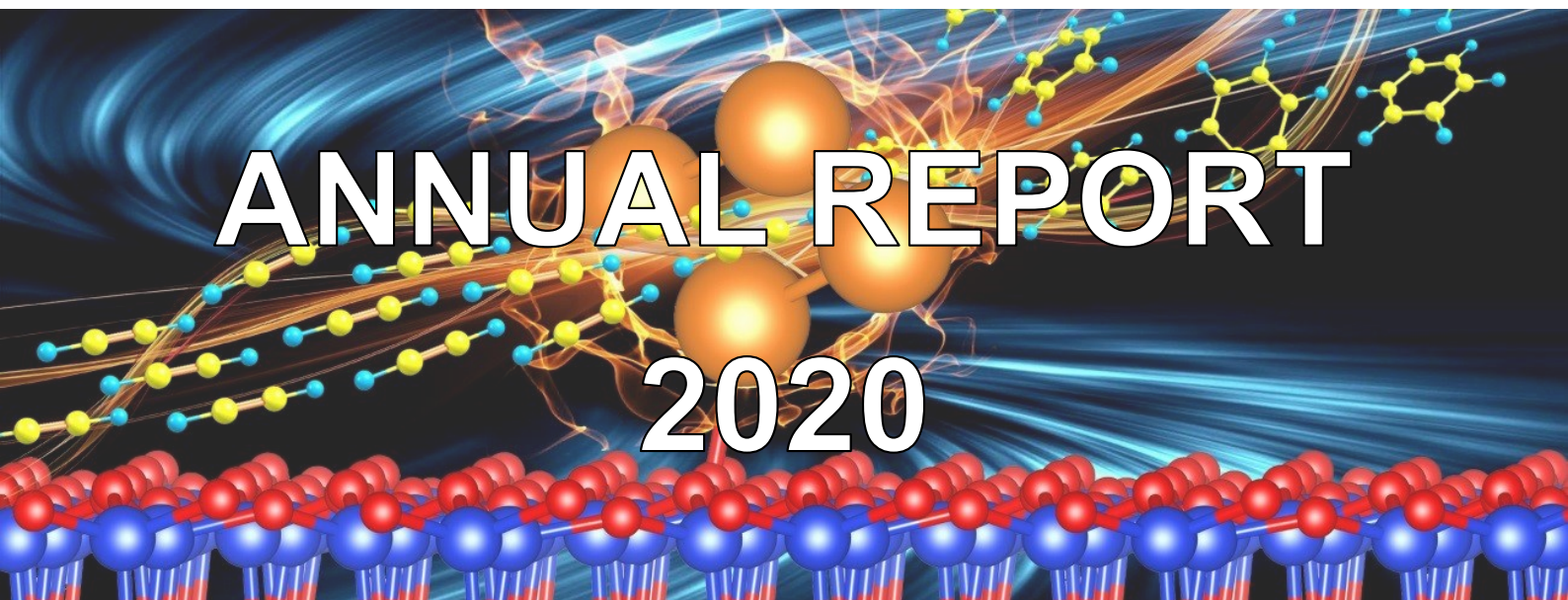


**Dipartimento di Scienza dei Materiali**  
**Department of Materials Science**

*Department of excellence 2018-2022*



**University of Milano - Bicocca**

# **Activity 2019**



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# THE DEPARTMENT OF MATERIALS SCIENCE

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Mail Secretariat: [lucia.rodolfi@unimib.it](mailto:lucia.rodolfi@unimib.it)

Head (Chairman): Prof. Alessandro Abboto

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, 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 optoelectronics, radiation detectors).

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

The 1<sup>st</sup> 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.

# SCIENTIFIC BOARD

## HEAD

Alessandro Abbotto

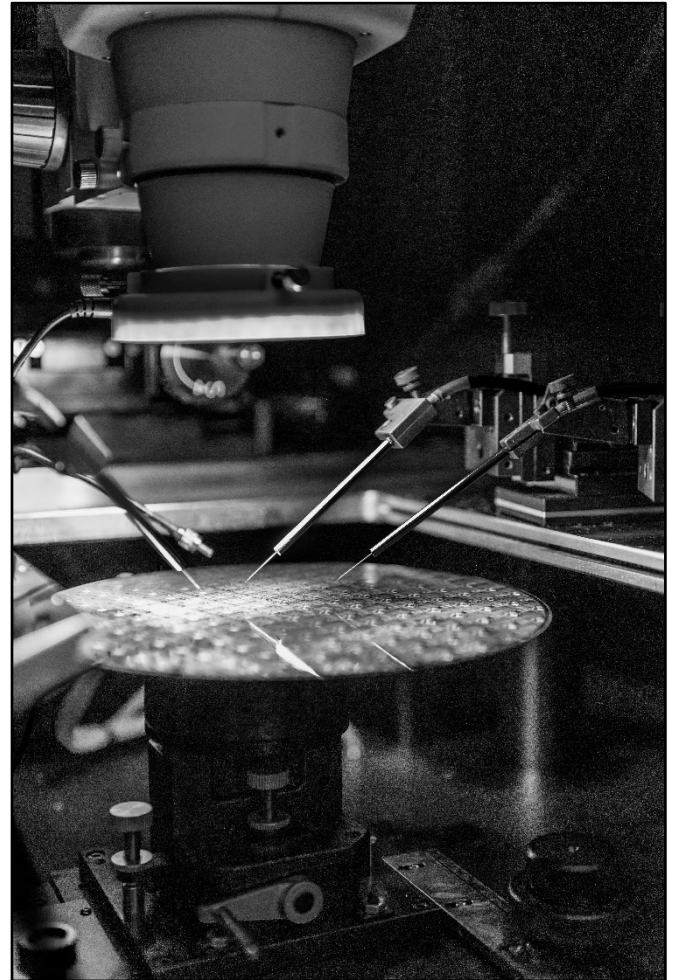
## DEPUTY HEAD

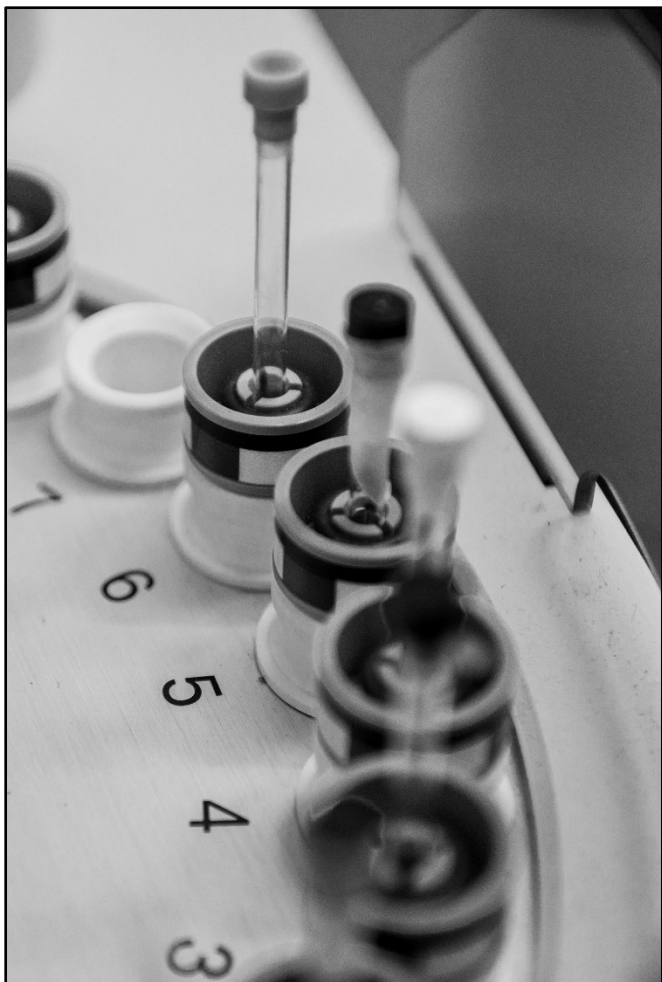
Anna Vedda

## DEPARTMENT BOARD

(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, Alberto Paleari, Adele Sassella, Norberto Manfredi, Antonio Papagni, Roberto Scotti, Giorgio Patriarca





# TEACHING BOARD

## CHEMICAL SCIENCE

Simona Binetti

## MATERIALS SCIENCE

Alberto Paleari

## OPTICS AND OPTOMETRY

Adele Sassella

## DOCTORATE

Marco Bernasconi

Francesco Montalenti (deputy)

# DEPARTMENT OF EXCELLENCE 2018-2022

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<sub>2</sub> 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  $\geq 4$ , 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 ( $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ) 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 ( $>4000 \text{ m}^2/\text{g}$ ) 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

- Richard Noetzel - South China Normal University, Guangzhou (China)
- Markus Niederberger - ETH, Zurich (Switzerland)
- Uve Posset - Fraunhofer Institut für Silikatforschung, Würzburg (Germany)
- Ivan Gordon - IMEC, Leuven (Belgium)
- Neil Mckeown - The University of Edinburgh, Edinburgh (UK)
- Stefano Passerini - Karlsruhe Institute of Technology, Helmholtz Institute Ulm (Germany)

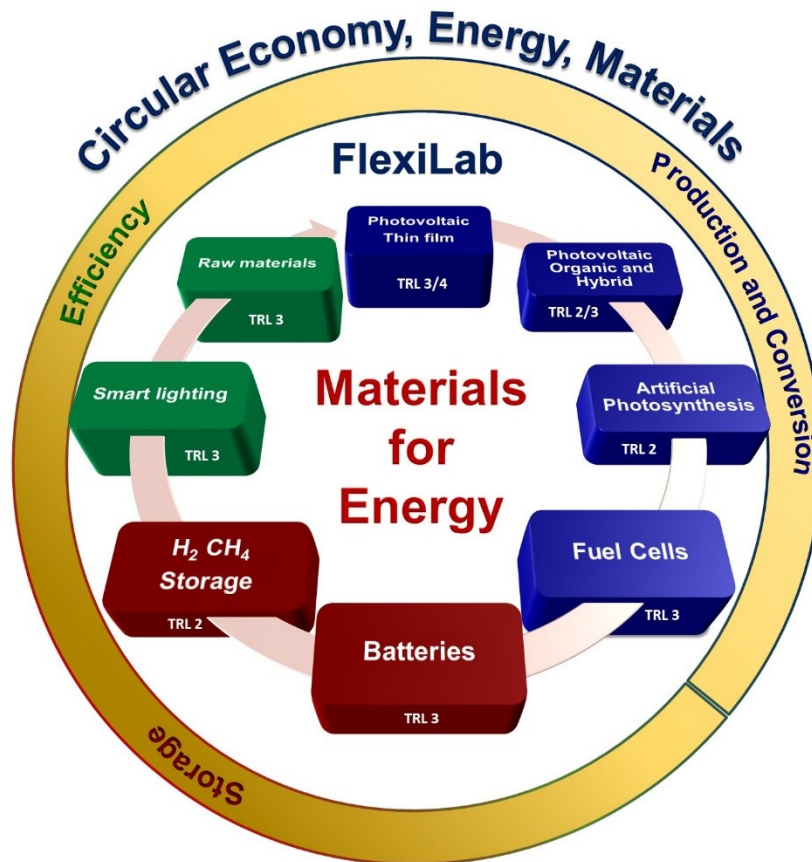
## STEERING COMMITTEE

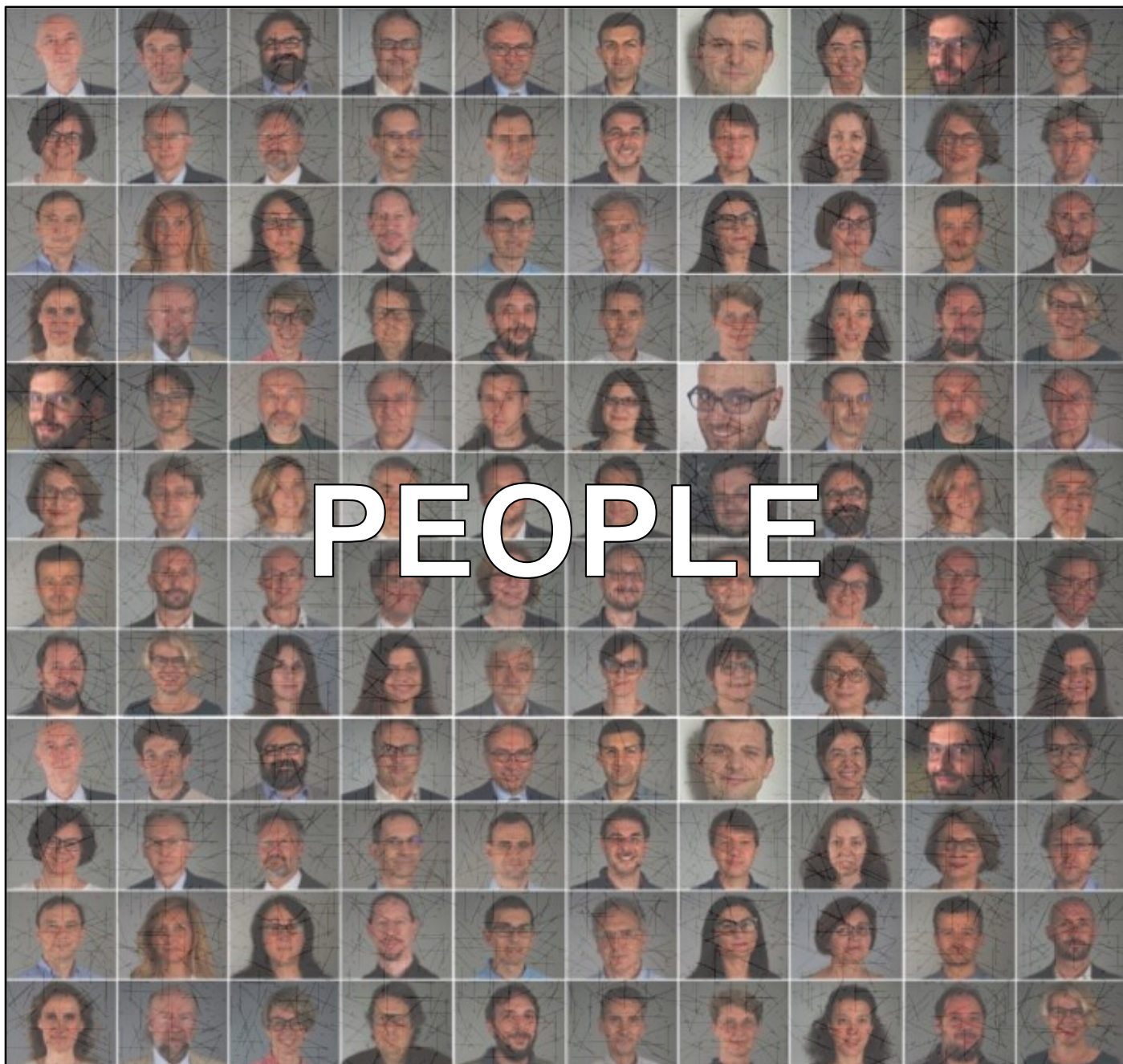
- Prof. Alessandro Abbotto (Principal Investigator)
- Prof. Luca Beverina
- Prof. Simona Binetti
- Prof. Angiolina Comotti
- Prof. Piercarlo Mustarelli
- Prof. Stefano Sanguinetti (Scientific Coordinator)
- Prof. Anna Vedda

## EVENTS

1st Workshop – The FLEXILAB project: 12/12/2019, University of Milano – Bicocca, Milan.







# Professors and researchers

## Professors Emeriti

Giorgio BENEDEK (FIS/03), Alessandro BORGHESI (FIS/01)

## Full Professors

Alessandro ABBOTTO (CHIM/06), Marco BERNASCONI (FIS/03), Luca BEVERINA (CHIM/06), Angiolina COMOTTI (CHIM/04), Cristiana DI VALENTIN (CHIM/03), Marco FANCIULLI (FIS/03), Marco MARTINI (FIS/07), Francesco MEINARDI (FIS/03), Leonida MIGLIO (FIS/03), Piercarlo MUSTARELLI (CHIM/02), Gianfranco PACCHIONI (CHIM/03), Alberto PALEARI (FIS/01), Antonio PAPAGNI (CHIM/06), Stefano SANGUINETTI (FIS/03), Adele SASSELLA (FIS/01), Piero SOZZANI (CHIM/04), Anna VEDDA (FIS/01)

## Associate Professors

Maurizio ACCIARRI (FIS/01), Simona BINETTI (CHIM/02), Emiliano BONERA (FIS/01), Silvia BRACCO (CHIM/04), Sergio BROVELLI (FIS/01), Massimiliano D'ARIENZO (CHIM/03), Mauro FASOLI (FIS/01), Angelo MONGUZZI (FIS/03), Francesco MONTALENTI (FIS/03), Massimo MORET (CHIM/03), Dario NARDUCCI (CHIM/02), Fabio PEZZOLI (FIS/01), Riccardo RUFFO (CHIM/02), Roberto SCOTTI (CHIM/03), Roberto SIMONUTTI (CHIM/04), Silvia TAVAZZI (FIS/01).

## Assistant Professors

Carlo ANTONINI (ING-IND/22), Roberto BERGAMASCHINI (FIS/03), Norberto CHIODINI (CHIM/07), Barbara DI CREDICO (CHIM/03), Chiara FERRARA (CHIM/02), Livia GIORDANO (CHIM/03), Roberto LORENZI (FIS/01), Norberto MANFREDI (CHIM/06), Fabrizio MORO (FIS/01), Mauro SASSI (CHIM/06), Emilio SCALISE (FIS/03), Daniele SELLI (CHIM/03), Emanuela SIBILIA (FIS/07), Sergio TOSONI (CHIM/03), Giovanni Maria VANACORE (FIS/03).

## PhD students

Abhinav ANAND, Luca BARBISAN, Denise BESGHINI, Simone BONIZZONI, Adiel Mauro CALASCIBETTA, Chiara CAPITANI, Francesco CARUSO, Chiara CERIANI, Roberta CORTI, Francesca COVA, Roberta CRAPANZANO, Martina DATTEO, Vito DE BELLIS, Cristina DECAVOLI, Raffaella DI LORENZO, Marianna DITERLIZZI, Gabriele FARAONE, Parisa FATEHBASHARZAD, Carlo Maria GAIFAMI, Antonio GENTILE, Marco Davide GIUSTRA, Antonio GUARDIANI, Atena HOSSEINEHFARAHAN, Iikpoemugh IMIETE ELO, Emanuele Maria LONGO, Stefano MAGAGNA, Paola MILANA, Andrea Maurizio MONTI, Mauro MONTI, Mattia NEGRONI, Jacopo PEREGO, Daniele PERILLI, Nicolò Pianta, Jacopo REMONDINA, Costanza RONCHI, Alessandra RONCHI, Simone ROSSI, Fabrizio

ROVARIS, Selena SILVANO, Dimosthenis TOLIOPOULOS, Laura TRIPALDI, Artur TUKTAMYSHEV, Chiara TULLIO, Aldo UGOLOTTI, Stefano VICHI, Matteo Luca ZAFFALON

## **Post-Docs and other Research Fellows**

Raziyeh AKBARI, Marco Giocondo ALBANI, Anu BABY, Charl Xavier BEZUIDENHOUT, Chiara Liliana BOLDRINI, Michele CACCIA, Valentina CANTATORE, Francesco CARULLI, Elkid COBANI, Francesca COVA, Tilak DAS, Giovanni DI LIBERTO, Daniele DRAGONI, Moloud KAVIANI, Hongsheng LIU, Bruno LORENZI, Sara MATTIELLO, Anna MARZEGALLI, Silvia MOSTONI, Mangelis PANAGIOTIS, Jacopo PARRAVICINI, Alessandro PEDRINI, Jacopo PEDRINI, Jacopo PEREGO, Valerio PINCHETTI, Francesca Rita POMILLA, Erika PONZINI, Fabrizio ROVARIS, Andrey SARIKOV, Valeria SECCHI, Paulo SIANI, Federico Ariel SORIA, Irene TAGLIARO, Dimosthenis TOLIOPOULOS, Giorgio TSEBERLIDIS, Shiro TSUKAMOTO, Luca VAGHI, Stefano VICHI, Irene VILLA, Elisa VITIELLO, Fabrizio ZERI.

## **Spinoffs**

Alberto BIANCHI (Graftonica), Francesco BRUNI (G2P), Chiara CAPITANI (G2P), Silvia FERRARIO (Graftonica), Marina GANDINI (G2P), Graziella GARIANO (G2P).

# **Administrative and technical staff**

## **Administrative staff**

Paola IANNACCONE, Lucia RODOLFI, Cristina VALENTINO, Stefano ZANINI.

## **Technical staff**

Sergio BIETTI, Enea BORIA, Carmen CANEVALI, Lorenzo FERRARO, Claudio LAGRASTA, Alessia LE DONNE, Francesco MASPERO, Laura PANZERI, Giorgio PATRIARCA, Luisa RAIMONDO, Silvia TRABATTONI, Bruno VODOPIVEC.

# 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 (MIB-SOLAR)**

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, Daniele Selli. **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**

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

Riccardo Ruffo. **Electrochemical activities**



# Materials for microelectronics and photonics

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

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

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

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

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

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

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

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, Emanuela Sibilio. **Dating and characterization of ancient materials. Materials science and cultural heritage**



## Mathematics

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



## Optics and optometry

Silvia Tavazzi. **Optics and optometry**



## Organic and polymeric materials

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

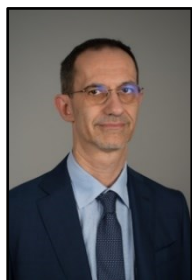
Silvia Bracco, Piero Sozzani. **Generation of nanospaces for polymerization and gas capture**

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

Roberto Simonutti. **Synthesis and characterization of novel polymeric nanostructure**

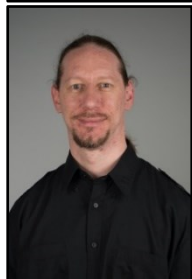


# Organic and hybrid materials and devices for solar fuels and artificial photosynthesis (MIB-SOLAR)



**Alessandro Abboto, Norberto Manfredi**

Present energy needs are classified into two main sectors: a) production of electricity; b) production of reactant and fuels for chemical industry and transportation. We focus our interest on the use of clean, no cost and abundant sources like sunlight, water, and carbon dioxide 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 and reduction of carbon dioxide. Water splitting is able to produce hydrogen, which can be used as a fuel or reactant in chemical industry. The reduction of CO<sub>2</sub> affords a number of 1C strategic chemicals and fuels, such as HCOOH, CO, CH<sub>3</sub>OH and CH<sub>4</sub>.

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 such as TiO<sub>2</sub> or NiO.

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.

## 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.



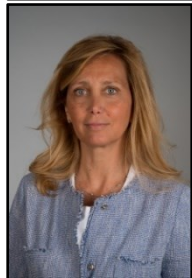




# Photovoltaics and Thermoelectrics (MIB-SOLAR)



**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<sub>2</sub> (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<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) and Cu<sub>2</sub>ZnSnSe<sub>4</sub> (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<sub>2</sub>MnSnS<sub>4</sub> (CMTS) and Cu<sub>2</sub>FeSnS<sub>4</sub> (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<sub>2</sub> (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) brings about research and innovation for the development of new technologies towards clean water and energy-efficient processes, two corner stones for sustainable development.

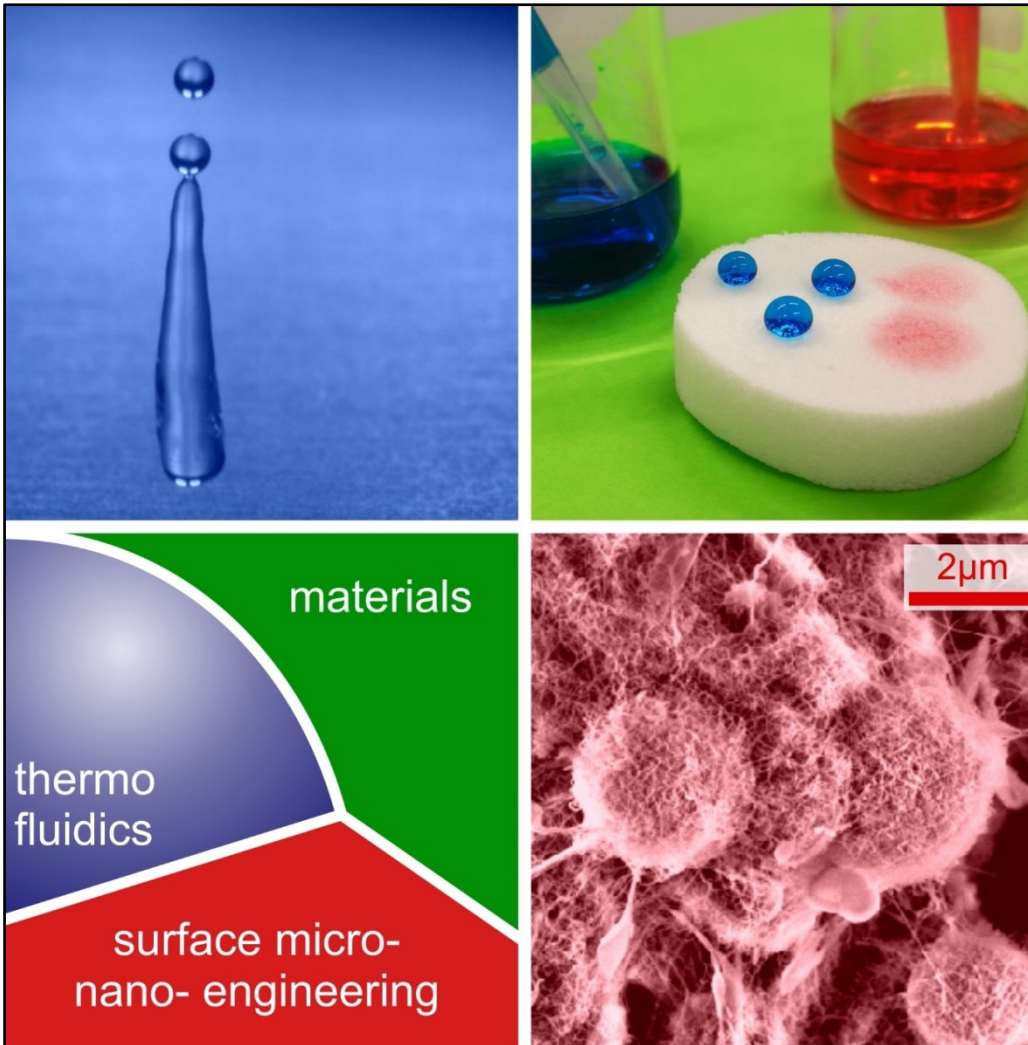
Research activities focus on understanding interfacial transport phenomena, for the design of innovative smart interfaces. SEFI Lab is characterized by an interdisciplinary approach, at the interface between thermofluidics, material science and surface micro- and nano-engineering.

## **SMART INTERFACES FOR ENERGY APPLICATIONS**

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

## **SMART INTERFACES FOR WATER**

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





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

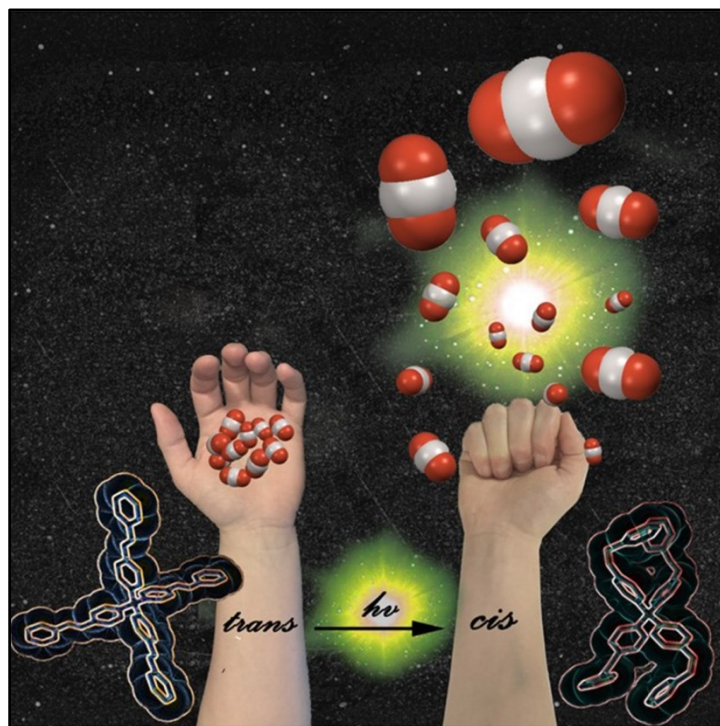


**Angiolina Comotti**

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  $\text{CO}_2$  from the gas phase.





# 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.  $\text{TiO}_2$ ,  $\text{ZnO}$ ,  $\text{MoO}_3$ ) and tuneable porous systems (macro/mesoporous silica or Metal Organic Frameworks, MOF), and at the study of their (photo)catalytic mechanism (formation and interfacial reactivity of paramagnetic defects) by spectroscopic and spectromagnetic techniques. In particular, the possibility of tailoring size, anisotropy and surface functionalities of these systems by employing catalysts (acid or bases), soft templates (e.g. amphiphilic surfactants), capping molecules or particular solvents, has been exploited for the modulation of the inorganic-organic interfaces. This play a crucial role in determining their properties and implementation for the development of advanced hybrid materials commonly utilized for water/air depollution,  $\text{CO}_2$  photoconversion in renewable fuels and Na-ion batteries.

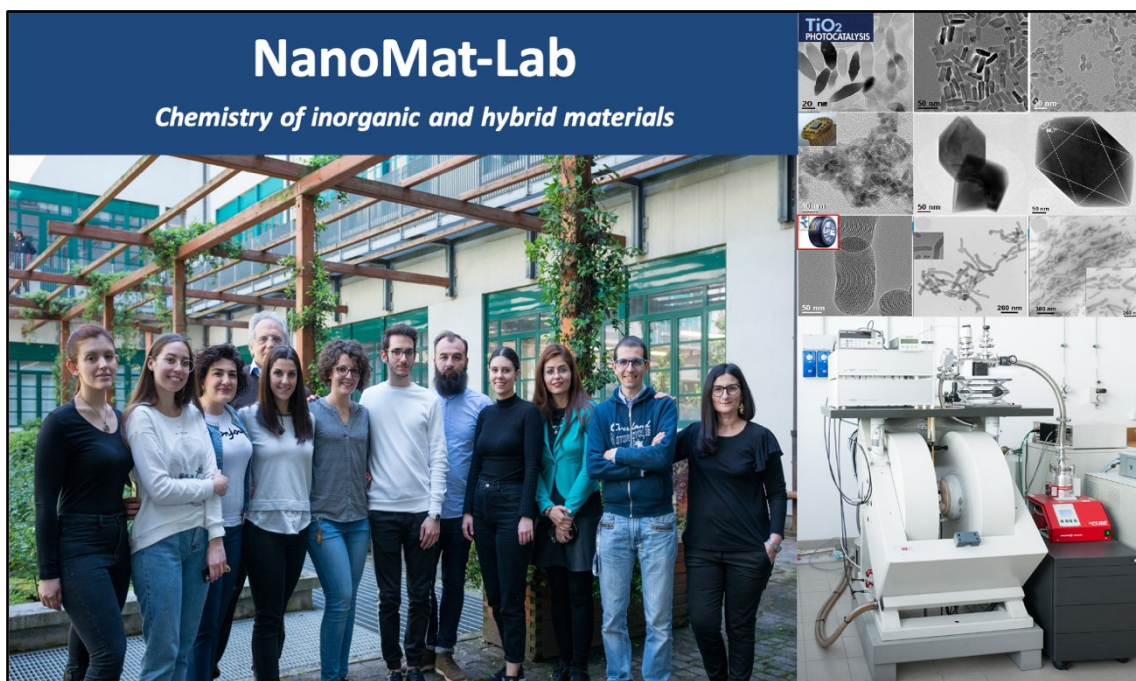
## **INORGANIC NANOFILLERS FOR MULTIFUNCTIONAL POLYMER NANOCOMPOSITES**

The research focus on the preparation by bottom-up approaches of oxides (mainly  $\text{ZnO}$  and  $\text{SiO}_2$ ) 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,  $\text{O}_2$  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  $1600^\circ\text{C}$ , 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  $1400^\circ\text{C}$  connected with MS station;
- Bruker ESR spectrometer equipped with liquid  $\text{N}_2/\text{He}$  Cryostat.









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



**Cristiana Di Valentin, Daniele Selli**

## COMPUTATIONAL NANOMEDICINE

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



## COMPUTATIONAL ELECTROCHEMISTRY AND FUEL CELLS

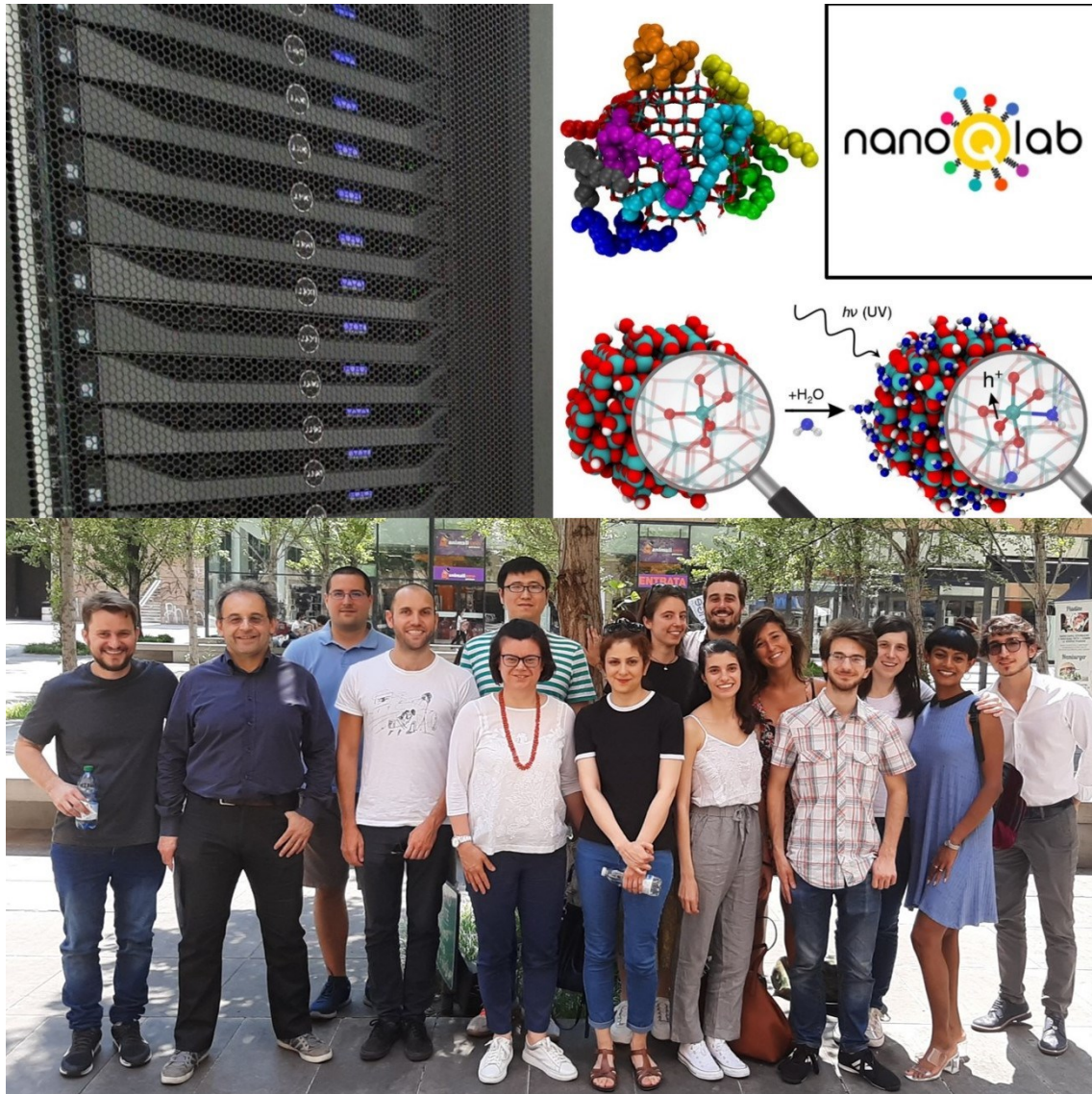
We use electronic structure calculations to design novel electrode materials for electrochemical devices and fuel cells, which are as efficient as or even more capable than precious and environmental unfriendly metal electrodes. Gibbs free energies of reaction in an aqueous environment for the all the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

## CATALYSIS UNDER COVER (2D LAYERS)

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

## GRAPHENIC NANOSTRUCTURES FROM MOLECULAR 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.





# 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

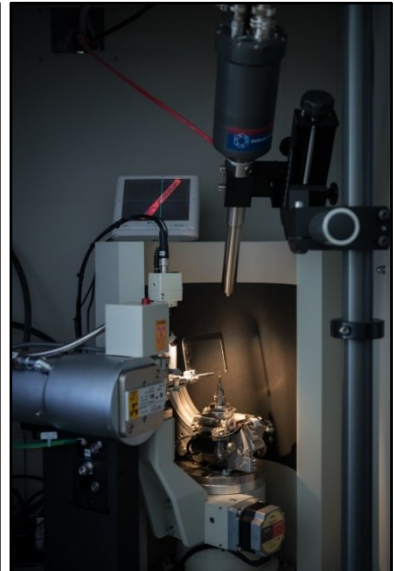
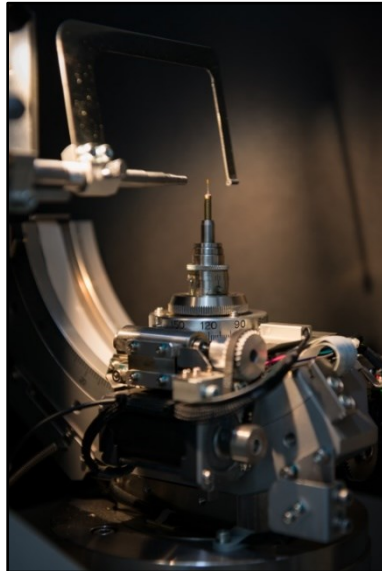
Growth of crystals with solution methods under ambient or solvothermal conditions (e.g. microporous coordination polymers exhibiting zeolite-like behavior or catalytic properties, aminoacids) allows preparation of crystals with size from centimeter to nanometer scale with control of morphology. Crystal 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 manufacturing plants (e.g. setting of cements/plasters in the presence of chemical additives) is directed toward acquisition 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
- Thermostatted crystallizers for crystal growth from solution, sublimation, vapor deposition
- Metallographic and stereoscopic microscopes equipped with analyzer/polarizer, DIC Nomarski prism, frame grabber for time lapse imaging, heating/freezing stage from 90 to 870 K.







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



**Chiara Ferrara, Piercarlo Mustarelli**



## **MEMBRANES AND MEMBRANE-TO-ELECTRODE ASSEMBLIES (MEAS) FOR POLYMER FUEL CELLS**

Polymer fuel cells operating at low temperature ( $< 100^{\circ}\text{C}$ ) 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<sup>TM</sup> 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  $100\text{--}200^{\circ}\text{C}$ , 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).





# Theory of oxide surfaces, interfaces, supported clusters



**Gianfranco Pacchioni, Sergio Tosoni**

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



## **OXIDE SURFACE AND THIN OXIDE FILMS**

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

## **SUPPORTED CLUSTERS**

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

## **DEFECTS AND DOPANTS IN OXIDES**

Nature of point defects in oxide materials for photocatalysis, photoelectrochemistry, microelectronics, fiber optics etc., in particular amorphous and crystalline  $\text{TiO}_2$ ,  $\text{ZnO}$ ,  $\text{WO}_3$ ,  $\text{SiO}_2$ , alkaline earth oxides. The activity is directed toward the determination of stability, structure, and spectral properties of intrinsic and extrinsic point defects (vacancies, metal and non-metal dopants, codopants, hydroxyl groups, trapped electrons, etc.) and their interplay through charge transfer processes. Particular attention is devoted to the study of optical absorption for activation in the visible region and of electron spin resonance spectra for identification of paramagnetic centres.

## **OXIDE SEMICONDUCTORS AND HETEROJUNCTIONS**

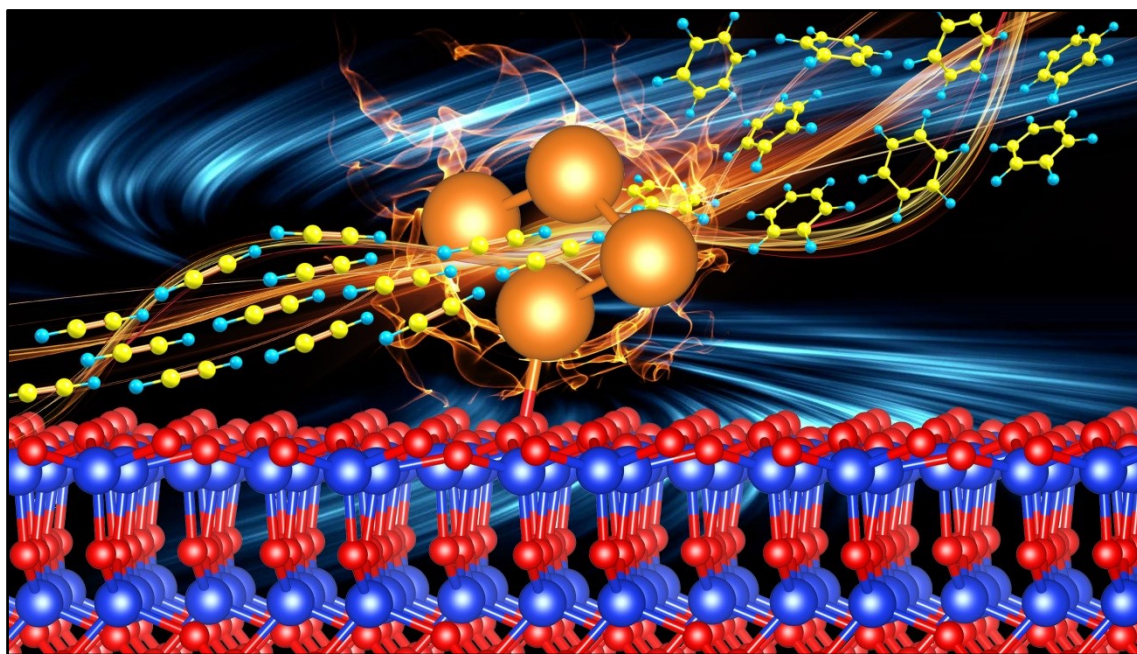
Heterojunctions between semiconductors (notably oxides) are a class of materials attracting growing attention in the field of photocatalysis. This research line aims at the accurate description of the band alignment, charge transfer phenomena, and charge carrier separation at the junction by means of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

## **MAIN FACILITIES**

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









# Electrochemical activities



**Riccardo Ruffo**

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

## **MATERIALS FOR ENERGY STORAGE AND PRODUCTION**

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

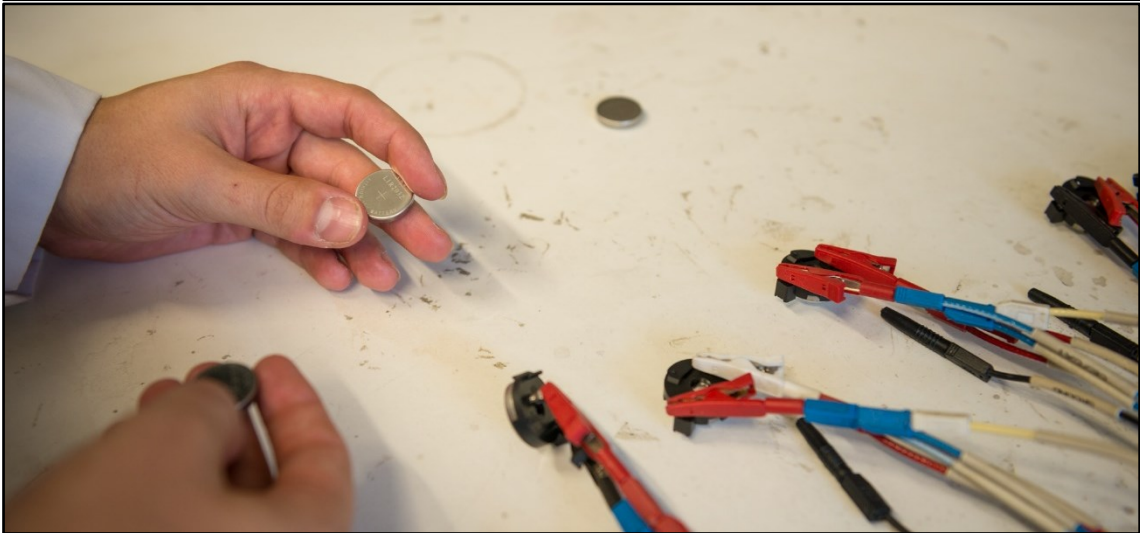
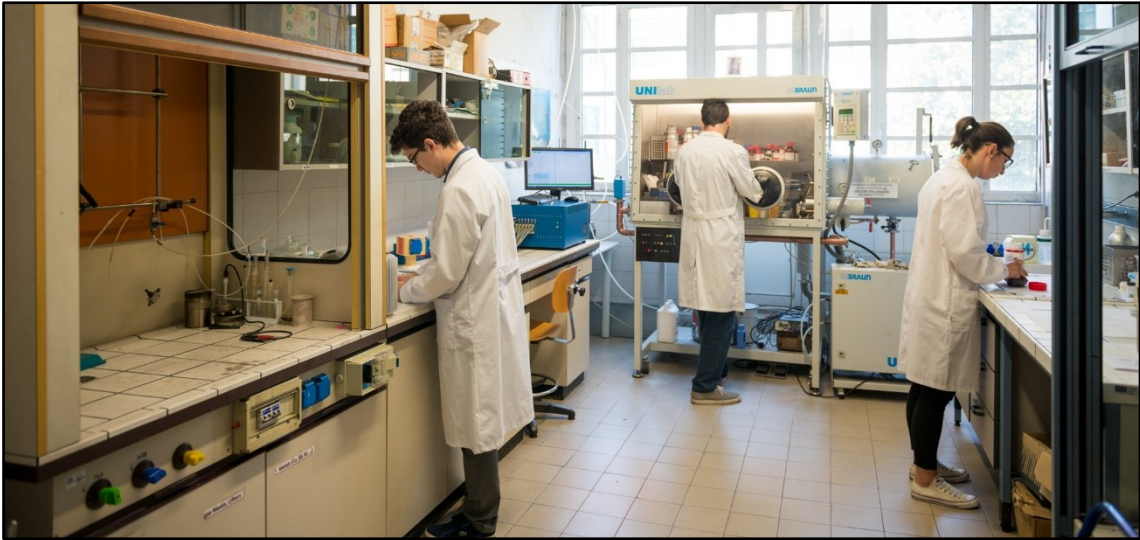
For all these PV absorbers, a comprehensive structural and spectroscopic characterization (including scanning electron microscopy, Raman spectroscopy, X-ray diffraction and photoluminescence) is performed. All the new absorber layers are tested in prototype solar devices.

## **MATERIAL FOR GAS SENSORS**

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

## **MATERIAL FOR ORGANIC OPTOELECTRONICS**

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





# First principles simulations of materials for microelectronics



**Marco Bernasconi**

## **PHASE CHANGE MATERIALS FOR DATA STORAGE**

Phase change materials ( $\text{Ge}_2\text{Sb}_2\text{Te}_5$  and related telluride alloys) are attracting an increasing interest worldwide for applications in optical disks (DVDs) and in a novel non volatile electronic memory, the phase change memory cell. Both applications rely on a fast (10-100 ns) and reversible transformation between the crystalline and amorphous phases induced by heating. The two states of the memory can be discriminated thanks to the large contrast in electronic conductivity and optical reflectivity between the two phases.

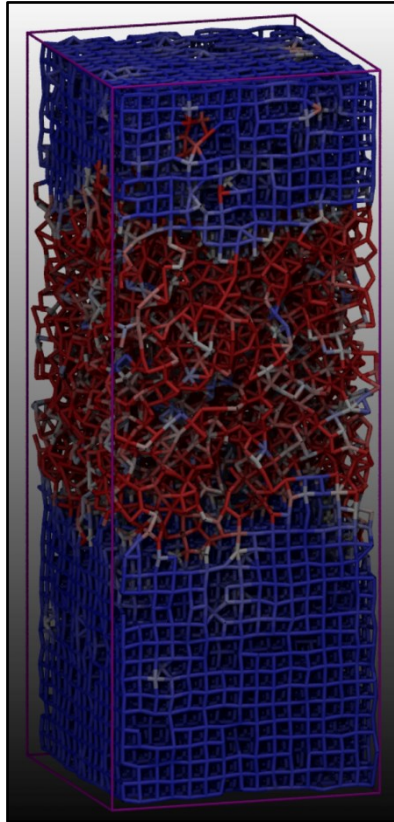
On the basis of density functional molecular dynamics simulations, we investigate the structural, dynamical and electronic properties of the amorphous and crystalline phases of materials in this class aiming at establishing correlations between the composition of the alloy and the electronic and optical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

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

## **SURFACE PHONONS AND TOPOLOGICAL INSULATORS**

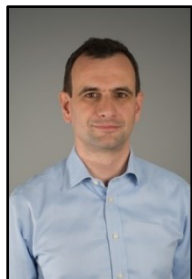
Some chalcogenide compounds of interest for phase change applications belong to the class of topological insulators, i.e. they are bulk insulators with a non trivial topology of the electronic bands which induces the formation of topologically protected metallic electronic bands at the surface. On the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







# Optical spectroscopy 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 in within the L-NESS interuniversity Centre.

## SIGE HETEROSTRUCTURES

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

- 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.



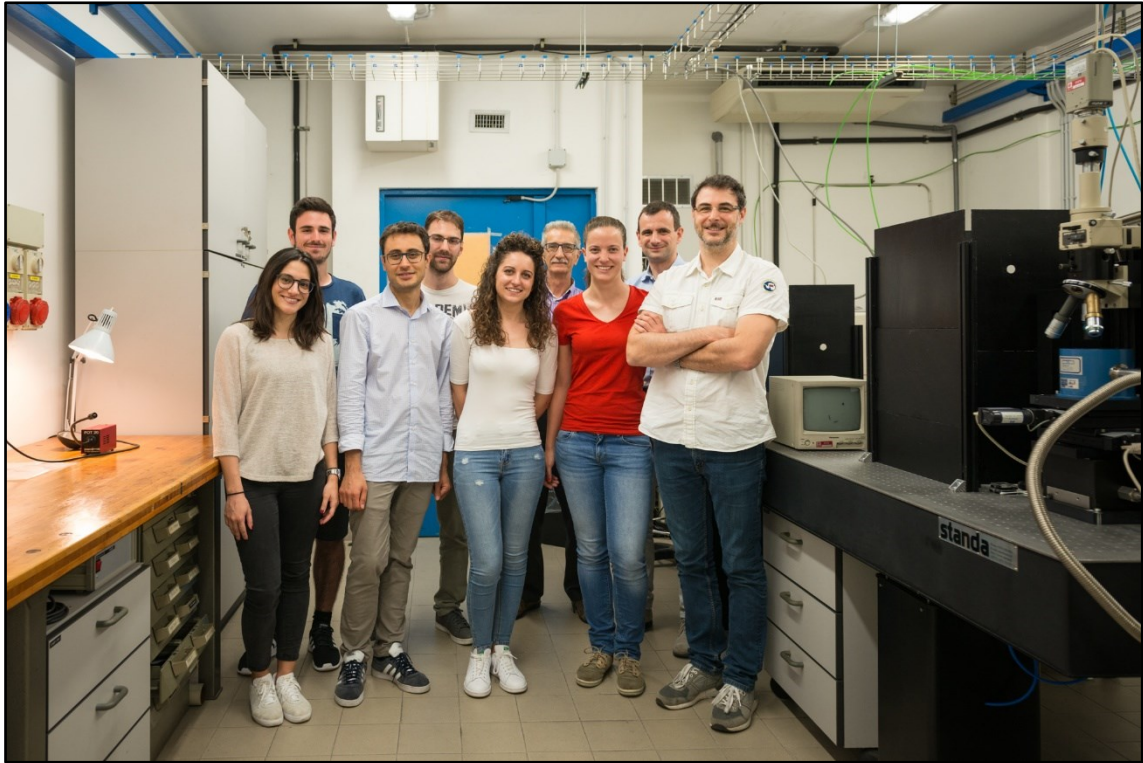
## QUANTUM STRUCTURES BASED ON III-V SEMICONDUCTORS

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<sup>-1</sup>. 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<sup>-8</sup> s can be measured with DPSS-QS lasers.







# 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.

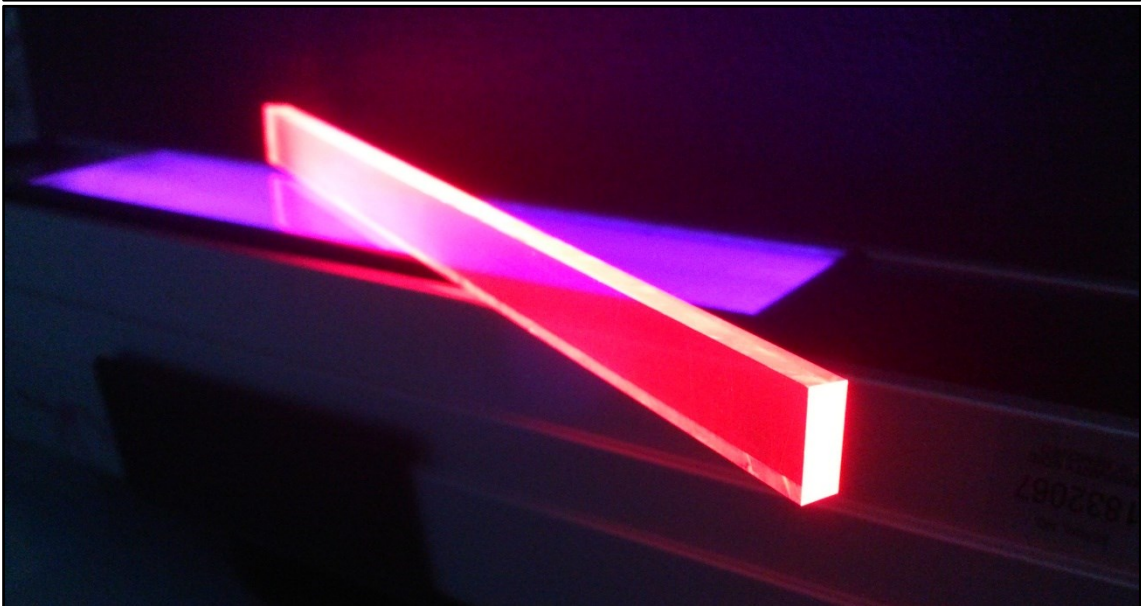
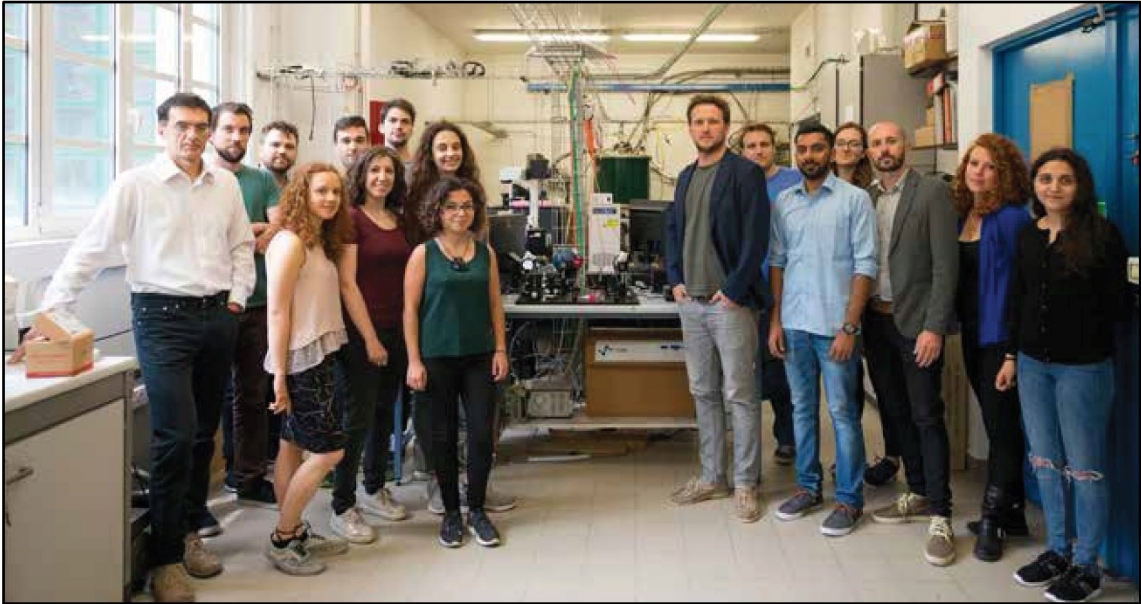


## **NON-COHERENT PHOTONS UP-CONVERSION**

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  $\mu\text{W}/\text{cm}^2$ . 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 heterostructures 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<sub>2</sub> growth, 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 and leading 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.

## **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<sub>2</sub>, WS<sub>2</sub>) 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 NEUROELECTRONICS**

Within the Neureka EU project ([www.neureka.gr](http://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.







# Oxide nanostructures and glass-based materials for optical technology



**Mauro Fasoli, Roberto Lorenzi, Alberto Paleari, Anna Vedda**

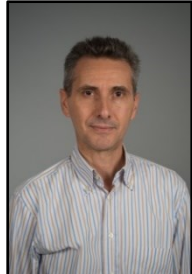
Our research is focused on the physical properties of silica-based glass and glass-ceramics for applications in photonics and optoelectronics. Bulk and film materials are synthesized and investigated looking at the particular optical properties one can obtain and control by doping with active ions and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



## RESEARCH LINES

Optical properties of rare earth ions such as Ce, Gd, Tb, Eu in bulk silica and in Hf-based oxide nanoparticles, studying the interaction with the host matrix, to obtain materials suitable to be used as scintillators in the detection of low-energy ionizing radiations for industrial and medical applications. The role of point defects in crystalline scintillators is also investigated.

Light-emission and non-linear optical properties of wide-band-gap oxide nanostructures in glasses, such as  $\text{Ga}_2\text{O}_3$  and  $\text{SnO}_2$  nanocrystals in silicates, analyzing the applicability as light-emitting systems, photo-sensitive optical materials, cubic non-linear components, and transparent conductors.



## FACILITIES

**SPECTROSCOPY LABORATORY:** optical absorption, photo- thermo- and radio-luminescence spectroscopy, micro-Raman scattering, refractive index and film thickness measurements, thermostimulated currents and complex impedance spectroscopy. Micro-ATR-FTIR analysis, micro-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;  $\mu$ -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).





# Fabrication and study of semiconductor quantum nanostructures (EpiLab)



**Stefano Sanguinetti**

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

## **QUANTUM DOT EMITTERS FOR QUANTUM PHOTONICS APPLICATIONS**

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

## **NANOSTRUCTURED SEMICONDUCTORS FOR OPTOELECTRONICS**

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**

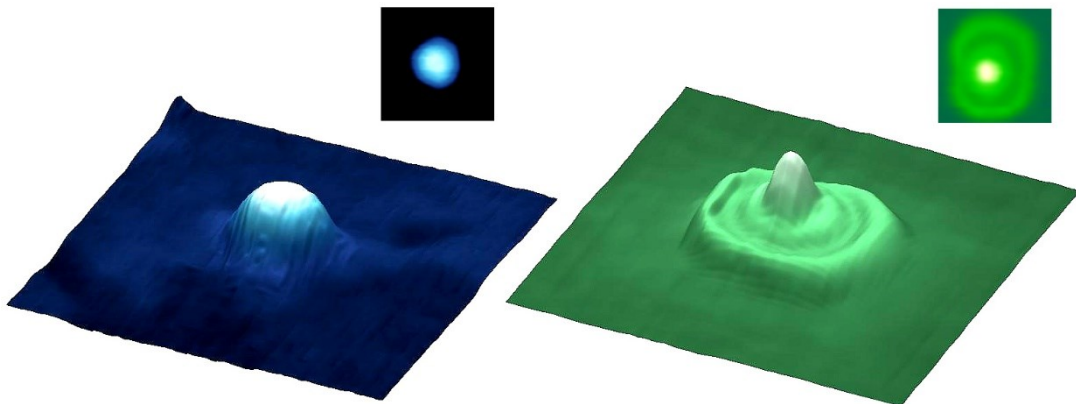
Growth and characterization of nanostructured InN/InGaN materials for photocatalytic electrodes for applications in biochemical sensors and hydrogen solar generation.

## **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



**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.

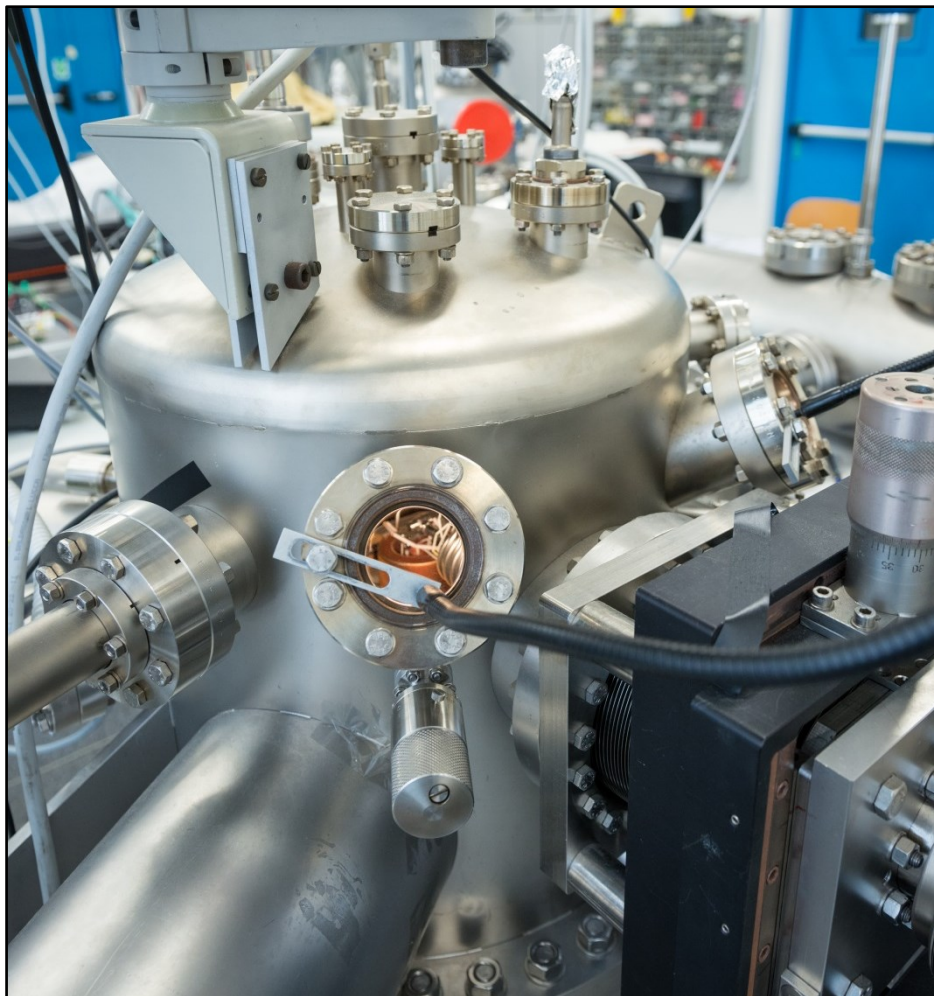
## HETEROSTRUCTURES

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 several  $\mu\text{m}^2$  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**

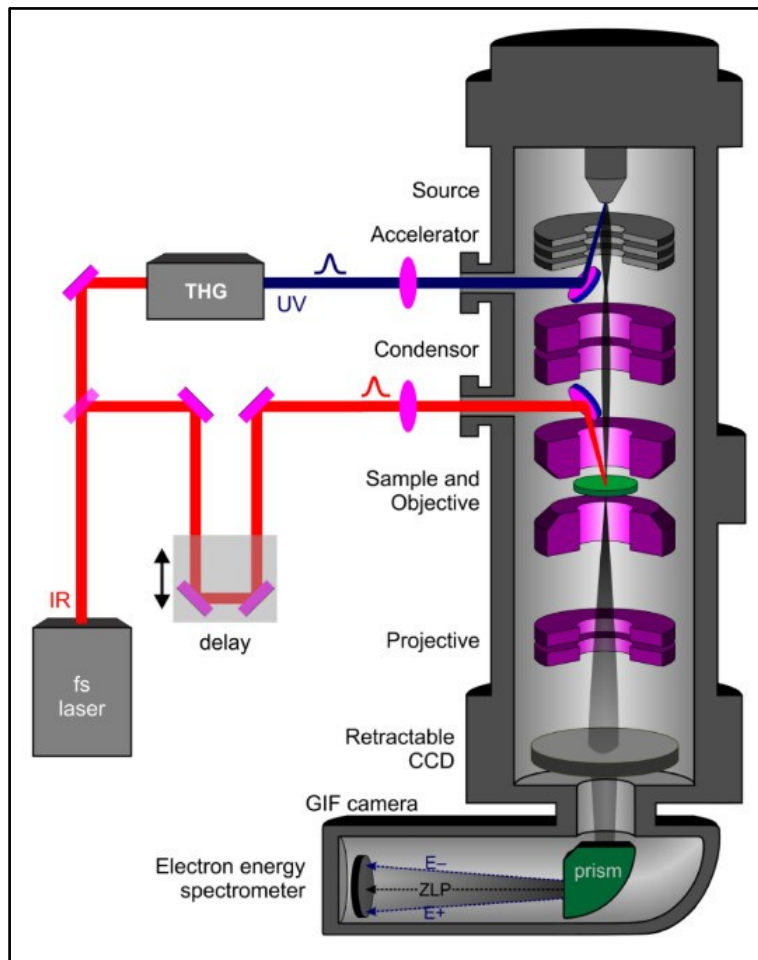
Our research activity is dedicated to the investigation of ultrafast phenomena in nanoscale low-dimensional materials. In particular, we focus on semiconductor quantum dots, nanowires, graphene and 2D van-der-Waals solids, nano-plasmonic structures, energy-related materials, topological insulators and 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 Laureate 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.





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



**Anna Galli, Marco Martini, Emanuela Sibilia**



## 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  $^{14}\text{C}$  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





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



**Veronica Felli**

The following problems are investigated:

## **SPECTRAL STABILITY FOR SINGULARLY PERTURBED PROBLEMS**

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

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

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

## **ASYMPTOTIC BEHAVIOR AND UNIQUE CONTINUATION PROPERTIES FOR ELLIPTIC EQUATIONS**

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



SHARP ESTIMATES FOR AHARONOV-BOHM VARYING POLE
15

$$(u + \psi_j) e^{\frac{i}{2}(\gamma_j - \gamma_j^0)} e^{\frac{i}{2}\gamma_j^0}$$

$$\int_{\Gamma} |u|^2 + \int_{\Gamma} \frac{\partial \psi_j}{\partial \nu} u$$

$$K = \{ \text{ack } g(\alpha) - \gamma^0(\alpha) - 2\psi_j \}$$

$$2 \int_{\Gamma} \nabla u \nabla \psi_j = - \int_{\Gamma} \frac{\partial u}{\partial \nu} \psi_j \quad \forall \psi_j \in K_0$$

$$\Delta u \leq 0 \quad \Gamma = \Gamma^+ \cup \Gamma^-$$

$$\gamma^0(u, \gamma) + \gamma^0(u, \gamma) = - \langle \gamma_j, u \rangle$$

$$\frac{\partial(u + \psi_j)}{\partial \nu} = \frac{\partial(u + \psi_j)}{\partial \nu} \quad \gamma_j \in \Gamma^+$$

$$-\int_{\Gamma} \frac{\partial \psi_j}{\partial \nu} \phi = \int_{\Gamma} \frac{\partial u}{\partial \nu} \phi$$

lemma nodele

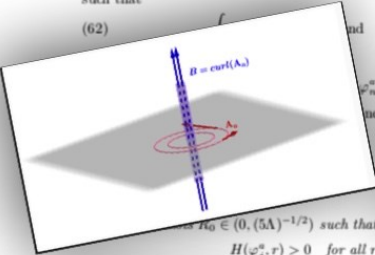
$$u \in K_0 \Rightarrow \int_{\Gamma} |\nabla u|^2 = - \int_{\Gamma} \frac{\partial \psi_j}{\partial \nu} u$$

$$\Rightarrow J(u) = \int_{\Gamma} |\nabla u|^2 - 2 \int_{\Gamma} |\nabla u|^2 = - \int_{\Gamma} |\nabla u|^2$$

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

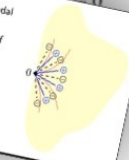
such that

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



$\lambda_V - \lambda_V^0 > 0$  if  $a$  is tangent to a nodal line of  $\varphi_V$  in  $\partial$ .

$\lambda_V - \lambda_V^0 < 0$  if  $a$  lies in the middle of the tangents to two nodal lines of  $\varphi_V$  in  $\partial$  (or in the middle between a tangent and the boundary).



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

$$H(\varphi_j^a, R_0) \geq C_0 \quad \text{for all } a \text{ with } |a| < \alpha_0 \text{ and } 1 \leq j \leq n_0.$$

and assume that, for all  $n$  sufficiently large, there exists  $r_n$  such that  $H(\varphi_{j_n}^{a_n}, r_n) = 0$ , i.e.  $\int_{D_{r_n}} |\nabla \varphi_{j_n}^{a_n}|^2 dx = 0$ . From the unique continuation principle (see [12 Corollary 1.4]) we conclude that  $\varphi_{j_n}^{a_n} \equiv 0$  in  $\Omega$ , a contradiction.

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



# Optics and Optometry



**Silvia Tavazzi**

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

- 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**

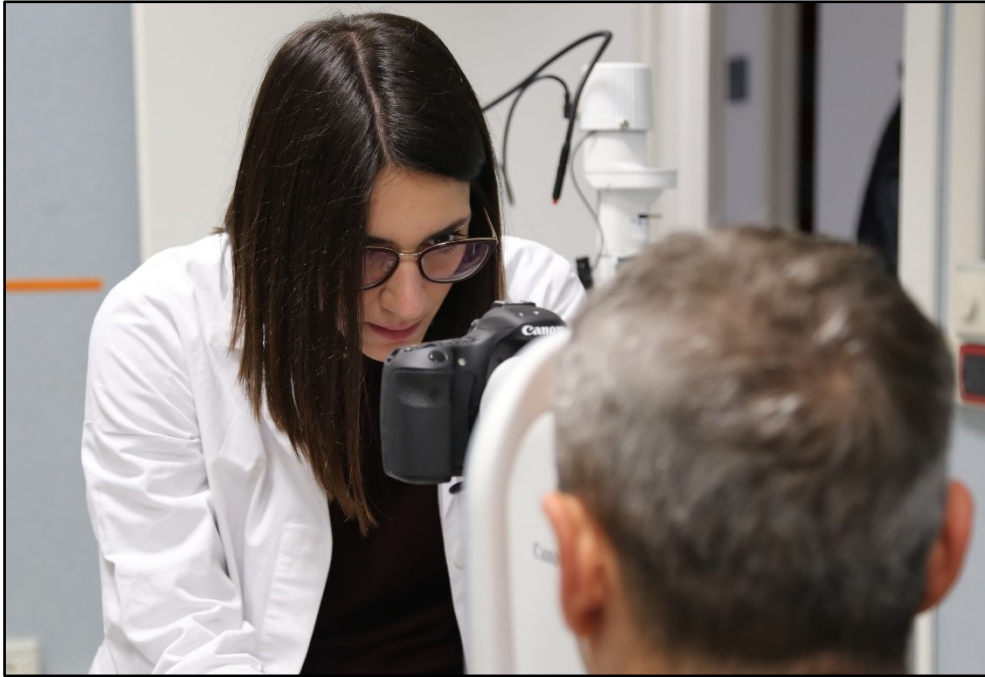
Recent studies were focused on the properties of materials for soft contact lenses in terms of microscopic structure and uptake/release of hyaluronan, lactoferrin, and drugs. Different materials were investigated. The uptake was studied in terms of loading capability, penetration depth in the lens, release 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-mydratic retinal camera with fundus autofluorescence, non-contact tonometer/pachymeter, corneal topographer, ocular aberrometer, keratometers, ophthalmoscopes, retinoscopes, etc.





# 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 mutated 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.

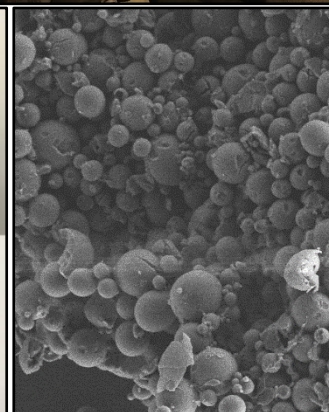
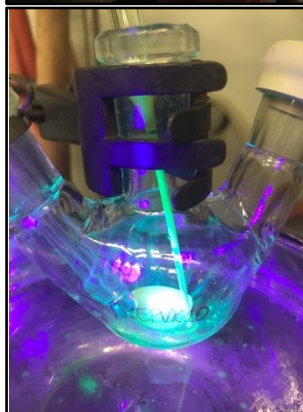
We routinely collaborate with large companies as well as PMI on both printed optoelectronics and formulation chemistry.

## DEVICES DEVELOPED ON COLLABORATION WITH COMPANIES AND RESEARCH INSTITUTIONS

OLEDs, OFETs, EGOFTs, 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).







# 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<sup>2</sup>/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 (<sup>129</sup>Xe, CO<sub>2</sub>, CH<sub>4</sub> and H<sub>2</sub>).

## 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<sup>-9</sup> torr) pump and equipment for hyperpolarized Xenon spectroscopy (laser-excited NMR). Gas-Vapor Adsorption Analyzers, Differential Scanning Calorimetry, Gel Permeation Chromatography, Dynamic Mechanical Analyzer.





# 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.

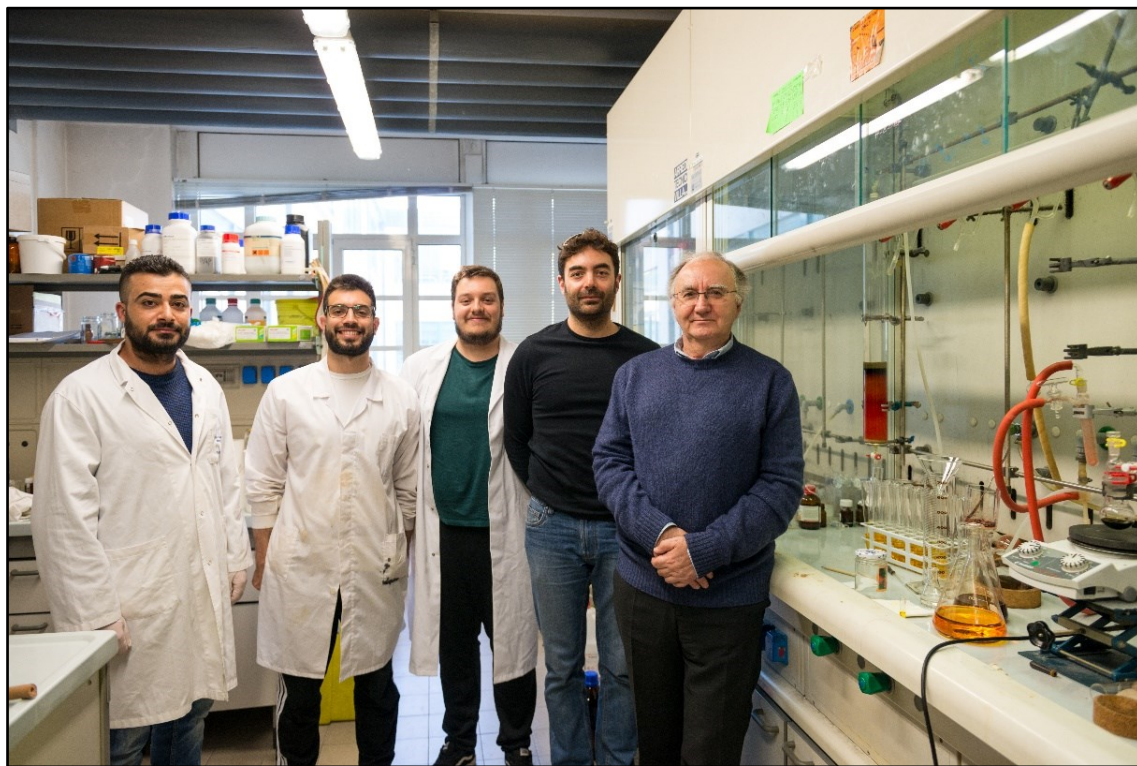
## ORGANIC SEMICONDUCTORS

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 systems able to produce, thermally and photochemically, highly reactive species (carbenes and nitrilimines). These species are involved in cross-linking processes of protein-base biomolecules or polymeric materials.







# Synthesis and characterization of novel polymeric nanostructures



**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 vesicles, 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**

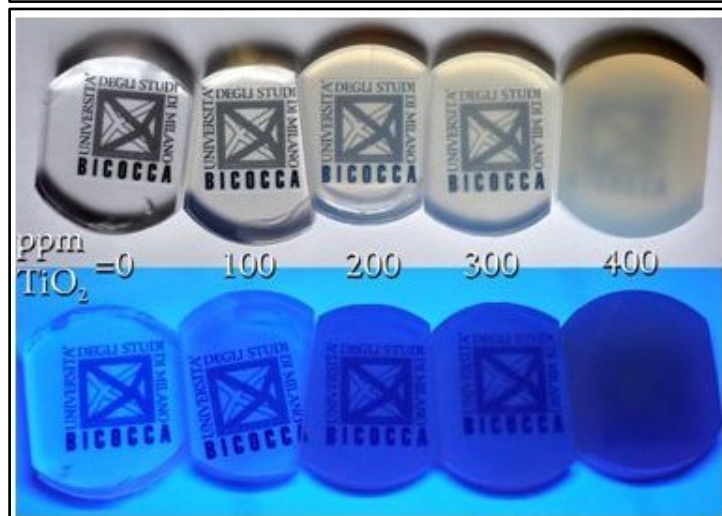
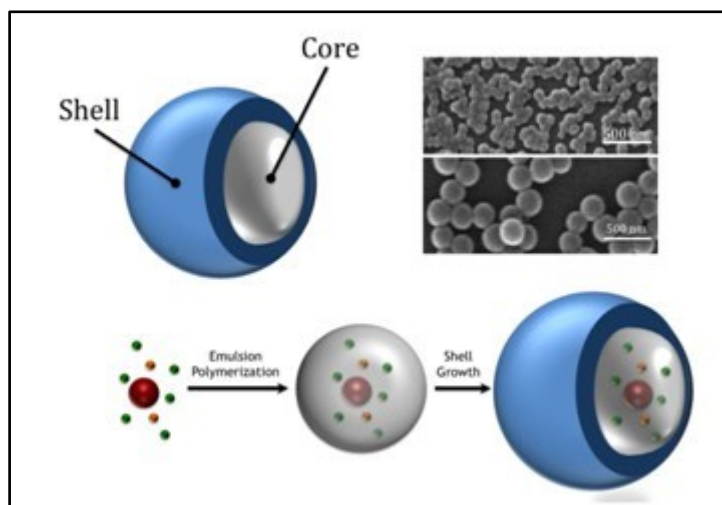
The mixing of polymers and inorganic nanoparticles, like oxides, semiconductors (usually defined as quantum dots) or noble metals, is opening pathways for engineering flexible composites that exhibit advantageous electrical, optical, or mechanical properties. In particular, the nanocomposite optical 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.





# 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
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
Caratterizzazione e la relativa analisi di celle solari ad alta efficienza tramite misure di risposta spettrale	RSE	S. Binetti
PLS - PN - SCIENZA DEI MATERIALI	MIUR	S. Binetti
Caratterizzazione e la relativa analisi di celle solari ad alta efficienza tramite misure di risposta spettrale	CESI	S. Binetti
KiC - RAISE - Raw Material Students Internship	EU	S. Binetti
KiC- Raw Materials @schools 3.0	EU	S. Binetti
Realizzazione di preforme e caratterizzazione di fibre scintillanti da impiegare come elementi di sensori di radiazione ionizzante	Prysmian	N. Chiodini
Nanoporous materials with tailored structure for high performance methane storage and purification	MIUR	A. Comotti
Biomethane low impact production and carbon dioxide bio-capture for circular economy BALANCE	FONDAZIONE CARIPLO	A. Comotti
KiC- LIGHTBODY- Infrastructure and expertise network for Lightweight mobility : body and chassis	EIT RAW MATERIALS GMBH	A. Comotti

<b>Project/Research Contract Title</b>	<b>Funded by</b>	<b>Principal Investigator</b>
<b>Meccanismi di attivazione della CO<sub>2</sub> per la progettazione di nuovi materiali per l'efficienza dell'energia e delle risorse</b>	MIUR	A. Comotti
<b>Additivi di vulcanizzazione per materiali elastomerici</b>	Pirelli Tyre SpA	B. Di Credico
<b>Materiali elastomerici rinforzati con fibre di sepiolite opportunamente modificate</b>	Pirelli Tyre SpA	B. Di Credico
<b>Design of innovative materials for tyres application</b>	CORIMAV	B. Di Credico
<b>La tecnologia SmartNET™ Silica per pneumatici altamente performanti</b>	UNIMIB-INNOVATION GRANT	B. Di Credico
<b>BIOINOHYB-Smart Bioinorganic Hybrids for Nanomedicine (ERC GRANT)</b>	EU	C. Di Valentin
<b>MADAM Metal Activated 2D Carbon-based Platforms</b>	MIUR	C. Di Valentin
<b>EIT QMforMA Designing New Materials with Quantum Mechanics</b>	EU	C. Di Valentin
<b>Valutazione dell'efficienza del trattamento di devulcanizzazione di granulati di gomma da pneumatici</b>	Previero	M. D'Arienzo, R. Scotti
<b>A new course on the Physics and technology of semiconductor devices with hand-on activity in a characterization and simulation lab</b>	MICRON TECHNOLOGY FOUNDATION INC	M. Fanciulli
<b>NEUREKA, "A smart, hybrid neural-computo device for drug discovery" H2020-FETOPEN-20</b>	EU	M. Fanciulli
<b>Variational methods, with applications to problems in mathematical physics and geometry</b>	MIUR	V. Felli
<b>NATUREChem - Unlocking Sustainable Technologies Through Nature-Inspired Solvents</b>	MIUR	N. Manfredi
<b>Leonardeschi oltre il visibile</b>	FONDAZIONE BRACCO	M. Martini
<b>MOBARTECH: una piattaforma mobile tecnologica, interattiva e partecipata per lo studio, la conservazione e la valorizzazione di beni storico-artistici</b>	REGIONE LOMBARDIA	M. Martini
<b>Multimodal nanotracking for exosome-based therapy in dmd (theoryenhancing)</b>	MINISTERO DELLA SALUTE	F. Meinardi
<b>Luminescent solar concentration windows for next generation buildingintegrated photovoltaics</b>	UNIMIB-INNOVATION GRANT	F. Meinardi

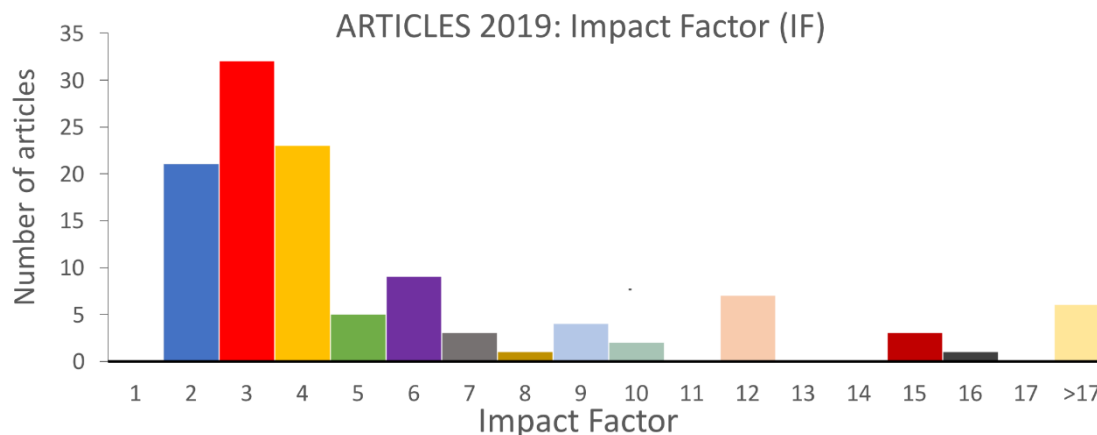
<b>Project/Research Contract Title</b>	<b>Funded by</b>	<b>Principal Investigator</b>
<b>CHALLENGE: 3C-SiCHetero-epitaxiALLY grown on silicon compliancE substrates and new 3C-SiC substrates for sustaiNable wide-band-Gap powEr devices</b>	EU	L. Miglio
<b>Materiali per Up-conversion a bassa potenza con applicazione nel Solare e nella Bio-teranostica Multimodale</b>	REGIONE LOMBARDIA	A. Monguzzi
<b>Theoretical analysis of the dislocation distribution in SILTRONIC SiGe/Si(001) graded layers</b>	SILTRONIC AG	F. Montalenti
<b>Towards sustainable, high-performing, all-solid-state sodium-ion batteries</b>	MIUR	P. Mustarelli
<b>Advanced Simulation Design of Nanostructured Thermoelectric Materials with Enhanced Power Factors</b>	EU	D. Narducci
<b>NANOTHERMA</b>	EU	D. Narducci
<b>Solar driven chemistry: new materials for photo- and electro-catalysis (SMARTNESS)</b>	MIUR	G. Pacchioni
<b>CASCADE DEOXYGENATION PROCESS USING TAILORED NANOCATALYSTS FOR THE PRODUCTION OF BIOFUELS FROM LIGNOCELLULOSIC BIOMASS</b>	EU	G. Pacchioni
<b>CATSENSE</b>	EU	G. Pacchioni
<b>Ossidi Nanostrutturati: multi-funzionalità e applicazioni</b>	MIUR	G. Pacchioni
<b>KiC- IMAGINE- Development and implementation of EIT KIC Raw Materials Master Program(s) in Sustainable Materials</b>	EU	A. Paleari
<b>Sviluppo di materiali elettrolici per batterie ricaricabili a sodio ione</b>	MINISTERO DEGLI ESTERI	R. Ruffo
<b>Give Sodium a Chance!Investigation of nanostructured mixed Na oxides as electrode materials for energy storage</b>	FONDAZIONE CARIPLO	R. Ruffo
<b>Preparazione e caratterizzazione elettrochimica di materiali elettrodi per batterie a ioni sodio (NIB)</b>	RSE S.p.A	R. Ruffo
<b>4PHOTON-Novel Quantum Emitters monolithically grown on Si, Ge and III-V substrates</b>	EU	S. Sanguinetti
<b>COSMITO - COMpressive Sampling Multispectral Imaging camera for remoTe Observation</b>	REGIONE LOMBARDIA	S. Sanguinetti

<b>Project/Research Contract Title</b>	<b>Funded by</b>	<b>Principal Investigator</b>
<b>FemToTera- Plasmon-enhanced Tera-Hertz emission by Femtosecond laser pulses of nanostructured semiconductor/metal surfaces</b>	EU	S. Sanguinetti
<b>TEcnologie INnovative per i VEicoli Intelligenti</b>	REGIONE LOMBARDIA/EU	S. Sanguinetti
<b>Micro-crystals Single Photon InfraREd detectors – <math>\mu</math>SPIRE – Horizon 2020 FET project</b>	EU	S. Sanguinetti
<b>EIT-KIC–Safer reduction of ZnO amount in rubber vulcanization process (SAFE-VULCA)</b>	EU	R. Scotti
<b>Studio dell'effetto di rinforzo di silice in compositi elastomerici</b>	Fluorsid Group	R. Scotti
<b>Next generation of molecular and supramolecular machines: towards functional nanostructured device, interfaces, surfaces and materials (NEMO)</b>	MIUR	P. Sozzani
<b>Augmented Environment for Control in amyotrophic lateral sclerosis</b>	ARISLA - AGENZIA DI RICERCA PER LA SCLEROSI LATERALE AMIOTROFICA	S. Tavazzi
<b>Influence of cylindrical power on visual functions and performance</b>	Hoya Holding	S. Tavazzi
<b>Analisi optometriche in soggetti non abbienti</b>	FONDAZIONE ONESIGHT	S. Tavazzi
<b>INTELUM-International and intersectoral mobility to develop advanced scintillating fibres and Cerenkov fibres for new hadron and jet calorimeters for future colliders</b>	EU	A. Vedda
<b>SCINTIGLASS</b>	EU	A. Vedda
<b>IDS-FunMat-Inno-2. International Doctoral School in Functional Materials &amp; Innovation</b>	EU	A. Vedda
<b>EIT-RM SPARK - Substitution and recycling of critical elements in materials for ionizing radiation detection</b>	EU	A. Vedda
<b>Brain adaptation to multifocal contact lenses</b>	Alcon Italia	F. Zeri



# PUBLICATIONS AND HIGHLIGHTS

In 2019 more than 150 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) of 5.8.



# HIGHLIGHTS

Macher, S.; Schott M.; **Sassi M.**; Facchinetti I.; **Ruffo R.**; **Patriarca G.**; **Beverina L.**; Posset U.; Giffin G.A.; Loebmann P.

*New Roll-to-Roll Processable PEDOT-Based Polymer with Colorless Bleached State for Flexible Electrochromic Devices.*

ADVANCED FUNCTIONAL MATERIALS 30(6), 1906254. (2020).

An Electrochromic Device (ECD) is designed for the control of optical properties through an electrical system. Transmissive ECDs can have a broad spectrum of applications, from smart windows to appliances, optical glasses, and automotive under the concept of energy savings. State of the art ECDs use as active materials inorganic oxides able to switch from a colored to a bleached state under a voltage stimulus. However, these materials are expensive, slow in switching between the optical states and required an integration in glasses.

The use of Electrochromic Conjugated (EC) polymers will open the doors to the production of low cost ECDs on flexible plastic supports, but EC generally lack a fully colorless bleached state. To overcome this drawback, we have designed of a new thiophene based polymer that can be deposited as thin-film in a customized high-throughput and large-area roll-to-roll polymerization process. The new polymer provides enhanced electrochromic properties in terms of color contrast and neutrality. Indeed, the intense blue-colored thin films exhibit high cycle stability (10000 cycles) and fast response times. Large area (up to A3 format), plastic, and flexible see-through ECDs were fabricated out integrating the new polymer with suitable components, i.e. electrolytes and ion storage material. These results have been obtained in the frame of three EU funded projects, namely NANO EFFECTS, INNOSHADE, and EELICON.



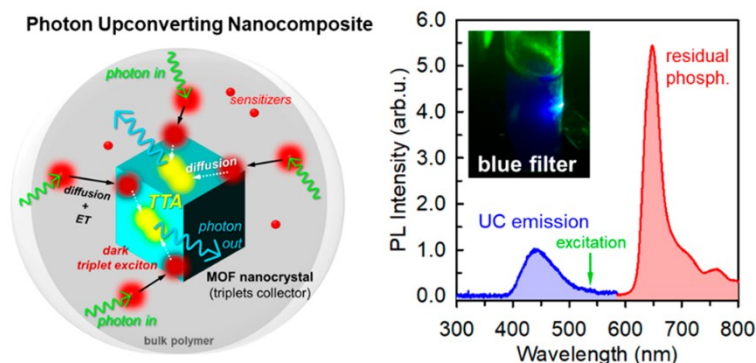
# HIGHLIGHTS

**Meinardi, F.**; Ballabio, M.; Yanai, N.; Kimizuka, N.; Bianchi, A.; Mauri, M.; **Simonutti, R.**; Ronchi, A.; Campione, M.; **Monguzzi, A.**

*Quasi-thresholdless Photon Upconversion in Metal–Organic Framework Nanocrystals.*

NANO LETTERS 19, 2169 (2019).

Photon upconversion based on sensitized triplet–triplet annihilation (sTTA) is a powerful strategy for the development of light-managing materials aimed to enhance the performance of solar devices by recovering unused low-energy photons. This work shows that the creation of triplet pairs in metal–organic framework nanocrystals (nMOFs) with size smaller than the exciton diffusion length implies a 100% TTA yield regardless of the illumination condition. This makes each nMOF a thresholdless, single-unit annihilator. A kinetic model of the upconversion dynamics in a nanocrystals ensemble reveals that, for materials based on such a thresholdless annihilator, the performances are limited only by the statistical distribution of the excitation energy among nanocrystals. The model is validated by fabricating a nanocomposite material based on nMOFs, which shows efficient upconversion under a few percent of solar irradiance, matching the requirements of real-world solar technologies.



In the figure: (Left) Sketch of a MOF nanocrystal which operates as a single-unit, thresholdless upconverter. (Right) Photograph and spectrum of the blue upconverted emission excited by low-power green light.

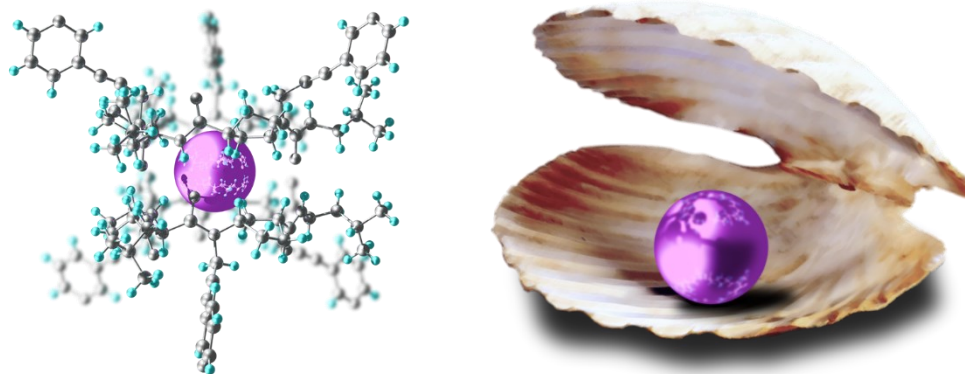
# HIGHLIGHTS

Pizzi, A.; Ozores, H.L.; Amarin, M.; Demistri, N.; Terraneo, G.; **Bracco, S.**; **Comotti, A.**; **Sozzani, P.**; Bezuidenhout, C. X.; Metrangolo, P.; Granja, J.R.

*Tight Xenon Confinement in a Crystalline Sandwich-like Hydrogen Bonded Dimeric Capsule of a Cyclic Peptide.*

ANGEWANDTE CHEMIE INTERNATIONAL EDITION 131, 14614. (2019).

We demonstrate that a cyclic hexapeptide self-assembles and forms a dimeric capsule, which tightly encapsulates a single xenon atom, like a pearl in its shell. The obtained molecular crystals of peptide dimers with encapsulated xenon can be manipulated in the open air at room temperature, with no gas release. Xenon receives the anisotropic imprint of the clamping dimers, as perceived by  $^{129}\text{Xe}$  NMR spectroscopy. The consequence of the present design is to provide a tool to construct supramolecular structures, based on biological building blocks, capable of capturing selectively rare gases, which find important applications in lighting, medical imaging, sensing and neuro-protection.



In the figure: a Xenon atom confined the cyclic hexapeptide, like a pearl in a shell.

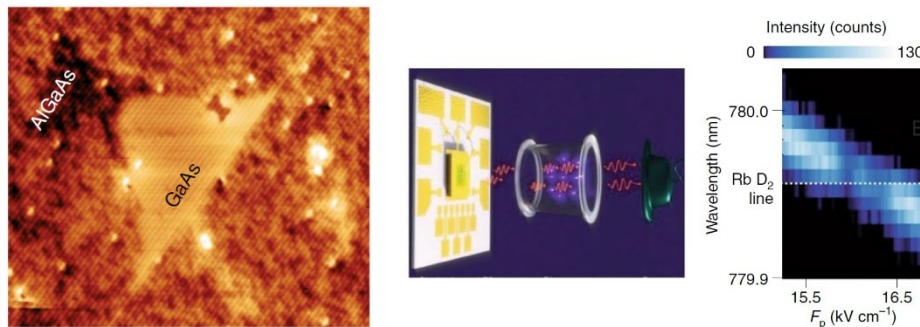
# HIGHLIGHTS

Gurioli, M., Wang, Z., Rastelli, A., Kuroda, T., **Sanguinetti, S.**

*Droplet epitaxy of semiconductor nanostructures for quantum photonic devices.*

NATURE MATERIALS 18, 799 (2019)

The long dreamed ‘quantum internet’ would consist of a network of quantum nodes (solid-state or atomic systems) linked by flying qubits, naturally based on photons, travelling over long distances at the speed of light, with negligible decoherence. A key component is a light source, able to provide single or entangled photon pairs. Among the different platforms, semiconductor quantum dots (QDs) are very attractive, as they can be integrated with other photonic and electronic components in miniaturized chips. Because of their robustness and simplicity QDs became the workhorse of quantum photonics permitting to achieve several breakthroughs in both fundamental and technological areas. The need for specific emission wavelengths or structural and optical properties has motivated further research on routes to obtain high-quality semiconductor nanostructures. The recent reports on the generation of highly entangled photon pairs, combined with good photon indistinguishability, show that droplet epitaxy outperforms conventional QDs obtained via Stranski–Krastanov growth mode as quantum emitters.



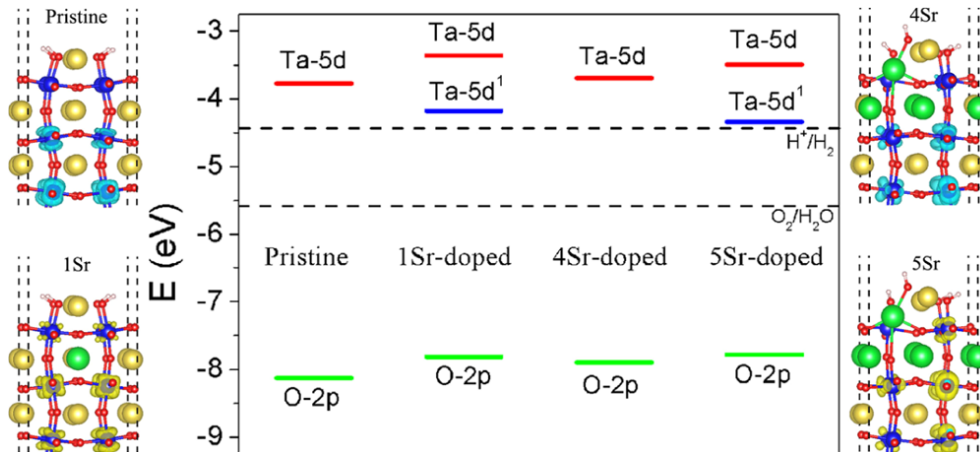
Left: topographic image of a QD by cross-sectional scanning tunnelling microscopy. Center: An LED based on GaAs QDs with emission energy tunable to transition lines of Rb atoms. Right: colour-coded electroluminescence spectra of a QD

# HIGHLIGHTS

Tang, Z.-K.; **Di Valentin, C.**; Zhao, X.; Liu, L.-M.; Selloni, A.

*Understanding the Influence of Cation Doping on the Surface Chemistry of NaTaO<sub>3</sub> from First Principles*  
ACS CATALYSIS 9, 10528. (2019).

Sodium tantalate, NaTaO<sub>3</sub>, is one of the few photocatalysts capable to perform overall water splitting, i.e. simultaneously produce O<sub>2</sub> and H<sub>2</sub> from water. In particular, an interesting and not fully understood observation is that the efficiency of NaTaO<sub>3</sub> increases dramatically in the presence of cation doping. To obtain better insight into the origin of this effect, we use first-principles calculations to investigate the fundamental structural, electronic, and chemical properties of pristine and Sr-doped NaTaO<sub>3</sub>. Our results show that Sr donor-acceptor codoping at Na and Ta sites significantly reduces the formation energy of the Sr dopants. Further study of the energetics of the oxygen evolution reaction (OER) shows a substantial reduction of its overpotential for the codoped material, consistent with recent suggestions that codoping is crucial for increasing NaTaO<sub>3</sub>'s efficiency. The detailed insights provided by our work could benefit the design and preparation of new efficient catalysts based on NaTaO<sub>3</sub>.



In the figure: Electronic states and models of pristine and Sr-doped NaTaO<sub>3</sub>.



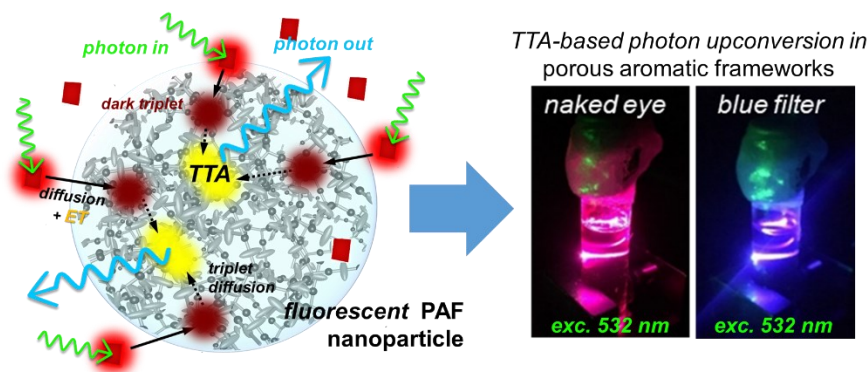
# HIGHLIGHTS

Perego, J.; Pedrini, J.; Bezuidenhout, C. X.; Sozzani, P. E.; Meinardi, F.; Bracco, S.; Comotti, A.; Monguzzi, A.

*Engineering Porous Emitting Framework Nanoparticles with Integrated Sensitizers for Low Power Photon Up-conversion by Triplet Fusion*

ADVANCED MATERIALS 31 (40), 1903309 (2019).

The conversion of low-energy light into photons of higher energy based on sensitized triplet–triplet annihilation (TTA) upconversion is the most promising wavelength-shifting methodology because it operates efficiently at excitation powers as low as the solar irradiance. The production of solid-state upconverters suited for direct integration in devices is solved here by fabricating porous fluorescent nanoparticles wherein the emitters are integrated into robust covalent architectures. These emitting porous aromatic framework (ePAF) nanoparticles allow intimate interaction with the included metallo-porphyrin as triplet sensitizers. The high concentration of framed chromophores ensures hopping-mediated triplet diffusion required for TTA, yet the low density of the framework promotes their high optical features without quenching effects, typical of the solid state. A green-to-blue photon upconversion yield as high as 15% is achieved: a record performance among annihilators in a condensed phase. Furthermore, the engineered ePAF architecture containing covalently linked sensitizers produces full-fledge solid-state bicomponent particles that behave as autonomous nanodevices.



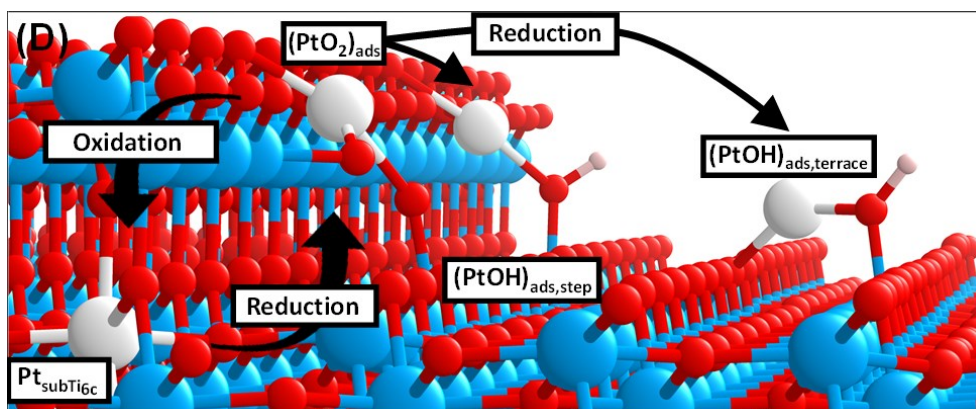
In the figure: Sketch of the ePAF structure and of the TTA upconversion process in the fluorescent nanoparticle. Digital picture of the green-to-blue upconversion obtained in a ePAFs dispersion.

De Rita, L; Resasco, J; Dai, S; Boubnov, A; Thang, H. V.; Hoffman, A. S.; Ro, I; Graham, G. W.; Bare, S. R.; **Pacchioni, G.**; Pan, X.; Christopher, P.

*Structural evolution of atomically dispersed Pt catalysts dictates reactivity*

NATURE MATERIALS 18, 746-751 (2019).

The use of oxide-supported isolated Pt-group metal atoms as catalytic active sites is of interest due to their unique reactivity and efficient metal utilization. However, relationships between the structure of these active sites, their dynamic response to environments and catalytic functionality have proved difficult to experimentally establish. Here, sinter-resistant catalysts where Pt was deposited uniformly as isolated atoms in well-defined locations on anatase TiO<sub>2</sub> nanoparticle supports were used to develop such relationships. Through a combination of in situ atomic-resolution microscopy- and spectroscopy-based characterization supported by first-principles calculations it was demonstrated that isolated Pt species can adopt a range of local coordination environments and oxidation states, which evolve in response to varied environmental conditions. The variation in local coordination showed a strong influence on the chemical reactivity and could be exploited to control the catalytic performance.



In the figure: Depending on the preparation and reaction conditions, Pt single atoms catalysts supported on anatase TiO<sub>2</sub> assume different positions and coordination.

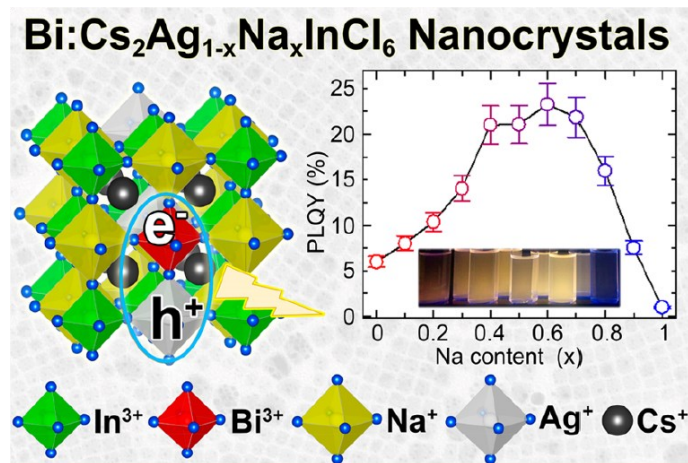
# HIGHLIGHTS

Locardi, F.; Sartori, E.; Buha, J.; Zito, J.; Prato, M.; Pinchetti, V.; Zaffalon, M.L.; Ferretti, M.; **Brovelli, S.**; Infante, I.; De Trizio, L.; Manna, L.

*Emissive Bi-Doped Double Perovskite  $\text{Cs}_2\text{Ag}_{1-x}\text{Na}_x\text{InCl}_6$  Nanocrystals*

ACS ENERGY LETTERS 4, 1976–1982 (2019)

Double perovskites, also termed *elpasolites*, have gained increasing attention as heavy-metal-free alternatives to lead halide perovskite materials for applications spanning from photovoltaics to artificial lighting and solar concentration. Such an environmentally friendly composition, however, comes with a cost in terms of a low emission performance due to the disadvantageous electronic structure of elpasolites. As a result, the excitonic photophysics of this material system is much more complex than lead halide perovskites. This calls for specific multidisciplinary investigations to trace rational guidelines for their optimization and, ultimately, device application. This work reports the composition-dependent optical properties of Bi-doped  $\text{Cs}_2\text{Ag}_{1-x}\text{Na}_x\text{InCl}_6$  nanocrystals having a double perovskite crystal structure. Spectroscopic investigations corroborated by density functional theory calculations revealed that the PL emission stems from trapped excitons between states localized in the  $\text{BiCl}_6$  and  $\text{AgCl}_6$  octahedra, respectively. Our findings indicated that both the partial replacement of  $\text{Ag}^+$  with  $\text{Na}^+$  ions and doping with  $\text{Bi}^{3+}$  cations are essential in order to optimize the PL emission of these systems.

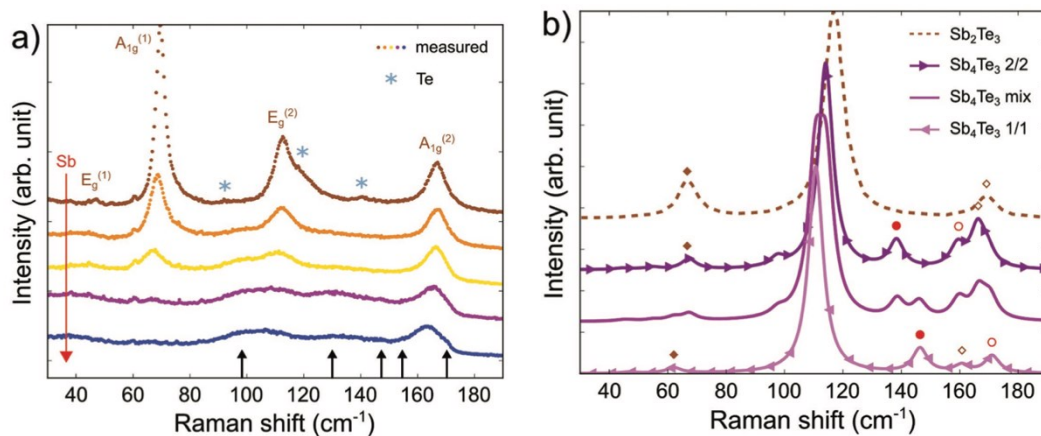


In the figure: Structure of  $\text{Cs}_2\text{Ag}_{1-x}\text{Na}_x\text{InCl}_6$  nanocrystals and their photoluminescence efficiency as a function of the sodium content.

# HIGHLIGHTS

Cecchi, S; Dragoni, D; Kriegner, D; Tisbi, E; Zallo, E; Arciprete, F; Holý, V; **Bernasconi, M**; Calarco, F.  
*Interplay between Structural and Thermoelectric Properties in Epitaxial  $\text{Sb}_{2+x}\text{Te}_3$  Alloys.*  
ADVANCED FUNCTIONAL MATERIALS 29, 1805184 (2019).

Antimony telluride alloys are of interest for applications in thermoelectric devices and in phase-change non-volatile electronic memories. Here, we report on the structural and thermoelectric properties of epitaxial  $\text{Sb}_{2+x}\text{Te}_3$  films grown by Molecular Beam Epitaxy. A combination of x-ray diffraction and Raman spectroscopy, aided by theoretical modeling based on electronic structure calculations, allowed unveiling the crystal structure of these layered alloys and its dependence on composition. The presence of both  $\text{Sb}_2$  and  $\text{Sb}_4$  blocks and a link between structural disorder and thermoelectric performances have been highlighted.



In the figure: Experimental (left) and theoretical (right) Raman spectra of  $\text{Sb}_{2+x}\text{Te}_3$  alloys.

# INTERNATIONAL JOURNALS

#	Publication	IF
1	Abbas, Z; Tawfilas, M; Khani, M; Golian, K; Marsh, Z; Jhalaria, M; Simonutti, R; Stefik, M; Kumar, S; Benicewicz, B, Reinforcement of polychloroprene by grafted silica nanoparticles, POLYMER 171, 96	3.771
2	Albani, M; Bergamaschini, R; Salvalaglio, M; Voigt, A; Miglio, L; Montalenti, F, Competition Between Kinetics and Thermodynamics During the Growth of Faceted Crystal by Phase Field Modeling, PHYSICA STATUS SOLIDI B-BASIC RESEARCH 256, 1800518	1.454
3	Ali, S; Imiete, I; Orlandi, M; Castellani, L; Hanel, T; Zoia, L, Novel CNC/silica hybrid as potential reinforcing filler for natural rubber compounds, JOURNAL OF APPLIED POLYMER SCIENCE, 48332	2.188
4	Anand, A; Zaffalon, M; Gariano, G; Camellini, A; Gandini, M; Brescia, R; Capitani, C; Bruni, F; Pinchetti, V; Zavelani-rossi, M; Meinardi, F; Crooker, S; Brovelli, S, Evidence for the Band-Edge Exciton of CuInS <sub>2</sub> Nanocrystals Enables Record Efficient Large-Area Luminescent Solar Concentrators, ADVANCED FUNCTIONAL MATERIALS , 1906629	15.62
5	Anemone, G; Al Taleb, A; Benedek, G; Castellanos-Gomez, A; Farías, D, Electron-Phonon Coupling Constant of MoS <sub>2</sub> from Helium Atom Scattering, JOURNAL OF PHYSICAL CHEMISTRY. C 123, 3682	4.309
6	Antonini, C; Wu, T; Zimmermann, T; Kherbeche, A; Thoraval, M; Nyström, G; Geiger, T, Ultra-Porous Nanocellulose Foams: A Facile and Scalable Fabrication Approach, NANOMATERIALS 9, 1142	4.034
7	Arnaboldi, S; Benincori, T; Penoni, A; Vaghi, L; Cirilli, R; Abbate, S; Longhi, G; Mazzeo, G; Grecchi, S; Panigati, M; Mussini, P, Highly enantioselective "inherently chiral" electroactive materials based on a 2,2'-biindole atropisomeric scaffold, CHEMICAL SCIENCE 10, 2708	9.556
8	Assali, S; Albani, M; Bergamaschini, R; Verheijen, M; Li, A; Kolling, S; Gagliano, L; Bakkers, E; Miglio, L, Strain engineering in Ge/GeSn core/shell nanowires, APPLIED PHYSICS LETTERS 115, 113102	3.521
9	Azadmand, M; Bonera, E; Chrastina, D; Bietti, S; Tsukamoto, S; Notzel, R; Sanguinetti, S, Raman spectroscopy of epitaxial InGaN/Si in the central composition range, JAPANESE JOURNAL OF APPLIED PHYSICS 58, SC1020	1.471
10	Azamat, D; Badalyan, A; Baranov, P; Fanciulli, M; Lancok, J; Hrabovsky, M; Jastrabik, L; Dejneka, A, Spin-lattice relaxation processes of transition metal ions in a heavily cobalt doped ZnO: Phonon heating effect, JOURNAL OF APPLIED PHYSICS 126, 123903	2.328
11	Bagolini, A; Scauso, P; Sanguinetti, S; Bellutti, P, Silicon Deep Reactive Ion Etching with aluminum hard mask, MATERIALS RESEARCH EXPRESS 6, 085913	1.449
12	Ballabio, A; Bietti, S; Scaccabarozzi, A; Esposito, L; Vichi, S; Fedorov, A; Vinattieri, A; Mannucci, C; Biccari, F; Nemcsis, A; Toth, L; Miglio, L; Gurioli, M; Isella, G; Sanguinetti, S, GaAs epilayers grown on patterned (001) silicon substrates via suspended Ge layers, SCIENTIFIC REPORTS 9, 17529	4.011
13	Balzani, V; Pacchioni, G; Prato, M; Zecchina, A, Solar-driven chemistry: towards new catalytic solutions for a sustainable world, RENDICONTI LINCEI. SCIENZE FISICHE E NATURALI 30, 443	1.087

#	Publication	IF
14	Bartlett, P; Berg, A; Bernasconi, M; Brown, S; Burr, G; Foroutan-Nejad, C; Gale, E; Huang, R; Ielmini, D; Kissling, G; Kolosov, V; Kozicki, M; Nakamura, H; Rushchanskii, K; Salinga, M; Shluger, A; Thompson, D; Valov, I; Wang, W; Waser, R; Williams, R, Phase-change memories (PCM)-Experiments and modelling: General discussion, FARADAY DISCUSSIONS 213, 393	3.712
15	Basset, F; Bietti, S; Tuktamyshev, A; Vichi, S; Bonera, E; Sanguinetti, S, Spectral broadening in self-assembled GaAs quantum dots with narrow size distribution, JOURNAL OF APPLIED PHYSICS 126, 024301	2.328
16	Beretta, D; Neophytou, N; Hodges, J; Kanatzidis, M; Narducci, D; Martin- Gonzalez, M; Beekman, M; Balke, B; Cerretti, G; Tremel, W; Zevalkink, A; Hofmann, A; Müller, C; Döring, B; Campoy-Quiles, M; Caironi, M, Thermoelectrics: From history, a window to the future, MATERIALS SCIENCE & ENGINEERING R-REPORTS 138, 100501	22.25
17	Beretta, M; Amirkhani, A; Brofferio, C; Brovelli, S; Buonanno, L; Cova, F; Capelli, S; Fasoli, M; Fiorini, C; Gironi, L; Vedda, A; Villa, I, The ESQUIRE project: Quantum Dots as scintillation detectors, IL NUOVO CIMENTO C 42, 188	NA
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147	Vaghi, L; Coletta, M; Coghi, P; Andreosso, I; Beverina, L; Ruffo, R; Papagni, A, Fluorine substituted non-symmetric phenazines: a new synthetic protocol from polyfluorinated azobenzenes, ARKIVOC 2019, 340	1.253
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152	Zianni, X; Narducci, D, Modelling the simultaneous increase of the conductivity and the Seebeck coefficient in highly B-doped nc-Si, MATERIALS TODAY: PROCEEDINGS 8, 706	NA
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# CONFERENCES AND SEMINARS

#	Authors & Title	Conference/Workshop
1	Albani, M; Assali, S; Bergamaschini, R; Scalise, E; Verheijen, M; Li, A; Kölling, S; Bakkers, E; Montalenti, F; Miglio, L, The interplay of morphology, composition and strain in metastable Ge/GeSn core/shell nanowires.	Nanowire Week - Pisa 2019, Pisa, Italia.
2	Albani, M; Bergamaschini, R; Salvalaglio, M; Voigt, A; Miglio, L; Montalenti, F, Modelling the kinetic growth and faceting of vertical micro- and nano-structures on Si.	EMRS fall Meeting 2019, Varsavia, Polonia.
3	Albani, M; Bergamaschini, R; Scalise, E; Montalenti, F; Miglio, L, Kinetic growth modeling of 3C-SiC micro-crystals on Si pillars.	EMRS Spring meeting 2019, Nizza, Francia.
4	Antonini, C, ApiTech - l'innovazione a portata di PMI. INVITED	Research, Innovation And Entrepreneurship Marie Curie Alumni Association (Mcaa) Gems Wg, Bologna, Italy.
5	Antonini, C; Blanken, N; Saleem, M; Thoraval, M, Self-lubrication of immiscible compound drops upon impact.	Materials Research Society Fall 2019, Boston, US.
6	Antonini, C; Wu, T; Nystrom, G; Kherbeche, A; Thoraval, M; Geiger, T, Ultra-porous nanocellulose foams with tailored wetting properties. INVITED	European Material Research Society 2019 Fall Meeting, Varsavia, Polonia.
7	Baby, A; Perilli, D; Liu, H; Kosmala, T; Lamana, L; Granozzi, G; Agnoli, S; Di Valentin, C, Tuning the hydrogen evolution reaction at the Pt(111) surface with 2D material and non-precious metal.	Materials for Today's Energy Challenges, Padova, Italia.
8	Barbisan, L; Marzegalli, A; Sarikov, A; Montalenti, F; Miglio, L, Multiple stacking fault formation via the evolution of related dislocations by molecular dynamics simulations.	2019 Spring Meeting of the European Materials Research Society (E-MRS 2019 spring meeting), Nizza, Francia.
9	Bergamaschini, R; Albani, M; Miglio, L; Montalenti, F; Salvalaglio, M, Kinetic growth and surface faceting of vertical micro- and nano-structures: theory and experiments.	3rd International conference on Applied Surface Science, Pisa.
10	Bergamaschini, R; Albani, M; Montalenti, F; Miglio, L, Continuum model of out-of-equilibrium crystal growth: theory and experiments.	EuroMBE 2019, Lenggriess.
11	Bergamaschini, R; Albani, M; Montalenti, F; Miglio, L, Phase-field modelling of compositional segregation during the growth of core-shell nanowires.	3rd International conference on Applied Surface Physics, Pisa.
12	Bernasconi, M, Atomistic simulations of phase change materials for electronic memories. INVITED	Nanomeeting 2019, Minsk, Bielorussia.



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13	Beverina, L, Bench-top, sustainable access to conjugated materials: how far you can go with tap water, a stirring plate, very little palladium and a little soap. INVITED	IFSOE 2019, Mosca.
14	Beverina, L, Green organic chemistry for advanced optoelectronic applications. INVITED	CNIST Winter Workshop IIT, Milano.
15	Beverina, L, Sustainable approaches for the design and synthesis of organic dyes and pigments for printed electronics. INVITED	International Workshop on Chemistry and Applications of Organic Chromophores, Cardiff.
16	Binetti, S, Earth-abundant chalcogenide thin film for PV application: the activity of MIB-SOLAR center at University of Milano-Bicocca. INVITED	School of Photovoltaic and Renewable Energy Engineering: Public Research Seminars, SYDNEY.
17	Binetti, S, Photoluminescence and infrared spectroscopy for impurities identification in silicon for photovoltaic applications. INVITED	School of Photovoltaic and Renewable Energy Engineering: Public Research Seminars, SYDNEY., SYDNEY (AUSTRALIA).
18	Binetti, S, Silicon, the key element for photovoltaic energy: past, present and future perspectives. INVITED	Avogadro Colloquia 2019: "Elements of the Periodic Table for Energy"., ROMAQ (ITALY).
19	Bonizzoni, S; Colombo, F; Tawfilas, M; Mauri, M; Simonutti, R; Ruffo, R; Mustarelli, P, PEO-grafted TiO <sub>2</sub> filler as Solid Polymer Electrolyte for rechargeable lithium batteries. INVITED	Giornate Italiane di elettrochimica (GEI), Padova, Italy.
20	Bracco, S, Riconoscimento e diffusione di gas in cavità ingegnerizzate di cristalli porosi. INVITED	BALANCE: Nanospugne e macchine molecolari: materiali innovativi per la produzione di biometano, Milano.
21	Campione, M; Villa, I; Villa, C; Torrente, Y; Vedda, A; Monguzzi, A, Self-assembled hybrid nanotubes for x-ray activated photodynamic therapy (X-PDT) on brain cancer.	The 2019 Spring Meeting of the European Materials Research Society, Nizza, France.
22	Comotti, A, Rotor and Gas Dynamics in Porous Materials. INVITED	Molecular Rotor Workshop, November 21-22, 2019, Praga, Repubblica Ceca.
23	Comotti, A, The Intriguing Dynamics of CO <sub>2</sub> and Xe in Molecular Crystals: The Imprint of the Crystal Structure.	ICCOSS XXIV - 24th International Conference on the Chemistry of the Organic Solid State, New York, USA.
24	Comotti, A; Bracco, S; Perego, J; Negroni, M; Bezuidenhout, C; Sozzani, P, Dynamics of CO <sub>2</sub> and Xe and Ultra-fast Molecular Rotors in Porous Crystals.	ISMSC2019 - 14th International Symposium On Macrocyclic And Supramolecular Chemistry, Lecce, Italy.

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25	Comotti, A; Bracco, S; Perego, J; Negroni, M; Bezuidenhout, C; Supino, I; Pedrini, A; Sozzani, P, Imprinting the pore symmetry to CO <sub>2</sub> and Xe, gas dynamics and ultra-fast molecular rotors in molecular porous materials with tetrahedral building blocks.	POOs - 2nd international symposium on porous organic polymers, Heidelberg, Germany.
26	Cova, F; Hostaša, J; Biasini, V; Fasoli, M; Moretti, F; Bourret, E; Vedda, A, Fabrication and Photo-Physical Characterization of Ce-doped Gd <sub>3</sub> (Ga,Al)5O <sub>12</sub> Transparent Ceramics.	15th International Conference on Scintillating Materials and their Applications, SCINT 2019, Sendai, Japan.
27	De Cesari, S; Balocchi, A; Vitiello, E; Jahandar, P; Amand, T; Marie, X; Myronov, M; Pezzoli, F, Carrier and Spin Coherent Dynamics in Strained Germanium-Tin Semiconductor on Silicon.	Joint ISTDM / ICSI 2019 Conference, 10th International SiGe Technology and Device Meeting (ISTDM), 12th International Conference on Silicon Epitaxy and Heterostructures (ICSI), Madison, USA.
28	Di Credico, B; Cobani, E; D'Arienzo, M; Giannini, G; Hanel, T; Tadiello, L; Scotti, R, From Research To Market: A New Family Of Silica Fillers. INVITED	International Rubber Conference - IRC 2019, Londra.
29	Di Valentin, C, MODELLING Stimuli-Responsive Nanomaterials for Biomedical Applications. INVITED	Nanomedicine2019, Milano.
30	Di Valentin, C, MODELLING Stimuli-Responsive Nanomaterials for Biomedical Applications. INVITED	Nasini Workshop 2019, Roma.
31	Di Valentin, C, MODELLING Stimuli-Responsive Nanomaterials for Biomedical Applications. INVITED	Women in science, Milano.
32	Di Valentin, C, Modeling photo and electro nanocatalysts for water splitting in water. INVITED	EMRS Fall meeting 2029, Varsavia.
33	Di Valentin, C, Polaronic effects in titanium and iron oxides by hybrid DFT calculations. INVITED	Polarons in the 21st century, Vienna.
34	Di Valentin, C, Theory of oxides and interfaces. INVITED	TCO 2019, Leipzig, Germany.
35	Facchinetti, I; Cobani, E; Brogioli, D; La Mantia, F; Ruffo, R, Thermally Regenerable Redox-Flow Batteries.	GEI 2019: Giornate dell'elettrochimica italiane, Padova, Italy.

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36	Ferrara, C; Brugnetti, G; Fiore, M; Mustarelli, P; Ruffo, R, Ilmenite nanoflowers as anode material for SIBs: the thin red line between morphology control and decomposition.	International Conference on Solid State Ionics, Pyeongchang (Corea).
37	Ferrara, C; Brugnetti, G; Fiore, M; Ruffo, R, FeTiO <sub>3</sub> as anode material for sodium ion batteries: from morphology control to decomposition.	Giornate dell'Elettrochimica Italiana GEI 2019, Padova, Italy.
38	Ferrara, C; Gentile, A; Ruffo, R, Tackling the structure and defect chemistry of MAX phases and the derived MXenes electrode materials.	2019 Annual School on Neutron Diffraction Data Treatment Using the FullProf Suite, Grenoble (Francia).
39	Ferrara, C; Vigo, E; Albini, B; Galinetto, P; Milanese, C; Tealdi, C; Quartarone, E; Passerini, S; Mustarelli, P, 31P solid-state NMR investigation of the Red-to-Black Phosphorus mechanochemical conversion.	XLVII Congresso Nazionale della Divisione di Chimica Fisica, Roma, Italy.
40	Galli, A; Bonizzoni, L; Caccia, M; Gargano, M; Ludwig, N; Poldi, G; Martini, M, From pigments to colour. Non invasive analyses on Bernardino Luini.	Technart 2019, maggio 2019, Bruges (Belgio)
41	Galli, A; Caglio, S; Bonizzoni, L; Gironda, M; Alberti, R; Martini, M, More than MA-XRF maps: the investigation of Chariot Race by de Chirico.	MA-XRF scanning in Conservation, Art and Archeology, ottobre 2019 Catania
42	Galli, A; Martini, M; Maspero, F; Panzeri, L; Sibilia, E, "MOBARTECH" A mobile, interactive and participatory platform for the study, conservation and promotion of Cultural Heritage,	Convegno tematico AIAR 2019. Dalla Conoscenza alla Valorizzazione: il Ruolo dell'archeometria nei Musei, Reggio Calabria, 27 – 29 Marzo 2019.
43	Gentile, A; Ruffo, R; Marchionna, S; Balordi, M; Cernuschi, F, Structure properties correlation in MXenes: 2D anodic materials for sodium ion batteries.	Giornate dell'Elettrochimica Italiana - GEI, Padova, Italy.
44	Hofmann, E; Scalise, E; Schofield, S; Capellini, G; Miglio, L; Curson, N; Klesse, W, Atomic scale insights into Sn on Ge(100): From submonolayers to the formation of Sn wetting layers.	Istmdm-icsi-2019, Madison, Wisconsin.
45	Li, H; Seifert, G; Di Valentin, C, Insights into magnetite bulk, surface and nanoparticles by first principles.	The 10th Joint European Magnetic Symposia (JEMS), Uppsala, Sweden.
46	Liu, H; Seifert, G; Di Valentin, C, Insights into magnetite bulk, surface and nanoparticles by first-principles.	III International Baltic Conference on Magnetism 2019, Kaliningrad, Russia.
47	Lorenzi, R; Golubev, N; Ignat'Eva, E; Sigaev, V; Paleari, A, Photocatalytic activity of germanosilicate glassceramics containing Ga <sub>2</sub> O <sub>3</sub> nanostructures.	International Congress on Glass, Boston, USA.
48	Lorenzi, R; Meinardi, F; Brovelli, S; Paleari, A, Interband decay and absorption mechanisms in amorphous silica probed by synchrotron light. INVITED	Photonics & Electromagnetics Research Symposium (PIERS), Roma, Italy.

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49	Marengo, M; Antonini, C, Understanding Surface Wettability Effects on Ice Formation. INVITED	Micro and Nanoscale Phase Change Heat Transfer Gordon Research Conference The Effects of Hydrodynamic, Interfacial and Intermolecular Forces on Phase Change Processes, Lucca.
50	Maspero, F; Sassella, A; Sibilia, E; Galli, A; Panzeri, L; Martini, M, A virtual approach to historical scientific instruments.	Convegno tematico AIAr 2019. Dalla Conoscenza alla Valorizzazione: il Ruolo dell'archeometria nei Musei, Reggio Calabria, 27 – 29 Marzo 2019
51	Miglio, L, From Science to Technology. INVITED	NANO-DAY IV, Milano, Italia.
52	Monguzzi, A, Triplet-triplet annihilation dynamics in nanosized fluorescent supramolecular systems for photon upconversion. INVITED	13th International Conference on Optical Probes of Organic and Hybrid Materials and Applications, Vilnius, Lithuania.
53	Mostoni, S; Marano, C; D'Arienzo, M; Di Credico, B; Susanna, A; Scotti, R, Effect of zinc oxide distribution on vulcanization efficiency and mechanical properties of rubber nanocomposites.	XII Convegno Nazionale INSTM, Ischia Porto.
54	Narducci, D, Silicon Reloaded - Novel Perspectives of Silicon as a Thermoelectric Material. INVITED	2019 Materials Research Meeting, Yokohama, Japan.
55	Narducci, D, Solar cogeneration and distributed microgeneration: novel opportunities for thermoelectrics? INVITED	2019 International Conference on Thermoelectrics, Gyeongju (Republic of Korea).
56	Narducci, D, Thermoelectricity beyond local and instantaneous approximations. INVITED	European Materials Research Society 2019 Fall Meeting, Warsaw (Poland).
57	Pacchioni, G, Catalysis design from first principles. Concepts, examples and perspectives. INVITED	International PCAM School "Future Perspectives in Catalysis", Bremerhafen (Germany).
58	Pacchioni, G, Catalyst design from first principles: modifying oxide reducibility by nanostructuring and metal/oxide interfaces. INVITED	American Chemical Society Meeting & Expo – Catalysis by metal-support interfaces, San Diego (USA).
59	Pacchioni, G, Electronic structure theory in catalysis: concepts, examples, and perspectives. INVITED	Past, present and future of inorganic chemistry in Italy: a path defined by the winners of the Nasini prize, Roma.

#	Authors & Title	Conference/Workshop
60	Pacchioni, G, Improving the activity of metal oxides in photocatalysis via doping and heterostructures: a theoretical perspective. INVITED	7th International Conference on Semiconductor Photochemistry, Milano.
61	Pacchioni, G, Nanoparticles versus bulk materials: dramatic changes of ZrO <sub>2</sub> properties by nanostructuring. INVITED	Gas-phase clusters: experiment and theory in concert, APS March Meeting, Boston.
62	Pacchioni, G, Oxide semiconductors for photocatalysis: doping versus heterostructures. INVITED	Design, Fabrication and Application of Devices for Energy Production, ICTP, Trieste.
63	Pacchioni, G, Oxide ultrathin films: new functions, new properties, new materials. INVITED	International Workshop on Layered Materials, Liblice (Repubblica Ceca).
64	Pacchioni, G, Role of nanostructuring and metal/oxide interfaces on the properties of heterogeneous catalysts for oxidation reaction. Single atom catalysts. INVITED	VIII Irsee Symposium – Advances in heterogeneous catalysis and electrocatalysis including new insights from surface science and quantum mechanics, Irsee (Germania).
65	Pacchioni, G, Searching new catalytic materials for CO <sub>2</sub> activation: ZnO/Cu(111) bilayer films. INVITED	Energy-X Workshop: Research needs towards sustainable production of fuels and chemicals, Bruxelles.
66	Pacchioni, G, Surfaces without secrets. INVITED	Crossroads in physical chemistry – Experiment meets theory, Berlin (Germany).
67	Pacchioni, G, Theory of magnetic impurities in oxides. Complex problem, pragmatic solution. INVITED	PARACAT – Paramagnetic species in catalysis research, Anversa (Belgio).
68	Pacchioni, G, TiO <sub>2</sub> and ZrO <sub>2</sub> in biomass conversion: why catalyst reduction helps. INVITED	American Chemical Society Meeting & Expo – Theoretical and mechanistic studies of biomass-derived oxygenates, San Diego (USA).
69	Pacchioni, G, Unveiling the nature of single atom catalysts. INVITED	2nd funCOS Workshop – Functional molecular structures on complex oxide surfaces, Erlangen (Germania).
70	Pacchioni, G, ZnO/Cu(111) bilayer films: new catalytic materials. INVITED	3rd International Workshop on Graphene and C <sub>3</sub> N <sub>4</sub> -based Photocatalysts, Wuhan (Cina).

#	Authors & Title	Conference/Workshop
71	Pedrini, A; Bracco, S; Castiglioni, F; Comotti, A; Galli, S; Maspero, A; Negroni, M; Sozzani, P, Fluorinated bis(pyrazole)-based MOFs for gas adsorption and separation.	ICS2019, Innovative Catalysis and Sustainability, International Winter School (Bardonecchia, 7-11 gennaio 2019), Bardonecchia, Italy.
72	Perego, J; Piga, D; Bracco, S; Sozzani, P; Comotti, A, Triphenylmethane Aromatic Frameworks (TAFs): Engineered Pore Chemistry for Targeted Gas Adsorption.	POPs - 2nd international symposium on porous organic polymers, Heidelberg, Germany.
73	Perilli, D; Selli, D; Liu, H; Di Valentin, C, Computational Electrochemistry of Water Oxidation on Metal-Doped and Metal-Supported Defective h-BN.	Graphene Week 2019, Helsinki, Finland.
74	Pezzoli, F, La fisica dello spin in nanostrutture a semiconduttore: spettroscopia ottica e applicazioni. INVITED	Conferenza Italiana degli Studenti di Fisica, Milano, Italy.
75	Pezzoli, F, Lattice-mismatched heterostructures based on group IV semiconductors as an advanced spin-optonics platform. INVITED	10th International Workshop on Bismuth-Containing Semiconductors, Toulouse, France.
76	Pezzoli, F, Unravelling spin-dependent properties of group IV semiconductors through optical investigations. INVITED	2nd AFRL Workshop on GeSn and GeSiSn, Dayton, Ohio, US.
77	Pezzoli, F; Pedrini, J; Biagioni, P; Barzaghi, A; Ballabio, A; Bonera, E; Miglio, L; Isella, G, Optical properties of micron-sized crystals grown via 3D heteroepitaxy.	2nd Joint ISTDM / ICSI 2019 Conference, 10th International SiGe Technology and Device Meeting (ISTDM), 12th International Conference on Silicon Epitaxy and Heterostructures (ICSI), Madison, USA.
78	Quartarone, E; MUSTARELLI, P; Ravelli, D; Samori, C, A Biomass-Derived Polyhydroxyalkanoate Biopolymer as Safe and Environmental-Friendly Skeleton in Highly Efficient Gel Electrolytes for Lithium Batteries.	MRS Fall Meeting, Boston (MA).
79	Remondina, J; Acciarri, M; Lorenzi, R; Golubev, N; Ignat'Eva, E; Sigaev, V; Paleari, A, Oxide-in-Oxide Ga2O3-Containing Glass-Ceramics: from Bulks to Thin-Film Devices.	GraFOx Summer School on Oxide Semiconductors for Smart Electronic Devices, Menaggio, CO.
80	Rovaris, F; Zoellner, M; Zaumseil, P; Marzegalli, A; Di Gaspare, L; De Seta, M; Schroeder, T; Storck, P; Schwalb, G; Capellini, G; Montalenti, F, Modeling the dynamics of cross-hatch evolution in heteroepitaxy.	Joint ISTDM / ICSI 2019 Conference, Madison, Wisconsin.
81	Ruffo, R; Gentile, A; Marchionna, S; Balordi, M; Cernuschi, F, Structure Properties Correlation in MXenes: 2D Anodic Materials for Sodium Ion Batteries. INVITED	236th ECS Meeting, Atlanta (US).



#	Authors & Title	Conference/Workshop
82	Sarikov, A; Marzegalli, A; Barbisan, L; Montalenti, F; Miglio, L, Molecular dynamics simulations of extended defects and their evolution in 3C-SiC by different potentials.	EMRS 2019 Spring Meeting, Nizza, Francia.
83	Sassella, A, Organic epitaxy as a tool for controlling crystallinity, orientation, and properties of organic thin films. INVITED	Fabrication processes and molecular organization in organic thin films: theory and simulation meet experiments - CECAM Workshop, Politecnico di Milano - sede di Lecco, Italy.
84	Scalise, E; Marzegalli, A; Montalenti, F; Miglio, L, Crystal free energy of SiC polytypes and stacking faults formation energy from DFT-based lattice-dynamics approach.	APS March meeting 2019, Boston.
85	Scalise, E; Marzegalli, A; Montalenti, F; Miglio, L, From the crystal free energy of SiC polytypes to the stacking faults formation energy: a DFT-based lattice-dynamics approach.	EMRS Spring meeting 2019, Nice.
86	Scotti, R; Mostoni, S; D'Arienzo, M; Di Credico, B; Susanna, A; Donetti, R, Nanosized and single site zinc-based activator onto silica for reducing ZnO in rubber vulcanization process.	International Rubber Conference IRC2019, Londra.
87	Tagliaro, I; Conzatti, L; Giannini, G; D'Arienzo, M; Scotti, R; Stagnaro, P; Tadiello, L; Di Credico, B, Sustainable synthetic strategy for preparing high-loaded clay-rubber nanocomposites.	Eurofillers Polymer Blends 2019, Palermo.
88	Tirelli, G; Lugli, S; Galli, A; Hajdas, I; Lindroos, A; Martini, M; Maspero, F; Olsen, J; Panzeri, L; Ringbom, A; Sibilia, E; Caroselli, M; Silvestri, E, Dating earthquake damage of the Modena cathedral vaults (Northern Italy): an integrated approach.	13th International Conference "Methods of Absolute Chronology, Tarnowskie Góry, 5 – 7 giugno 2019
89	Trifiletti, V; Mostoni, S; Scotti, R; Binetti, S, In situ gel formation of high quality kesterite thin films.	MCEC 2019 - Materials for Clean Energy Conference, National Physics Laboratory, London, UK.
90	Vedda, A, Silica-based scintillating fibers for ionizing radiation sensing. INVITED	PIERS 2019 - Photonics & Electromagnetics Research Symposium, Roma, Italy.
91	Villa, I; Bonaldo, C; Crapanzano, R; Tawfilas, M; Villa, C; Torrente, Y; Vedda, A; Campione, M; Monguzzi, A, CHRYSOTILE NANOTUBES FOR X-RAY ACTIVATED PHOTODYNAMIC THERAPY.	15th International Conference on Scintillating Materials and their Applications, SCINT 2019, Sendai, Japan, Sendai, Japan.
92	Zeri, F, Moving a step ahead in Multifocal CL fitting. INVITED	5th Annual Palestinian Jordanian Optometry Conference., Arab American University- Ramallah, Palestine.
93	Zeri, F, Quale rapporto tra ametropie e contattologo nell'era di internet? INVITED	XIII Congresso Assottica, Roma.

#	Authors & Title	Conference/Workshop
94	Zeri, F, The Italian version of ICLC INVITED	IACLE Educator Meeting at EAEO 2019, Roma.
95	Zeri, F, The compliance issue: a missing link in CL complications? INVITED	5th Annual Palestinian Jordanian Optometry Conference., Arab American University- Ramallah Palestine.
96	Zorloni, G; Cova, F; Caresan, M; Vedda, A, Development of a prototype thermal neutron dosimeter based on a color-based quasi-digital neutron/ $\gamma$ discrimination.	19th International Conference on Solid State Dosimetry (SSD19), Hiroshima, Japan.

# BOOKS AND CONTRIBUTIONS

Authors	Title	Details
<b>Benedek, G</b>	High-Tc Superconductivity: the Erice Legacy	Nuovo Saggiatore 35, 47.
<b>Bonizzoni, L; Bruni, S; Castiglioni, I; Galli, A; Gargano, M; Interlenghi, M; Longoni, M; Martini, M; Passaretti, A; Salvatore, C</b>	Leonardeschi oltre il visibile	in Leonardo e la Madonna Litta (Skira, 2019)
<b>Caglioti, G; Benedek, G</b>	Graphics and Quantum Mechanics – The Necker Cube as a Quantum-Like Two-Level System	in ICGG 2018 - Proc. 18th Int. Conf. on Geometry and Graphics:Advances in Intelligent Systems and Computing 809, Ed. by L. Cocchiarella (Springer, 2019), pp. 161-172
<b>Martini, M; Fasoli, M</b>	Luminescence and Defects in Quartz	Advances in Physics and Applications of Optically and Thermally Stimulated Luminescence, Ed. R. Chen and V. Pagonis (World Scientific, 2019), Chapter 5 (pp. 173-204)
<b>Tavazzi, S; Parodi, A; Colciago, S; Nigrotti, G; Borghesi, S; Zeri, F</b>	Corneal Pachymetry and Endothelial Microscopy by Slit-Lamp	in Novel Diagnostic Methods in Ophthalmology (IntechOpen, 2019)
<b>Trifiletti, V; Manfredi, N</b>	Dye-Sensitized Solar Cells: Photophysics of Coordination Complex	in Emerging Photovoltaic Technologies: Photophysics and Devices, Ed. C.S. Ponseca jr. (CRC Press, 2019)

# PATENTS

Authors	Title	Details
<b>Grandi, S; Mustarelli, P; Nulli, A</b>	Sol-Gel Process for the Production of Silica Aerogels	Patent; Patent number US20190375644
<b>Monguzzi, A; Villa, C; Torrente, Y</b>	Nanocluster d'oro nel trattamento atassia di Friedreich	Patent (deposited)

# 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
Albani, M	Modeling of 3D heteroepitaxial structures by continuum approaches
Andreosso, I	Functionalization of unsaturated polymers backbone for tyre compounding application
Azadmand, M	PA-MBE Growth and Characterization of Nitride Semiconductors, from InGaN Thin-films to GaN and AlN Self-assembled Nanowires
Boldrini, C	Materials and devices for solar generation of electricity and fuels
Castiglioni, F	Design of Functional Porous Materials with Stimuli-Responsive Mobile Elements
Cristofalo, M	Nanomechanics of DNA and DNA-ligand interactions: focus on structural polymorphism and DNA condensation
Mostoni, S	From nanosized to single sites zinc-based activators for rubber vulcanization process
Tagliaro, I	Novel colloidal approach to prepare highly-loaded silica-based elastomeric nanocomposites
Tawfilas, M	Surface decoration of inorganic nanoparticles for novel polymer-based nanocomposite materials



# CONSULTANCY

<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
- Consultancy
- 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

## Consultancy

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

## Research Projects

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





## CUDAM

CENTRO UNIVERSITARIO DATAZIONI E ARCHEOMETRIA MILANO  
BICOCCA

[cudam.mater.unimib.it](http://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](mailto: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.



**ABCD**  
Centro Interdipartimentale  
per gli Studi di Genere

## 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](http://www.mibsolar.mater.unimib.it)

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

Main objectives of MIB-SOLAR are:

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

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

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

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 electronic 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 offers the possibility to use the service to all the staff of the University of Milano-Bicocca and other universities, to the staff belonging to public research centers for their institutional activities, as well as to the staff of no-profit centers. 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.



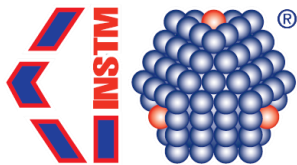
## **CNISM**

CONSORZIO NAZIONALE INTERUNIVERSITARIO PER LE SCIENZE FISICHE DELLA MATERIA

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



## GALATEA BIOTECH- THE WHITE BIOTECH COMPANY

<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](http://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](http://www.glasstopower.com)

**GLASS to POWER**

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.

