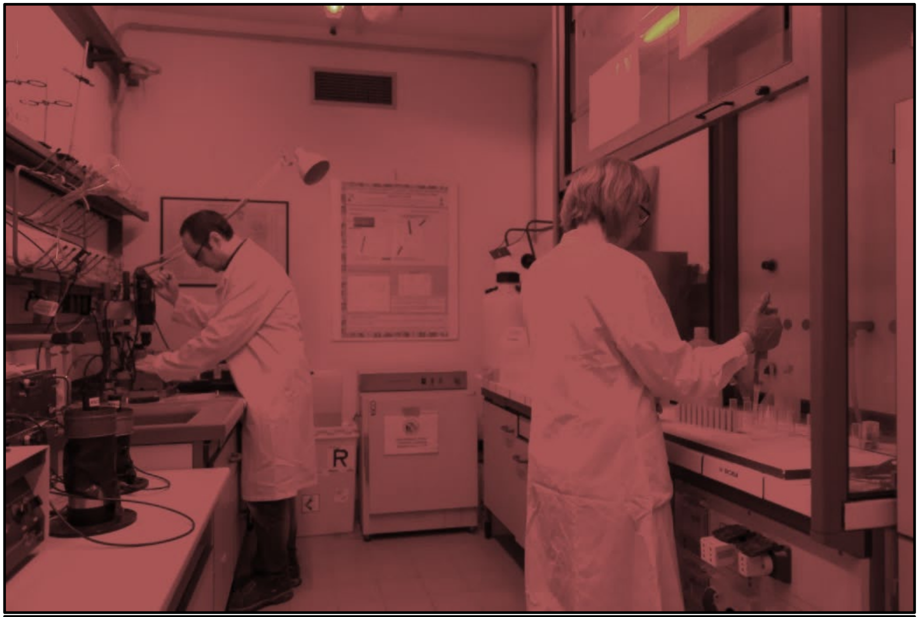
The laboratory is member of CUDAM (Centro Universitario Datazioni e Archeometria, Università di Milano Bicocca) and of BIPAC, Centro Ricerche per il Patrimonio Storico, Artistico e Culturale.

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 peaks 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 ^{14}C 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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Optics and Optometry

Alessandro Borghesi, Silvia Tavazzi, Fabrizio Zeri

The research activities concern materials science, optics, and spectroscopy applied to systems of interest for optometry and/or ophthalmology. Few examples are:

- the development and characterization of polymers for contact lenses and also for drug release by contact lenses;
- the material characterization before and after wear (surface morphology, roughness, rheology, geometry, etc.);
- the characterization of the preservative solutions for contact lenses and also of tears for diagnostic purposes;
- the development of specific instrumentation;
- the study of the mechanisms of vision, also in collaboration with specialists of this field.

MATERIALS FOR CONTACT LENSES

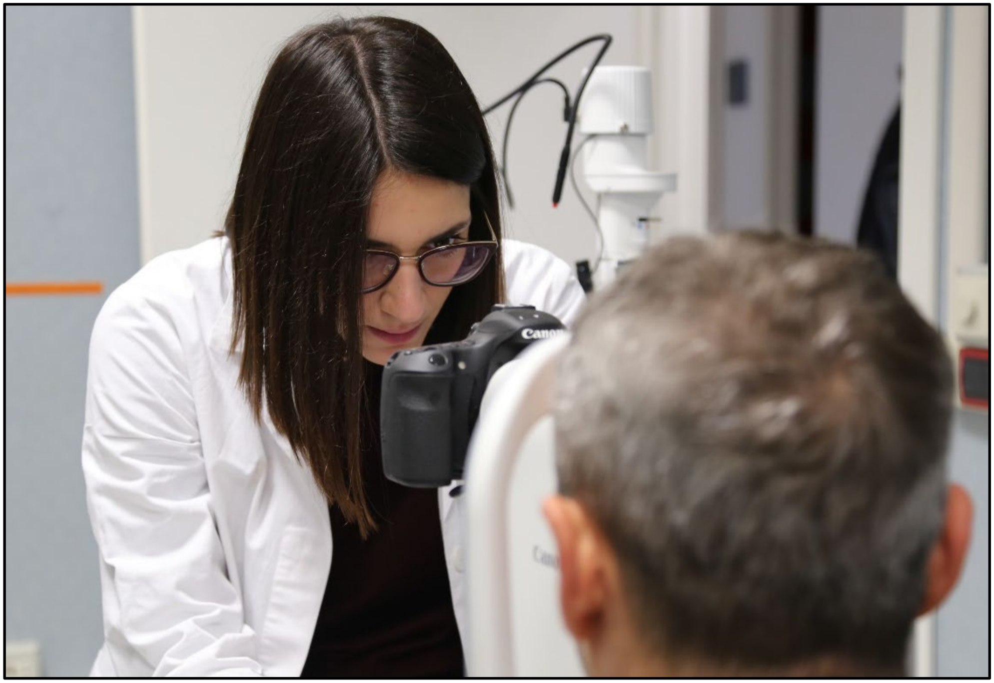
Recent studies were focused on the properties of materials for soft contact lenses in terms of microscopic structure and uptake/release of hyaluronan, lactoferrin, and drugs. Different materials were investigated. The uptake was studied in terms of loading capability, penetration depth in the lens, release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

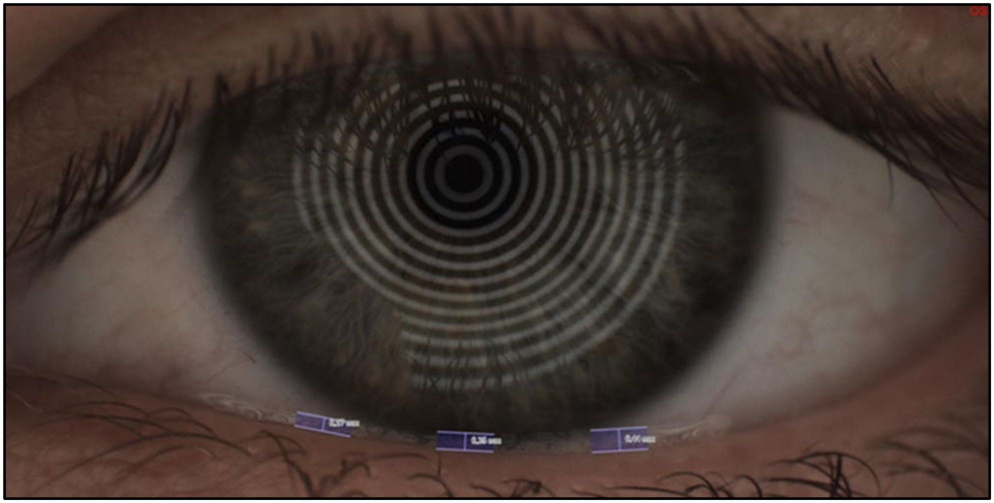
OPTICAL SYSTEMS

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


Canon



Functional dyes and pigments for photonics, electronics and optoelectronics


Luca Beverina, Mauro Sassi

The main goal of our research is the development of efficient and sustainable organic semiconductors for printed optoelectronics and related applications. In the last 20 years the community of researchers devoted to the development of such materials established reliable structure property characteristics providing guidelines to the development of performing active materials for a wide platform of devices. OLEDs, OFETs, OPVs, LEECs and biosensors are amongst the most representative examples.
We have been contributing to such activities, profiting from our expertise in the field of heteroaromatic chemistry and in the development of high performances pigments and dyes.
Recently, the organic semiconductor community started to face the Lab to Fab transition, thus realizing that performances are a necessary but not sufficient condition for successful technological transfer. Stability, reliability and sustainability of the production processes are at least as important as the absolute performance.
We are actively working with partners from Italian and foreign institutions on the development of strategies mutuated from the formulation chemistry approach to develop inks of performing organic semiconductors – polymeric and molecular – whose preparation and handling mainly rely on the use of water and alcohols as reaction media and processing solvents. While gearing up for such an endeavor, we complemented our background in synthetic organic chemistry with a solid knowledge of formulation chemistry.
We routinely collaborate with large companies as well as PMI on both printed optoelectronics and formulation chemistry.

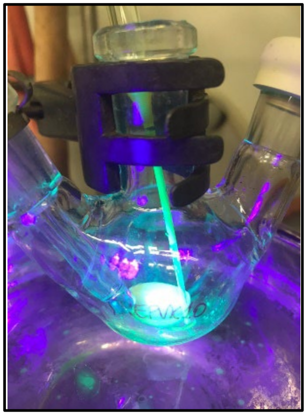
DEVICES DEVELOPED ON COLLABORATION WITH COMPANIES AND RESEARCH INSTITUTIONS

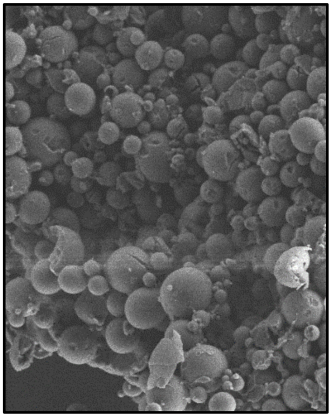
OLEDs, OFETs, EGOFETs, OPVs, fluorescent molecular probes for bioimaging, electrochromic devices, luminescent solar collectors

FACILITIES

Fully equipped organic chemistry lab, capable of scaling up of relatively complex materials up to the 100 g scale. Full chemical characterization (identity and purity).

La^{32}SMO





Generation of nanospaces for polymerization and gas capture

Silvia Bracco, Piero Sozzani

The preparation and characterization of novel nanostructured materials showing permanent porosity or including polymers in supramolecular architectures are the main target of our research group. The effort for designing suitable nanospaces and optimizing extended interfaces enabled the fabrication of materials containing gases and polymers endowed with unusual properties and controlled morphologies. The link between structure and properties is provided by a detailed characterization by magic angle spinning nuclear magnetic resonance (MAS NMR) and wide-line NMR. Laboratories for synthesis and NMR spectroscopy, dedicated to the preparation and the characterization of solid materials, are available.

CURRENT RESEARCH PROJECTS

The current research topics are dedicated to the general themes of confinement of gases and macromolecules to galleries and nanochannels of various cross-sections (0.5 up to 4.5 nm). Nanoporous materials are synthesized and exploited for this sake, realizing absorption of gases and polymerization in the confined state.

The matrices encompass molecular crystals (including dipeptides), metal organic frameworks (MOFs), hybrid mesoporous structures, hyper-crosslinked polymers and porous organic frameworks. The matrices, showing extended interactive areas (1000 - 5000 m^2/g), form intimate host-guest adducts, realizing extraordinarily robust organic materials and solids containing molecular-rotors, whose dynamics is regulated by species diffusing-in.

The study of reactivity and interactions of the guests included in nanometric vessels and supramolecular architectures encompasses also morphological replicas by polymerization and thermal transformation of included polymers to conjugated polymers or carbon nanofibers. Diffusion processes of gases into the porous materials and the direct detection of gases diffusing into solids is performed by MAS and hyperpolarized NMR (^{129}Xe, CO_2, CH_4 and H_2).

FACILITIES

NMR Bruker Avance_300 MHz spectrometer with wide bore magnet operating at 7.05 T and dedicated to the solid state, fully equipped for high power output, 7 kHz and 15 kHz magic angle spinning probes and several heads for wide-line spectroscopy, including deuterium.

NMR Bruker Avance III_600 MHz spectrometer equipped with cryoprobe, with HR MAS and 35 kHz spinning-speed CP-MAS probes.

High vacuum (10^{-9} torr) pump and equipment for hyperpolarized Xenon spectroscopy (laser-excited NMR).

Gas-Vapor Adsorption Analyzers, Differential Scanning Calorimetry, Gel Permeation Cromatography, Dynamic Mechanical Analyzer.


TYPHOON TWIN

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

Antonio Papagni

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.

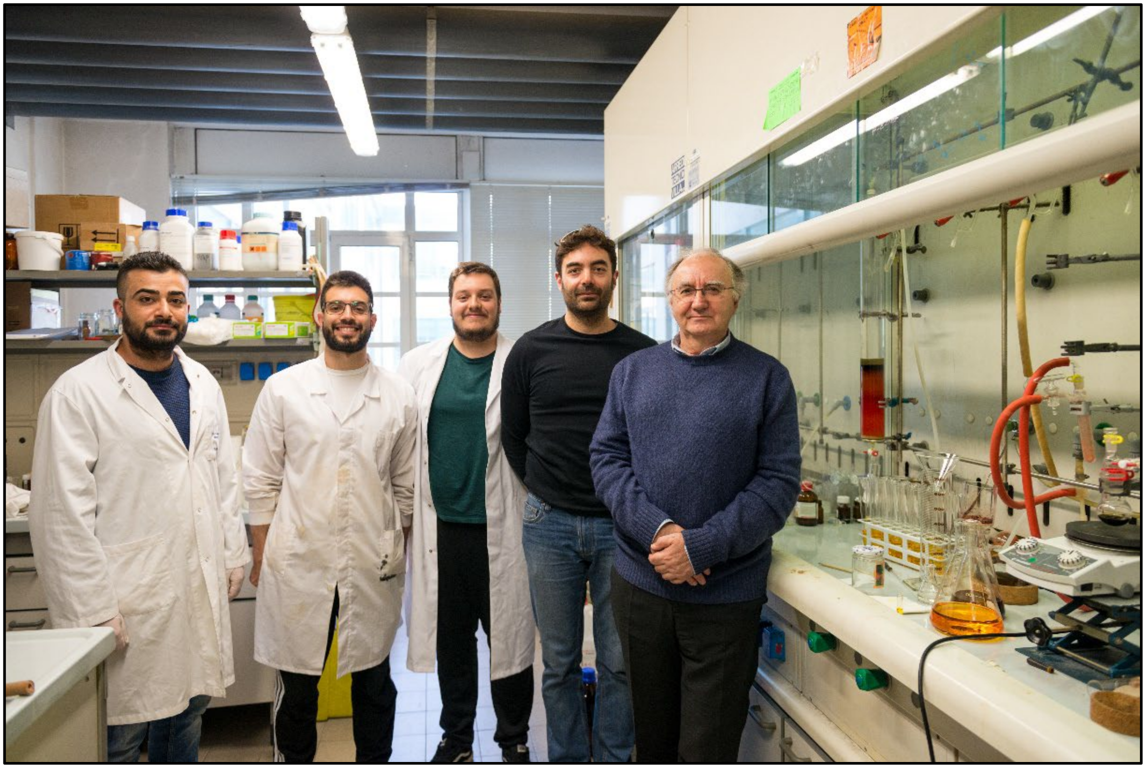
ORGANIC SEMICONDUCTORS

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 systemsable 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


Michele Mauri, Roberto Simonutti

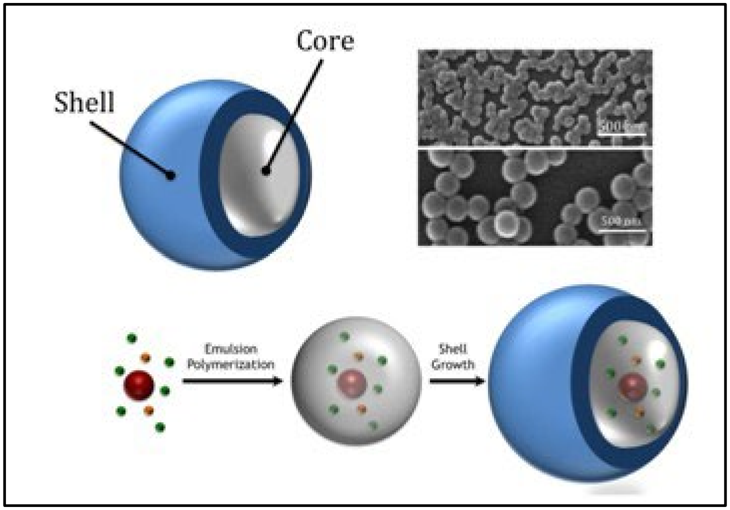
Nanostructured polymer materials have attracted growing interest due to their applicability in many different areas: from microelectronics to photonics, from catalysis to water purification, from biomedical to military applications. Among many different strategies used for preparing polymeric nanostructures,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

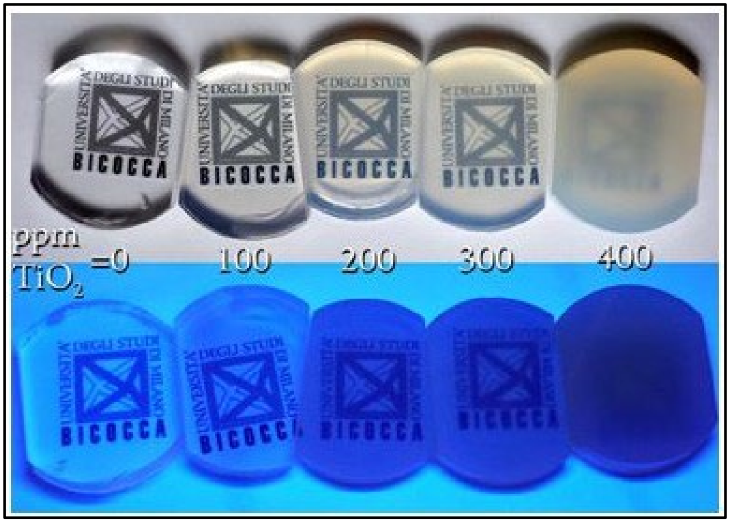
NEW MATERIALS BASED ON BLOCK COPOLYMERS

Block copolymers are constituted by two or three different types of polymer chains connected at the ends with a covalent bond. They display self-organization on the nanometre scale modulated by the external environment. For example, the interaction between block copolymer and solvent produces a diversity of self assembled shapes, including vescicles, spheres, cylinders, that can be tuned by concentration, solvent polarity, temperature and other external stimuli. The morphology in the solid state can also be very complex and is finely tuned by the conditions and the method of solid formation (melt cooling, casting from solvent).
Recently, by implementing advanced polymerization techniques like RAFT (Reversible Addition-Fragmentation chain Transfer polymerization) we synthesized several samples of highly controlled amphiphilic block copolymers. Our interest is currently focused on innovative techniques for their characterization in liquid and solid state, as well as the almost unexplored intermediate soft matter states: highly concentrated solutions, gels and sponge-like materials.

NANOPARTICLE POLYMER NANOCOMPOSITES

The mixing of polymers and inorganic nanoparticles, like oxides, semiconductors (usually defined as quantum dots) or noble metals, is opening pathways for engineering flexible composites that exhibit advantageous electrical, optical, or mechanical properties. In particular, the nanocomposite optical characteristics, as the refractive index, absorption of UV light, birefringence or scattering properties, can be modulated by carefully choosing the particle size and electronic structure of the nanoparticle used for its preparation.
Our research is now directed to the use of oxide nanoparticles with all the dimensions less than 100 nm. A key point of the experimental activity is the surface modification of the nanoparticles by a capping agent in order to increase the stability of the colloidal dispersion.
Nanocomposite molecular structure, morphology and mechanical properties are characterized by a comprehensive suite of advanced techniques, (among others: FTIR, TGA, NMR, DLS, AFM). The measurement of optical properties (absorption, transmission, angular scattering) of nanocomposite monolithic objects is done in collaboration with the University of Insubria.
Another possible application of these nanocomposites is in the conservation of cultural heritage, as protective layer that can protect the painting surface from UV radiation, preserving the aesthetics.


Core
Shell
Emulsion
Polymerization
Shell
Growth


ppm
TiO2 =0
100
200
300
400

FUNDED PROJECTS

Project/Research Contract Title	Funded by	Principal Investigator
Perform Water 2030	Regione Lombardia	M. Acciarri
REPHOB: Superfici superidrofobiche resilienti in condizioni avverse	MIUR	C. Antonini
Efficient separation of compound drops for clean water	Xi'an Jiaotong University	C. Antonini
Metal additive manufacturing (3D printing) based on Digital Light Processing	Regione Lombardia	C. Antonini
SURFICE - Smart surface design for efficient ice protection and control	EU	C. Antonini
Supporto attività di ricerca e sviluppo nella piccola e media impresa	ApiTech srl	C. Antonini
Engineering bio-inspired atmospheric Water Harvesters through fog collection with Badgir architecture	UNIMIB	C. Antonini - R. Akbari
Ab initio simulation of chalcogenide materials	Micron Semiconductor Italia	M. Bernasconi
BeforeHand-Boosting Performance of Phase Change Devices by Hetero- and Nano-Structure Material Design	EU	M. Bernasconi
Nuovi materiali coniugati per celle solari organiche	ENI	L. Beverina
Nanocapps – Nanoencapsulation made easy	FONDAZIONE U4I	L. Beverina
Booster - BOOSTING SUSTAINABILITY IN ORGANIC ELECTRONICS: THE KEY ROLE OF FUNCTIONAL SURFACTANTS AS REACTION MEDIA AND DISPERSING AGENTS	MIUR	L. Beverina
Joint Lab Intercos-Unimib	Intercos	L.Beverina
Sviluppo di inchiostri e di buffer layer alternativi al CdS mediante ALD per celle solari a base di kesteriti	ENEA	S. Binetti
BEST- 4U - Tecnologia per celle solari bifacciali ad alta Efficienza a 4 terminali per 'utility scale'	MIUR	S. Binetti
Enhancing Photosynthesis	Regione Lombardia	S. Bracco
Realizzazione di preforme e caratterizzazione di fibre scintillanti da impiegare come elementi di sensori di radiazione ionizzante	Prysmian	N. Chiodini
Scintillating Porous Architectures for RadioacTivE gas detection – SPARTE	EU	A. Comotti
La tecnonologia SmartNETTM Silica per pneumatici altamente performanti	UNIMIB	B. Di Credico

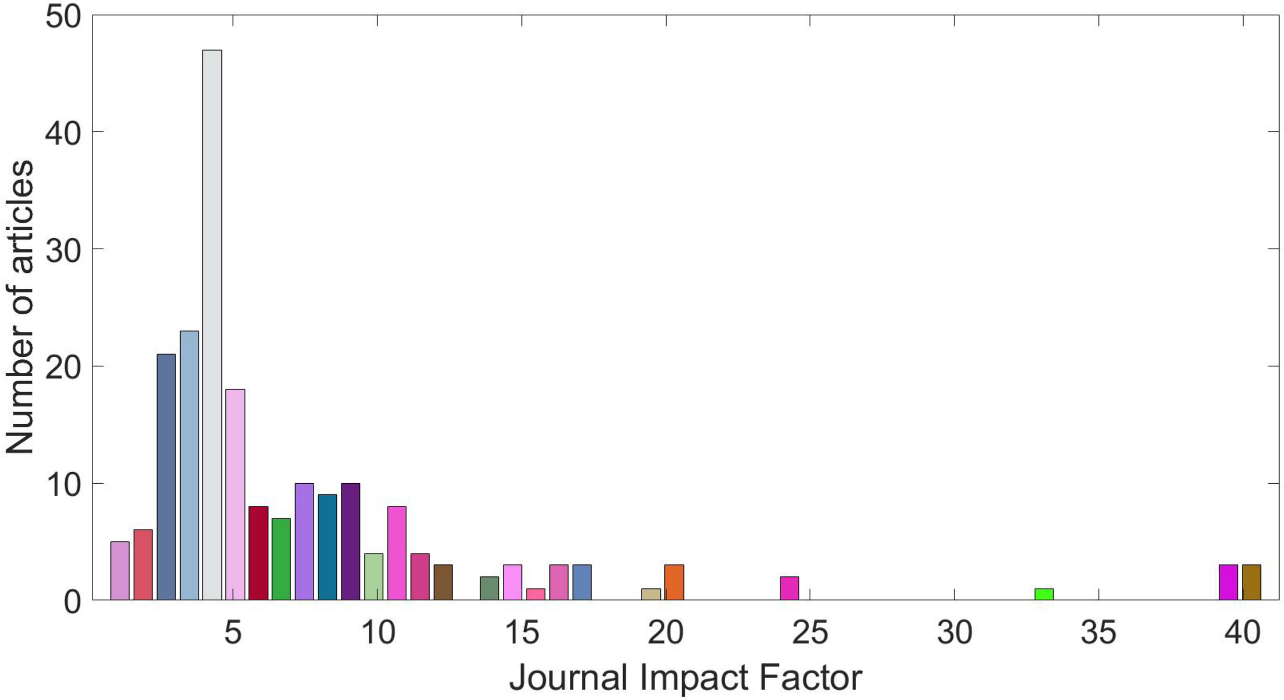
Project/Research Contract Title	Funded by	Principal Investigator
Chimica di 6PPD e derivati	Pirelli-Corimav	B. Di Credico
BIOINOHYB-Smart Bioinorganic Hybrids for Nanomedicine (ERC GRANT)	EU	C. Di Valentin
MADAM Metal Activated 2D Carbon-based Platforms	MIUR	C. Di Valentin
EIT QMforMA Designing New Materials with Quantum Mechanics	EU	C. Di Valentin
Photodynamic therapy for brain tumors by multifunctional particles using in situ Cerenkov and radioluminescence light	UNIMIB	C. Di Valentin
On demand BIOdegradable STARrch-derived composites for PACKaging (BIOSTAR-PACK)	Fondazione Cariplo	M. D'Arienzo
A new course on the Physics and technology of semiconductor devices with hand-on activity in a characterization and simulation lab	MICRON TECHNOLOGY FOUNDATION INC	M. Fanciulli
NEUREKA – A smart hybrid neural-computo device for drug discovery	EU	M. Fanciulli
NATUREChem - Unlocking Sustainable Technologies Through Nature-Inspired Solvents	MIUR	N. Manfredi
MOBARTECH: una piattaforma mobile tecnologica, interattiva e partecipata per lo studio, la conservazione e la valorizzazione di beni storico-artistici	REGIONE LOMBARDIA	M. Martini
Multimodal nanotracking for exosome-based therapy in dmd (theoryenhancing)	MINISTERO DELLA SALUTE	F. Meinardi
Luminescent solar concentration windows for next generation buildingintegrated photovoltaics	UNIMIB	F. Meinardi
CHALLENGE: 3C-SiCHetero-epitaxiALLy grown on silicon compliancE substrates and new 3C-SiC substrates for sustaiNable wide-band-Gap powEr devices	EU	L. Miglio
X-RAY ACTIVATED PHOTODYNAMIC THERAPY FOR TARGETED TREATMENT OF ALZHEIMER'S DISEASE (X-PATH)	MINISTERO AFFARI ESTERI	A. Monguzzi
Theoretical analysis of the dislocation distribution in SILTRONIC SiGe/Si(001) graded layers	SILTRONIC AG	F. Montalenti
Towards sustainable, high performing, all-solid-state sodium-ion batteries	MIUR	P. Mustarelli
ENVIRONMENTALIST - New green and environmentally friendly materials for lithium and beyond-lithium batteries.	Accordo bilaterale Italia-Israele	P. Mustarelli

Project/Research Contract Title	Funded by	Principal Investigator
Advanced Simulation Design of Nanostructured Thermoelectric Materials with Enhanced Power Factors (NanoThermMA)	EU	D. Narducci
Solar driven chemistry: new materials for photo- and electro-catalysis (SMARTNESS)	MIUR	G. Pacchioni
Cascade deoxygenation process using tailored nanocatalysts for the production of biofuels from lignocellulosic biomass	EU	G. Pacchioni
CATSENSE	EU	G. Pacchioni
Ossidi Nanostrutturati: multi-funzionalità e applicazioni	MIUR	G. Pacchioni
CREW - Codesign for REhabilitation and Wellbeing	FONDAZIONE CARIPLO	A. Paleari
KiC- IMAGINE- Development and implementation of EIT KIC Raw Materials Master Program(s) in Sustainable Materials	EU	A. Paleari
Preparazione e caratterizzazione elettrochimica di materiali elettrodi per batterie a ioni sodio (NIB)	RSE S.p.A	R. Ruffo
4PHOTON-Novel Quantum Emitters monolithically grown on Si, Ge and III-V substrates	EU	S. Sanguinetti
FemToTera- Plasmon-enhanced Tera-Hertz emission by Femtosecond laser pulses of nanostructuredsemiconductor/metal surfaces	EU	S. Sanguinetti
TEcnologie INnovative per i VEicoli Intelligenti	REGIONE LOMBARDIA/EU	S. Sanguinetti
Micro-crystals Single Photon InfraREd detectors – μSPIRE – Horizon 2020 FET project	EU	S. Sanguinetti
Pyrolysis processes for valorizing waste biomass and plastic through transformation into platinum-free catalysts for oxygen reduction and hydrogen evolution.	MIUR	C. Santoro
Hexagonal allotropes for group IV photonics	UNIMIB	E. Scalise
EIT-KIC–Safer reduction of ZnO amount in rubber vulcanization process (SAFE-VULCA)	EU	R. Scotti
Studio dell'effetto di rinforzo di silice in compositi elastomerici	Fluorsid Group	R. Scotti
PROtein THErmoplastIcs from FOod Refuse for food packaging Materials -PROTHEIFORM	CARIPLO	R. Simonutti
Next generation of molecular and supramolecular machines: towards functional nanostructured device, interfaces, surfaces and materials (NEMO)	MIUR	P. Sozzani
Design e protocolli applicativi di lenti oftalmiche multifocali e progressive	GrandVision Italia	S. Tavazzi

Project/Research Contract Title	Funded by	Principal Investigator
Assessment of Three Basic Progressive Lens Designs	Hoya Corporation	S. Tavazzi
Analisi optometriche in soggetti non abbienti	FONDAZIONE ONESIGHT	S. Tavazzi
MyExpert Master Fit (myopia progression)	Essilor Italia	S. Tavazzi
SMART-electron	EU	G. M. Vanacore
LUMiNaD	UNIMIB	G. M. Vanacore
SCINTIGLASS	EU	A. Vedda
IDS-FunMat-Inno-2. International Doctoral School in Functional Materials & Innovation	EU	A. Vedda
EIT-RM BRIEFCASE – Learning the use of minerals through non conventional teaching tools	EU	A. Vedda
Brain adaptation to multifocal contact lenses	Alcon Italia	F. Zeri
Stability of the Hoya soft contact lens toric	Hoya Holdings NV, Amsterdam, The Netherlands	F. Zeri
Stability of the Hoya soft contact lens toric: phase II	Hoya Holdings NV, Amsterdam, The Netherlands	F. Zeri
Study on the causes of non-adaptation to progressive addition ophthalmic lenses”	Hoya Corporation Vision Care Section Technical Research & Development Department, Tokyo, Japan	F. Zeri, S.Tavazzi

PUBLICATIONS AND HIGHLIGHTS

In 2021 more than 210 scientific articles authored (or co-authored) by members of the Department were published in international peer-reviewed journals, with an average impact factor (based on ISI WOS, Journal of Citation Reports 2021) of 7.5.

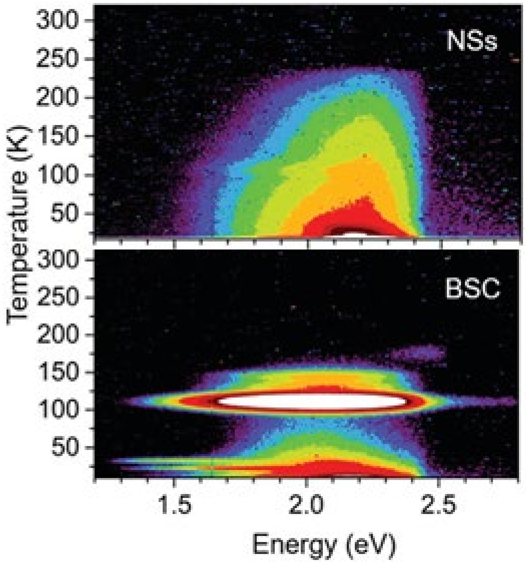


Rodà C., **Fasoli M.**, Zaffalon M.L., Cova F., Pinchetti V., Shamsi J., Abdelhady A.L., Imran M., **Meinardi F.**, Manna L., **Vedda A.**, and **Brovelli S.**

Understanding Thermal and A-Thermal Trapping Processes in Lead Halide Perovskites Towards Effective Radiation Detection Schemes.

ADVANCED FUNCTIONAL MATERIALS **31**, 2104879 (2021).

Lead halide perovskites (LHP) are rapidly emerging as efficient, low-cost, solution-processable scintillators for radiation detection. Carrier trapping is arguably the most critical limitation to the scintillation performance. Nonetheless, no clear picture of the trapping and detrapping mechanisms to/from shallow and deep trap states involved in the scintillation process has been reported to date, as well as of the role of the material dimensionality. Here, this issue is addressed by performing, for the first time, a comprehensive study using radioluminescence and photoluminescence measurements side-by-side to thermally-stimulated luminescence (TSL) and afterglow experiments on $CsPbBr_3$ with increasing dimensionality, namely nanocubes, nanowires, nanosheets, and bulk crystals. All systems are found to be affected by shallow defects resulting in delayed intragap emission following detrapping via athermal tunneling. TSL further reveals the existence of additional temperature-activated detrapping pathways from deeper trap states, whose effect grows with the material dimensionality, becoming the dominant process in bulk crystals. These results highlight that, compared to massive solids where the suppression of both deep and shallow defects is critical, low dimensional nanostructures are more promising active materials for LHP scintillators, provided that their integration in functional devices meets efficient surface engineering.



In the figure: TSL contour plots of $CsPbBr_3$ nanosheets (NSs) and bulk single crystal (BSC).

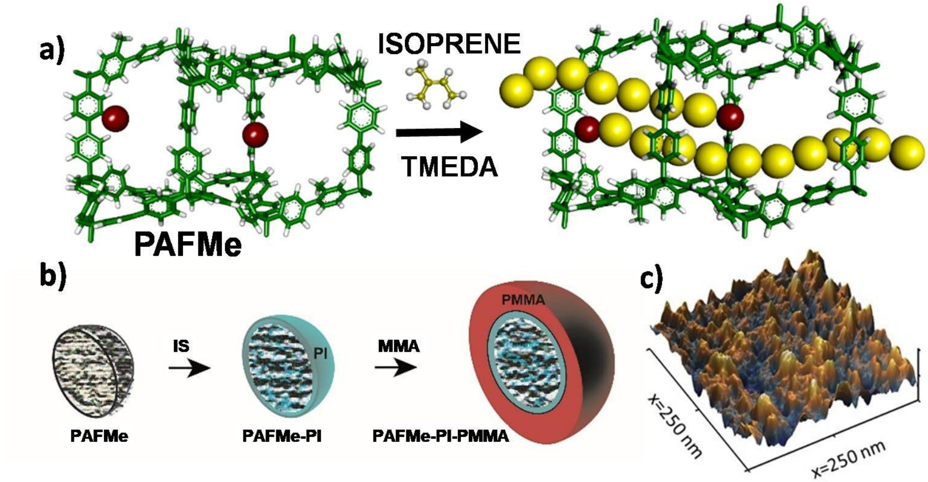
HIGHLIGHTS

Perego, J.; **Bracco, S.**; **Comotti, A.; Piga, D.; Bassanetti, I.**; **Sozzani, P.**

Anionic Polymerization in Porous Organic Frameworks: A Strategy to Fabricate Anchored Polymers and Copolymers.

ANGEWANDTE CHEMIE INTERNATIONAL EDITION 60, 6117 (2021).

An anionic mechanism is used to create polymers and copolymers as confined to, or anchored to, high-surface area porous nanoparticles. For the first time, linear polymers with soft and glassy chains, such as polyisoprene (PI) and polymethylmethacrylate (PMMA), were produced by confined anionic polymerization in 3D networks of porous aromatic frameworks (PAFs). Alternatively, multiple anions were generated on the frameworks and initiate chain propagation, resulting in chains covalently connected to the 3D network. Sequential reactions were promoted by the living character of this anionic propagation, yielding nanoparticles that were covered by a second polymer anchored by anionic block copolymerization. The intimacy of the matrix and the grown-in polymers was demonstrated by 2D ^{1}H-^{13}C-HETCOR NMR spectra.



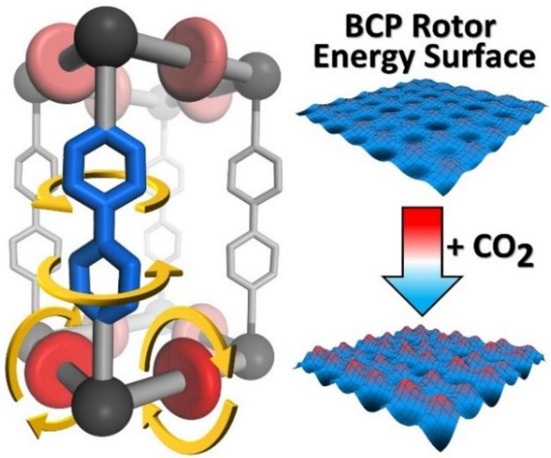
In the figure: a) Porous framework of PAFMe with covalently connected polymer chains resulting from polymerization. b) Living anionic copolymerization from pure PAFMe to the PAFMe-PI and to PAFMe-PI-PMMA nanocomposite. c) AFM images of PAFMe nanoparticles upon copolymerization.

Perego, J.; Bezuidenhout, C. X.; **Bracco, S.**; Prando, G.; Marchiò, L.; Negroni, M.; Carretta, P.; **Sozzani, P.**; **Comotti, A.**

Cascade Dynamics of Multiple Molecular Rotors in a MOF: Benchmark Mobility at a Few Kelvins and Dynamics Control by CO_2.

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 143, 13082 (2021).

Achieving sophisticated juxtaposition of geared molecular rotors with negligible energy-requirements in solids enables fast yet controllable and correlated rotary motion to construct switches and motors. Our endeavor was to realize multiple rotors operating in a MOF architecture capable of supporting ultrafast motional regimes, even at extremely cold temperatures (10^7 Hz at 4 K). Two distinct ligands coordinated to Zn clusters fabricated a pillar-and-layer 3D array of orthogonal rotors. Variable temperature XRD, ^{2}H solid echo, and ^{1}H T_1 relaxation NMR, collected down to a temperature of 2 K revealed the hyperfast mobility of BCP and an unprecedented cascade mechanism modulated by distinct energy barriers starting from values as low as 24 cal mol^{-1}, a real benchmark for complex arrays of rotors. These rotors explored multiple configurations of conrotary and disrotary relationships, switched on and off by thermal energy, a scenario supported by DFT modeling. CO_2 diffused through the open pores, dramatically changed the global rotation mechanism.

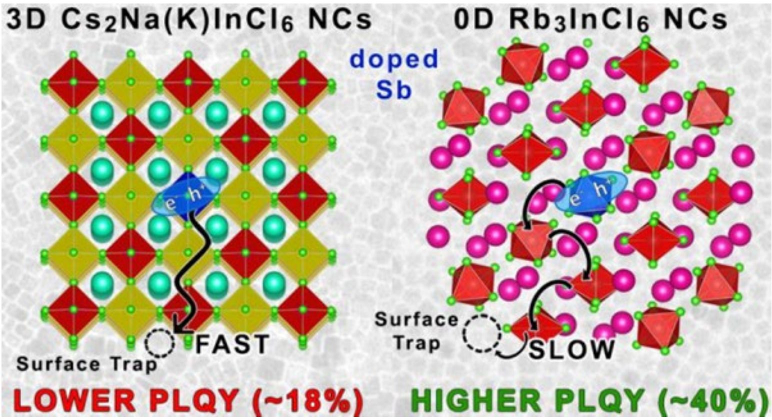


In the figure: MOF architecture made by 4,4′-bipyridine (bipy) and bicyclopentanedicarboxylate (BCP) coordinated to Zn clusters. Bipyridine molecules act as pillars whilst BCP moieties lie in the 2D sheets (left). Energy landscape of BCP rotors in empty MOF and after CO_2 loading: an increase of energy barrier after the external stimulus is observed (right).

HIGHLIGHTS

Zhu, D.; Zaffalon, M. L.; Zito, J.; Cova, F.; **Meinardi**, **F.**; De Trizio, L.; Infante, I.; **Brovelli**, S.; Manna, L.
Sb-Doped Metal Halide Nanocrystals: A 0D versus 3D Comparison
ACS ENERGY LETTERS 6, 2283–2292 (2021)

We synthesize colloidal nanocrystals (NCs) of Rb_3InCl_6, composed of isolated metal halide octahedra (“0D”), and of $Cs_2NaInCl_6$ and Cs_2KInCl_6 double perovskites, where all octahedra share corners and are interconnected (“3D”), with the aim to elucidate and compare their optical features once doped with Sb^{3+} ions. Our optical and computational analyses evidence that the photoluminescence quantum yield (PLQY) of all these systems is consistently lower than that of the corresponding bulk materials due to the presence of deep surface traps from under-coordinated halide ions. Also, Sb-doped “0D” Rb_3InCl_6 NCs exhibit a higher PLQY than Sb-doped “3D” $Cs_2NaInCl_6$ and Cs_2KInCl_6 NCs, most likely because excitons responsible for the PL emission migrate to the surface faster in 3D NCs than in 0D NCs. We also observe that all these systems feature a large Stokes shift (varying from system to system), a feature that should be of interest for applications in photon management and scintillation technologies. Scintillation properties are evaluated via radioluminescence experiments, and re-absorption-free waveguiding performance in large-area plastic scintillators is assessed using Monte Carlo ray-tracing simulations.



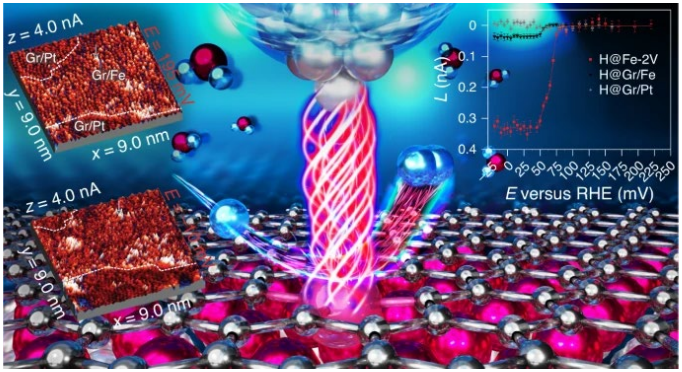
In the figure: sketch of the crystal lattices of undoped and Sb-doped “3D” double perovskites and “0D” NCs studied in this work, and the identified excitonic quenching pathways.

Kosmala, T; Baby, A; Lunardon, M; Perilli, D; Liu, H; Durante, C; **Di Valentin, C**; Agnoli, S; Granozzi, G.

Operando visualization of the hydrogen evolution reaction with atomic-scale precision at different metal–graphene interfaces.

NATURE CATALYSIS 55, 7998. (2021).

The development of catalysts for the hydrogen evolution reaction is pivotal for the hydrogen economy. Thin iron films covered with monolayer graphene exhibit outstanding catalytic activity, surpassing even that of platinum, as demonstrated by a method based on evaluating the noise in the tunnelling current of electrochemical scanning tunnelling microscopy. Using this approach, we mapped with atomic-scale precision the electrochemical activity of the graphene–iron interface, and determined that single iron atoms trapped within carbon vacancies and curved graphene areas on step edges are exceptionally active. Density functional theory calculations confirmed the sequence of activity obtained experimentally. This work exemplifies the potential of electrochemical scanning tunnelling microscopy as the only technique able to determine both the atomic structure and relative catalytic performance of atomically well-defined sites in electrochemical operando conditions and provides a detailed rationale for the design of novel catalysts based on cheap and abundant metals such as iron.



In the figure: STM images during catalytic activity for HER by Gr/Fe/Pt(111).

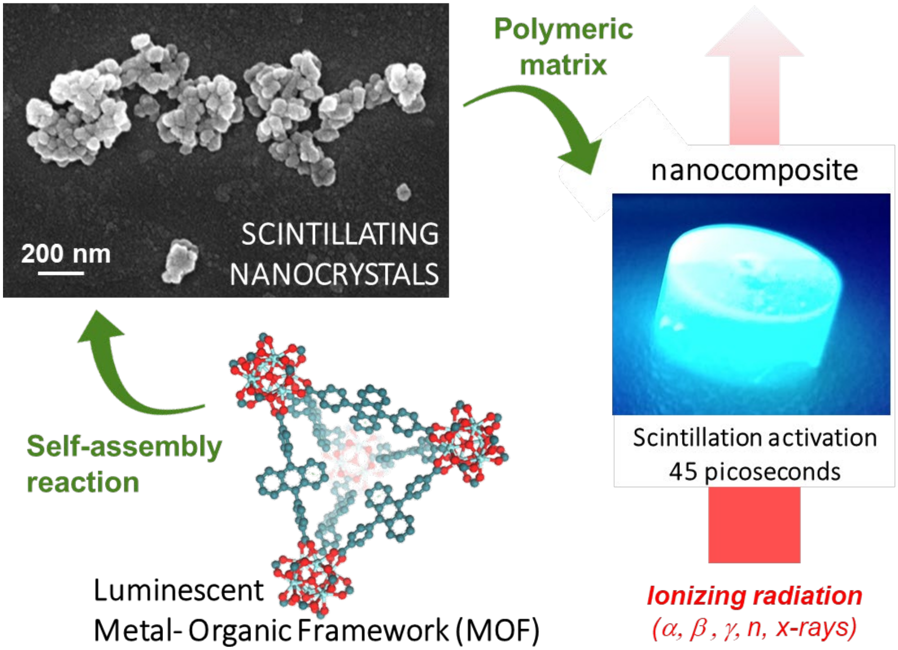
HIGHLIGHTS

Perego, J; Villa, I; Pedrini, A; Padovani, E. C; Crapanzano, R; **Vedda, A**; Dujardin, C; Bezuidenhout, C. B.; **Bracco, S**; **Sozzani, P. E**; **Comotti, A**; Gironi, L; Beretta, M; Salomoni, M; Kratochwil, N; Gundacker, S; Auffray, E; **Meinardi, F**; **Monguzzi, A**.

Composite fast scintillators based on high-Z fluorescent metal–organic framework nanocrystals.

NATURE PHOTONICS, 15(5), 393-400 (2021).

In this study, the researchers designed a composite material, made of a processable polymeric matrix that incorporates scintillating Metal- Organic Frameworks (MOFs) nanocrystals, thus demonstrating an improvement in the scintillation efficacy. This multicomponent material would allow the fabrication of radiation detector more sensitive and with a better time response to be employed in TOF-PET to enhance the imaging accuracy and scanner sensitivity.



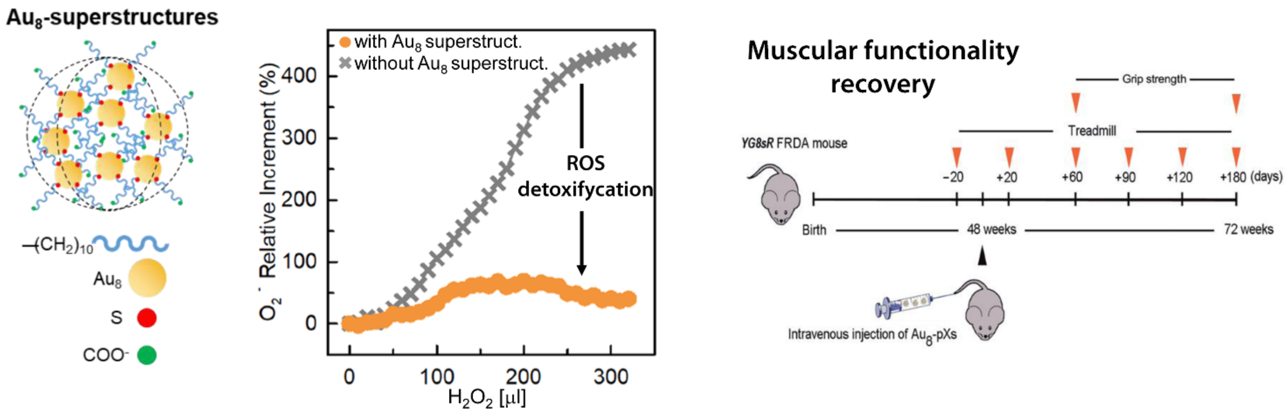
In the figure: Molecular structure and SEM imaging of scintillating MOF nanocrystals. Picture of the composite scintillator fabricated by embedding MOF nanocrystals in a polymer matrix under X-ray excitation.

Villa C; Legato, M; Umbach, A; Riganti, C; Jones, R; Martini, B; Boido, M; Medana, C; Facchinetti, I; Barni, D; Pinto, M; Arguello, T; Belicchi, M; Fagiolari, G; Liaci, C; Moggio, M; **Ruffo, R**; Moraes, C. T; **Monguzzi, A**; Merlo, G, R; Torrente, Y.

Treatment with ROS detoxifying gold quantum clusters alleviates the functional decline in a mouse model of Friedreich ataxia.

SCIENCE TRANSLATIONAL MEDICINE 13, 607 (2021).

The Friedreich Ataxia (FRDA) is a neurodegenerative disease caused by an abnormality in the gene that codes for a protein called frataxin. This disease mainly affects the central and peripheral nervous system and generally arises in the age of puberty, manifesting itself with ataxia of the limbs. In this work, we demonstrate how reactive oxygen species (ROS) scavenging quantum cluster of gold atoms improve the mitochondrial activity and function, thus reducing the oxidative damage in the patients affected by the FRDA.

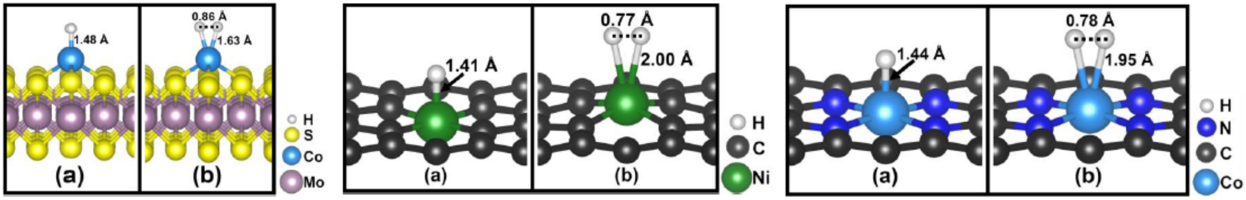


In the figure: Structure of the gold quantum clusters employed in this study (left), the measure of their efficiency as ROS scavengers (center), and recovery of muscular functionality in FRDA mice upon treatment with gold clusters (right).

HIGHLIGHTS

Di Liberto, G.; Cipriano, L; **Pacchioni, G.**
Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts.
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 143, 20431 (2021).

The hydrogen evolution reaction (HER) has a key role in electrochemical water splitting. A lot of attention has been dedicated to HER from Single Atom Catalysts (SAC) and the activity of SACs in HER is rationalized or predicted using models derived for metal surfaces where the only intermediate that forms are H atoms adsorbed on the metal electrode. However, SACs differ substantially from metal surfaces, and can be considered analogs of coordination compounds. In coordination chemistry, at variance with metal surfaces, stable dihydride or dihydrogen complexes (HMH) can form. We have shown that stable HMH intermediates, in addition to MH ones, can form on SACs and that this changes the kinetics of the process. The work provides an example of the important analogies between the chemistry of SACs and that of coordination compounds.



CoH/MoS_2 and HCoH/MoS_2 NiH@DV-Gr and HNiH@DV-Gr CoH@4N-Gr and HCoH@4N-Gr

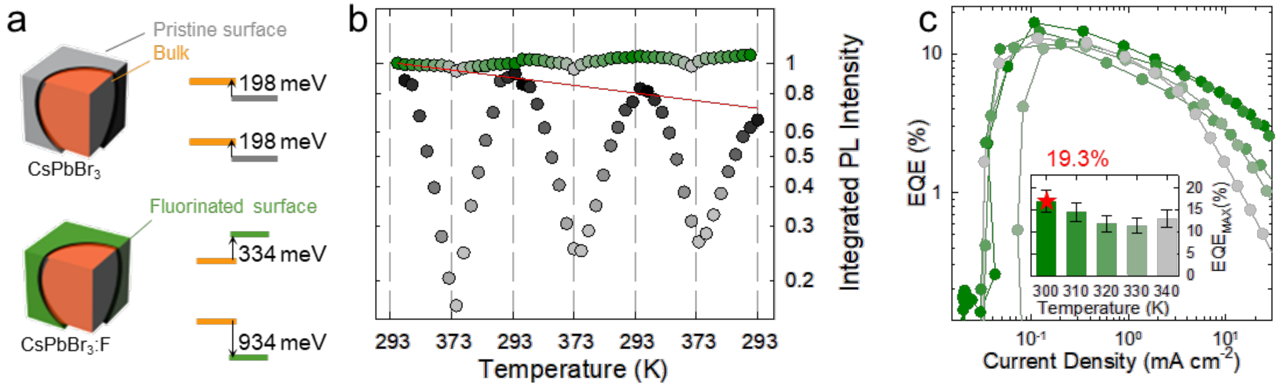
In the figure: structure of mono- and di-hydrogen complexes formed on single atom catalysts on different supports.

Liu, M.; Wan, Q.; Wang, H.; Carulli, F.; Sun, X.; Zheng, W.; Kong, L.; Zhang, Q.; Zhang, C.; Zhang, Q.; **Brovelli, S.;** Liang Li.

Suppression of temperature quenching in perovskite nanocrystals for efficient and thermally stable light-emitting diodes.

NATURE PHOTONICS, 15, 379-385 (2021).

The thermal quenching of light emission is a critical bottleneck that hampers the real-world application of lead halide perovskite nanocrystals (PVK NCs) in light-emitting diodes. Here, we report $CsPbBr_3$ perovskite nanocrystals with a temperature-independent emission efficiency of near unity and constant decay kinetics up to a temperature of 373 K. This regime is obtained by a fluoride post-synthesis treatment that produces fluorine-rich surfaces with a wider energy gap than the inner NCs core, yielding suppressed carrier trapping, improved thermal stability and efficient charge injection. Light-emitting diodes incorporating these fluoride-treated PVK NCs show a low turn-on voltage and spectrally pure green electroluminescence with an external quantum efficiency as high as 19.3% at 350 cd m^{-2}. Importantly, nearly 80% of the room-temperature external quantum efficiency is preserved at 343 K, in contrast to the dramatic drop commonly observed for standard $CsPbBr_3$ PVK NCs light-emitting diodes. These results provide a promising pathway for high-performance, practical light-emitting diodes based on PVK nanostructures.

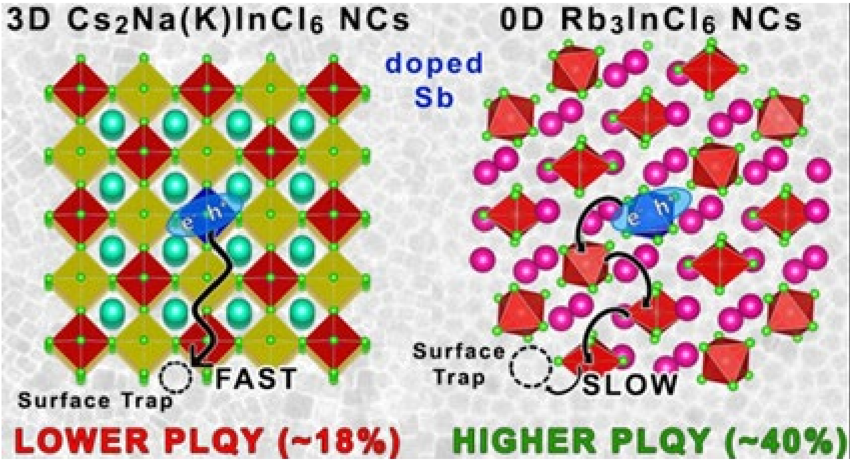


In the figure: a) fluorination effect on energy position of surface levels. b) Thermal stability of pristine and fluorinated PVK NCs 3 thermal cycles. c) EQE–current density curves collected at different temperature.

HIGHLIGHTS

Zhu, D.; Zaffalon, M.L.; Zito, J; Cova, F.; **Meinardi, F.**; De Trizio; L.; Infante, I.; **Brovelli, S.**; Manna, L.
Sb-Doped Metal Halide Nanocrystals: A 0D versus 3D Comparison.
ACS ENERGY LETTERS 6, 2283 (2021).

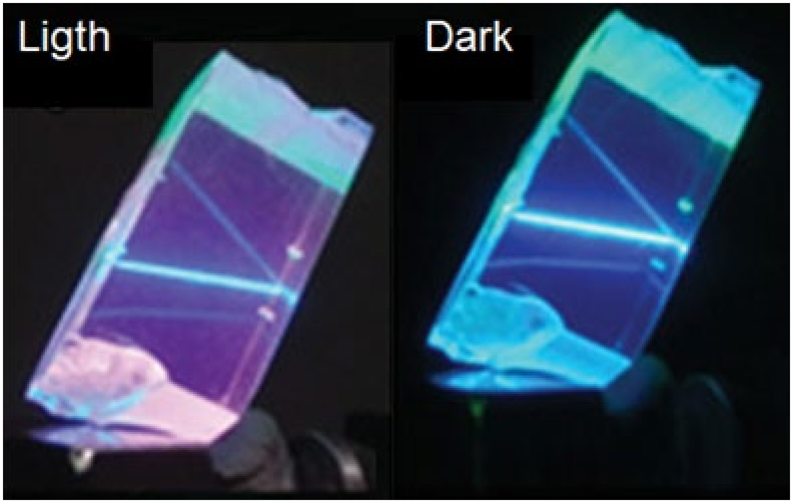
Lead halide perovskite nanocrystals (NCs) feature a bright and narrow photoluminescence (PL) emission that can be varied over the whole visible spectrum by compositional tuning. On the other hand, these materials are inherently toxic. Hence, the current quest is to replace such Pb-based perovskites with alternative non-toxic metal halide NCs. Here, we reported the syntheses of colloidal nanocrystals of Rb_3InCl_6 ("0D") metal halide and of $Cs_2NaInCl_6$ and Cs_2KInCl_6 ("3D") double perovskites and their doping with Sb^{3+} cations. Sb-doped "0D" NCs exhibit a higher PLQY compared to the corresponding "3D" ones. We explained this finding to the different connectivity of metal halide octahedra characterizing 0D and 3D structures: isolated octahedra in the 0D structure reduce the exciton diffusion, thus minimizing non-radiative decay. The applicability of the systems as scintillator materials is assessed via RL measurements and corroborated by Monte Carlo ray-tracing simulations, highlighting their potential for re-absorption-free plastic scintillators of very large size.



In the figure: Sketch of the Crystal Lattices of Sb-Doped "3D" Double Perovskites and "0D" Nanocrystals with a pictorial representation of the exciton trapping process.

Saenz, F.; Ronchi, A.; **Mauri, M.**; Vadrucci, R.; **Meinardi, F.**; **Monguzzi, A.**; Weder, C.
Nanostructured Polymers Enable Stable and Efficient Low-Power Photon Upconversion
ADVANCED FUNCTIONAL MATERIALS 31, 2004495 (2021).

Photon upconversion based on sensitized triplet–triplet annihilation (sTTA-UC) is a wavelength-shifting technique with potential use in actuators, sensing, and solar technologies. In sTTA-UC, the upconverted photons are the result of radiative recombination of high-energy singlets, which are created through the fusion of metastable triplets emitter molecules. The emitter triplets are populated via energy transfer (ET) from a proper sensitizer. The process is highly efficient at low powers in solution but becomes relatively ineffective in solid matrices where the diffusion-assisted bimolecular interactions are prevented. Here, we report nanophase-separated polymer systems synthesized under ambient conditions that contain the upconverting dyes in liquid nanodomains. The nanostructured polymers show an excellent optical quality, an outstanding upconversion efficiency of up to ≈23%, and excellent stability in air. Moreover, the dyes' confinement in nanosized domains <50 nm results in an increased effective local density of chromophores that enables hopping-assisted ET and TTA and confers to the upconversion process peculiar kinetics that enhances the material performance at low powers.



In the figure: Pictures of a free-standing upconverting polymer sample under excitation at 532 nm taken under ambient light and in the dark.

PUBLICATIONS IN INTERNATIONAL JOURNALS

#	Publication details	IF
1	Abou El Kheir, O; Bernasconi, M, High-throughput calculations on the decomposition reactions of off-stoichiometry gesbte alloys for embedded memories, NANOMATERIALS 11, 2382	5.719
2	Abou El Kheir, O; Dragoni, D; Bernasconi, M, Density functional simulations of decomposition pathways of Ge-rich GeSbTe alloys for phase change memories, PHYSICAL REVIEW MATERIALS 5, 095004	3.980
3	Acciarri, M; Checola, S; Galli, P; Magatti, G; Stefani, S, Water resource management and sustainability: A case study in faafu atoll in the Republic of Maldives, SUSTAINABILITY 13, 3484	3.889
4	Adriani, O; Agnesi, A; Albergo, S; Antonelli, M; Auditore, L; Basti, A; Berti, E; Bigongiari, G; Bonechi, L; Bongi, M; Bonvicini, V; Bottai, S; Brogi, P; Castellini, G; Cattaneo, P; Checchia, C; D'Alessandro, R; Detti, S; Fasoli, M; Finetti, N; Italiano, A; Maestro, P; Marrocchesi, P; Mori, N; Orzan, G; Olmi, M; Pacini, L; Papini, P; Pellegriti, M; Pirzio, F; Pizzolotto, C; Poggiali, C; Rappoldi, A; Ricciarini, S; Sciuto, A; Spillantini, P; Starodubtsev, O; Stolzi, F; Suh, J; Sulaj, A; Tiberio, A; Tricomi, A; Trifiro, A; Trimarchi, M; Vedda, A; Vannuccini, E; Zampa, G; Zampa, N, The CaloCube calorimeter for high-energy cosmic-ray measurements in space: Performance of a large-scale prototype, JOURNAL OF INSTRUMENTATION 16, P10024	1.121
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BOOKS AND CONTRIBUTIONS

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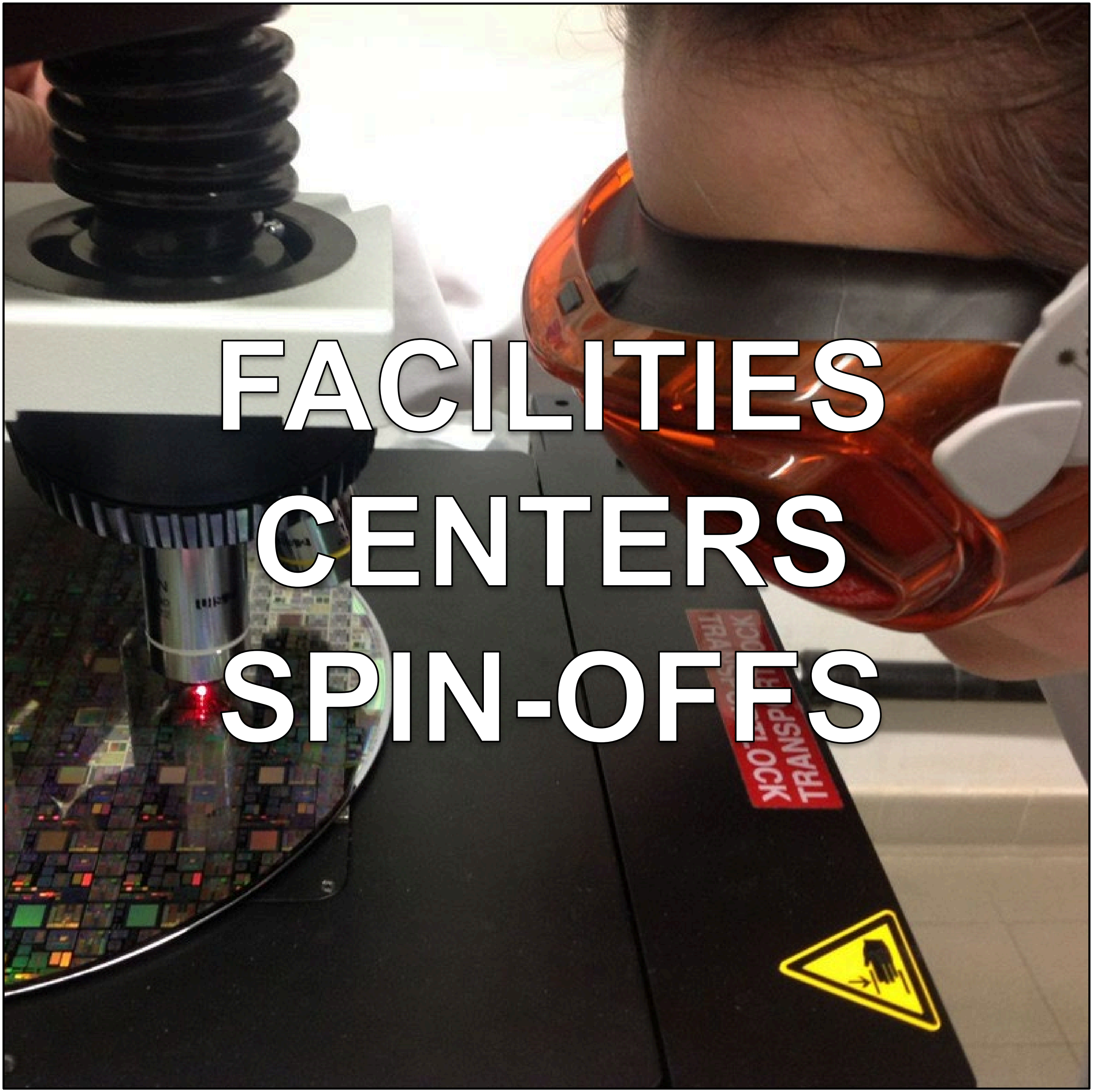
PhD THESES

DOCTORATE IN MATERIALS SCIENCE AND NANOTECHNOLOGY

https://en.unimib.it/education/doctoral-research-phd-programmes/phd-programmes/materials-science-and-nanotechnology

Authors	Title
CALASCIBETTA, ADIEL MAURO	Sustainable synthetic methodologies for the preparation of organic semiconducting materials: organic (opto)electronics growing “green”
IMIETE, IIKPOEMUGH ELO	Light weight polysaccharides as biofillers for elastomeric compounds
TOLIOPOULOS, DIMOSTHENIS	Single photon sources integrated on ge mie resonator fabricated by solid state dewetting
GUARDIANI, ANTONIO	Quantum engineering at the single photon level
LONGO, EMANUELE MARIA	Heterostructures based on the large-area Sb_2Te_3 topological insulator for spin-charge conversion
MAGAGNA, STEFANO	Thermoelectric nanostructured silicon obtained by metal-assisted chemical etching
MONTI, ANDREA MAURIZIO	Point defects in quartz: role in trapping and luminescence
ANAND, ABHINAV	Spectroscopic avenues and photophysical phenomena in colloidal nanocrystals
FACCHINETTI, IRENE	Thermally regenerable redox-flow batteries
GAIFAMI, CARLO MARIA	Plasma technology application on tyre reinforcing materials
MONTI, MAURO	Synthesis of innovative multifunctional thermally-activated reactive species for elastomeric nanocomposite technology
PERILLI, DANIELE	Quantum mechanical modeling of chemical activated 2D-materials for electrocatalysis and sensing
TULLIO, CHIARA	Development of an effective tumor-targeted contrast agent for magnetic resonance imaging based on Mn/H-ferritin nanocomplexes
FARAONE, GABRIELE	Two-dimensional phosphorus: from the synthesis towards the device integration
TUKTAMYSHEV, ARTUR	Droplet epitaxy quantum dots on GaAs (111)a substrates for quantum information applications
VICHI, STEFANO	Bandgap and intrinsic electric field engineering in nitrides: towards efficient red leds


FACILITIES
CENTERS
SPIN-OFFS

CONSULTING

https://www.mater.unimib.it/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
- Consulting
- Training

Materials Characterization

Investigating the properties of materials

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

Consulting

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

Research Projects

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

CUDAM

CENTRO UNIVERSITARIO DATAZIONI E ARCHEOMETRIA MILANO BICOCCA

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, DEPARTMENT OF EARTH AND ENVIRONMENTAL SCIENCES, DEPARTMENT OF PHYSICS “G. OCCHIALINI”, DEPARTMENT 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 Cultural 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, DIPARTIMENTO DI INFORMATICA, SISTEMISTICA E COMUNICAZIONE; DIPARTIMENTO 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, METODI QUANTITATIVI E STRATEGIE DI IMPRESA; DIPARTIMENTO DI SCIENZE ECONOMICO-AZIENDALI E DIRITTO PER L’ECONOMIA; DIPARTIMENTO DI STATISTICA E METODI QUANTITATIVI.

L-NESS

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

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

L-NESS (Laboratory for Epitaxial Nanostructures on Silicon and Spintronics)

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

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

CENTRO INTERDIPARTIMENTALE PER GLI STUDI DI GENERE

https://abcd.unimib.it/

The ABCD research center of University of Milano – Bicocca promotes and disseminates gender research and gender studies. The main aims of the Center are:

- to encourage scientific cooperation between scholars from different disciplines, with the aim of identifying new directions for gender-sensitive research, at both national and international level;
- to disseminate gender-sensitive knowledge through research projects and research publications;
- to organize conferences, seminars, meetings and to support events to disseminate gender knowledge and gender studies;
- to facilitate opportunities for discussion within and outside the University about gender issues and to support cooperation with communities, associations, and institutions for a better integration of the gender dimension in research programs
- to promote education activities on gender differences and inequalities.

MIB-SOLAR

SOLAR ENERGY RESEARCH CENTER

www.mibsolar.mater.unimib.it

MIB-SOLAR was constituted in July 2010 with the goal to assemble and organize the diverse experiences of research in the field of materials and devices for solar energy applications at the University of Milano-Bicocca. Through MIB-SOLAR the department of Material Science supports the national business community in research and development of new materials and technologies for solar energy application, mainly photovoltaics and solar fuels (artificial photosynthesis and water splitting). The Centre presently counts about 25 members. MIB-SOLAR has been included amongst the top players in the power industry 'made in Italy' (“100 italian energy stories” by Enel and Symbola).

Main objectives of MIB-SOLAR are:

- study and research of new materials and devices related to solar energy in its various forms;
- the aggregation and coordination of researchers in the field of solar energy;
- training of young researchers in the field of materials science and technology for solar energy;
- the development of intellectual property of the University of Milano-Bicocca in the field of solar energy;
- cooperation with institutions, public and private research centers, and Fondazioni in the field of solar energy;
- support and technology transfer to companies operating in the field of solar energy;
- promotion of seminars, conferences, meetings and discussions for the study and exchange of information and knowledge in the field of solar energy.

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

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

COMiB

UNIVERSITY RESEARCH CENTER IN OPTICS AND OPTOMETRY OF MILANO-BICOCCA

The University Research Center in Optics and Optometry of Milano-Bicocca (COMiB), established in 2015 at the Department of Materials Science, is a platform for the coordination and aggregation of the various skills that operate in the field of vision science.
The main objectives of the Center are:

- promote and develop new research in the field of optometry and contact lenses, supporting the interaction and collaboration between different disciplines such as Optics and Optometry, Physics, Materials Science, Psychology, Biology, Chemistry, Medicine, IT, Biostatistics
- activate collaborations with public and private bodies (eg. schools, sports centers, companies) for the creation of screening and visual analysis in the field
- activate both national and international research projects in the field of vision science.
- organize events, seminars, training activities for professionals in the sector, also proposing itself as an Academy to companies interested in training courses of high professional level by making available the structure and skills of the Center.

Interdepartmental Microscopy Platform

The Interdepartmental Microscopy Platform aims at bringing together the interdepartmental services of optical and electron microscopies under a single structure. At the University of Milano-Bicocca an electron microscopy service has been active since 2004 and finally became part of the Microscopy Platform in 2017. The Platform was born from the collaboration of the Departments of Biotechnology and Biosciences, Physics, Earth and Environmental Sciences, and Materials Science. The Microscopy Platform provides service to the personnel of the University of Milano-Bicocca, as well as to the personnel of other universities, public research centers and no-profit centers for their institutional activities. Access to the microscopes is also open to individuals in the form of commissioned research. All services are regulated by a regulation and a tariff.

FACILITIES

- Scanning Electron Microscope (SEM) ZEISS FEG Gemini 500
- Transmission Electron Microscope JEOL (TEM) JEM 2100+
- Dual Beam SEM-FIB FEI Quanta 3D
- Scanning Electron Microscope (SEM) Tescan VEGA TS 5136XM
- Transmission Electron Microscope (TEM) JEOL JEM 1220
- Confocal microscope Nikon A1R.

CNISM

CONSORZIO NAZIONALE INTERUNIVERSITARIO PER LE SCIENZE FISICHE DELLA MATERIA

www.cnism.it

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

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

INSTM

CONSORZIO INTERUNIVERSITARIO NAZIONALE PER LA SCIENZA E LA TECNOLOGIA DEI MATERIALI

www.instm.it

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

General Fields of Research are: Advanced mechanics, construction and transport, Energy and environment, Systems for the preparation, transmission and storage of information, Health and Nutrition. The success of INSTM is underlined by the sheer number and quality of the domestic and international projects involving INSTM's research groups that have been financed to date.

CORIMAV

CONSORZIO PER LA RICERCA SUI MATERIALI AVANZATI

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

DELTATI RESEARCH

DeltaTi Research was founded in 2011 as a joint spin-off between the University of Milano-Bicocca and ERG SpA. The consortium, fully financially supported by ERG, has aimed at the development of nanostructured silicon-based thermoelectric generators. Thermal harvesting is actually a key enabling technology to power the so-called Internet of Things, further to be a way to recover waste heat released at low temperatures by industrial plants, cars, and buildings.
Over the last five years DeltaTi Research has empowered a novel technological approach developed at the Department of Materials Science and protected now by eleven international patents. Low-cost, high-efficiency generators based upon silicon nanocomposites have now reached full technological maturity. Technology was pre-industralised in 2014 and has then been transferred to LFoundry srl, which has joined the Consortium in 2015.
Over its five years of activity the Consortium R&D has signed research contacts for more than four million euros with a number of external institutions, including CNR, the Universities of Modena, Naples, and Vienna, the Fondazione Bruno Kessler, the Demokritos Research Center, and Altran SpA.

PILEGROWTH TECH S.R.L.

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 collaboration with Swiss federal institutions, such as ETH Zürich, CSEM SA (Swiss Center for Electronics and Micromachining) Neuchatel, and EMPA (Federal Institute of Materials Certification) are particularly active, within a collaboration for developing a new Ge-based X-ray imaging detector, integrated on a Si CMOS chip.

GALATEA BIOTECH- THE WHITE BIOTECH COMPANY

http://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.

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 Professor Sergio 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 radiation and 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 absorption and emission of light. This makes it possible to obtain colorless poly acrylate panels, with an electrical generation efficiency close to 5%, made of non-toxic materials 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.

Bicocca Quantum Technologies

https://biqute.unimib.it/

Interdepartmental initiative to strengthen Quantum Technology research and innovation, training, and technology transfer in University of Milano-Bicocca. The initiative encompasses research on superconducting quantum devices, advanced quantum materials, non-classical single photon sources and detectors, semiconductor spin qubits, quantum computing and artificial intelligence.

The initiative leverages collaborations with national and international research institutes, such as Istituto Nazionale di Fisica Nucleare (INFN), Fondazione Bruno Kessler (FBK), Istituto Nazionale per la Ricerca Metrologica (INRiM), National Institute for Science and Technology (NIST), and Superconducting Quantum Materials and Systems Center (SQMS) at Fermilab.

Scientific Committee: Prof. Marco Fanciulli (Dipartimento di Scienza dei Materiali), Prof. Claudio Ferretti (Dipartimento di Informatica, Sistemistica e Comunicazione), Prof. Alberto Leporati (Dipartimento di Informatica, Sistemistica e Comunicazione), Prof. Angelo Nucciotti, Scientific Director (Dipartimento di Fisica “G. Occhialini”), Prof. Stefano Sanguinetti (Dipartimento di Scienza dei Materiali), Prof. Alberto Zaffaroni (Dipartimento di Fisica “G. Occhialini”).