Scienza dei Materiali Materials Science

ANNUAL REPORT 2015

Università degli Studi di Milano-Bicocca



INDEX

THE MATERIALS SCIENCE DEPARTMENT	р.	2
NUMBERS	р.	7
RESEARCH	р.	8
PUBLICATIONS & PHD THESIS	р.	56
HIGHLIGHTS	р.	77
FUNDED PROJECTS	р.	82
PEOPLE	р.	84
RESEARCH FACILITIES	р.	88
DOWNTOWN	р.	97
TEACHING	р.	99
CREDITS	р.	110



THE MATERIALS SCIENCE DEPARTMENT

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

ABOUT US

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

The main research fields are:

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

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

STRATEGIC GOALS

General goals of the Materials Science Department include competitive Research & Development and Advanced Training, both in basic and applied research, in the field of new materials and their industrial applications.

Theoretical and experimental studies are carried out in several fields such as ionic conductors, electrochemistry, molecular electronics, laser, molecular modelling, insulator oxides, non-linear optics, polymers, semiconductors, sensors, organic and inorganic synthesis, superconductors, luminescence, glass, optical fibres. Beside the main spectroscopic and electrical characterization techniques, advanced materials analysis is achieved by means of many experimental techniques like AFM, STM, ESR, FIB, NMR and a number of other advanced optical, magnetic and electrical instrumentations.

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

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

The educational project aims at forming young professionals highly qualified in both physics and chemistry, able to fit their knowledge to the contemporary requirements of the related labour market. Milano-Bicocca University is in fact located in an area where highly specialized high-tech companies are abundant, offering stimulating employment opportunities in consolidated applications (nanotechnology, elastomers, polymers, insulators, semiconductors, ceramics) as well as in innovative materials (optical fibres, ionic conductors, superconductors, organic and inorganic semiconductors, materials for non linear optics, micro and opto-electronics, radiation detectors).

Degrees in Materials Science and in Chemical Science and Technology include a basic degree (Laurea, three years), followed by a possible two-year specializing course (Laurea Magistrale).

The three-years course of Optics and Optometry gives interesting professional opportunities.

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

BOARDING

DIRECTOR Marco Martini

DEPUTY DIRECTOR Franca Morazzoni

Alessandro Abbotto Marco Bernasconi Simona Binetti Alberto Paleari Luisa Raimondo Adele Sassella Emanuela Sibilia





DIDACTICS

Alessandro Abbotto Chemical Science Courses, Chairman

> Marco Bernasconi Students career commission

Farncesco Montalenti Study advisory

Dario Narducci Library Board, Chairman

Alberto Paleari Materials Science Courses, Chairman

Antonio Papagni Optics and Optometry Course, Coordinator

> Piero Sozzani Erasmus

Anna Vedda Thesis commission



NUMBERS 2015

PERSONNEL	#
Researchers	41
Administration/Didactics	3
Technical personnel	8
Post graduate	74
Total	126

FUNDINGS	£
PRIN-FIRB	381.240
EU	1.810.890
OTHER	984.870
Total	3.177.000



Organic and polymeric materials



Alessandro Abbotto

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

Luca Beverina

Functional dyes and pigments for photonics, electronics and optoelectronics

Massimo Moret

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

Antonio Papagni

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

Roberto Simonutti

Synthesis and characterization of novel polymeric nanostructures

Piero Sozzani

Nanostructured materials and magic angle spinning NMR

Materials for microelectronics and photonics



Marco Bernasconi

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

Emiliano Bonera, Emanuele Grilli, Stefano Sanguinetti

Optical spectroscopy and fabrication of semiconductors and semiconductor quantum structures

Silvia Tavazzi Optics and optometry

Adele Sassella Organic molecular films and heterostructures

Sergio Brovelli, Francesco Meinardi Photophysics of molecular semiconductors

Norberto Chiodini, Alberto Paleari, Anna Vedda

Oxide nanostructures and silica-based materials for optical technology

Marco Fanciulli

Materials and Spectroscopies for Nanoelectronics and Spintronics – MSNS Laboratory

Leo Miglio, Francesco Montalenti

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

Materials for energy and environment



Maurizio Acciarri, Simona Binetti, Dario Narducci

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

Gian Paolo Brivio

Theory and computations of adsorbate interfaces

Michele Catti

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

Angiolina Comotti

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

Cristiana Di Valentin, Livia Giordano, Gianfranco Pacchioni

Theory of oxide surfaces, interfaces, and supported clusters

Claudio Maria Mari, Riccardo Ruffo

Electrochemical activities

Franca Morazzoni, Roberto Scotti

Chemistry of inorganic and organometallic materials

Materials for cultural heritage

Anna Galli, Marco Martini, Emanuela Sibilia

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



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





ALESSANDRO ABBOTTO

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

ORGANIC AND HYBRID 3RD GENERATION PHOTOVOLTAICS

We investigate last generation organic and hybrid photovoltaics, namely:

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

Furthermore we study tandem multijunction cells in combination with silicon and thin film inorganic technologies, in order to access higher performances.

A large variety of materials (organic and organometallic dyes, electron and hole transporting materials, electrolytes, semiconductor oxides, electrodes) are investigated as well as lab-scale and pre-industrial photovoltaic panels.

ARTIFICIAL PHOTOSYNTHESIS: CLEAN AND RENEWABLE SOLAR FUELS

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

MAIN FACILITIES

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

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



Functional dyes and pigments for photonics, electronics and optoelectronics





LUCA BEVERINA

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

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

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

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



Crystal growth and characterization of organic and inorganic crystals





MASSIMO MORET

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

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

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

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

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



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





ANTONIO PAPAGNI

The current research interests are essentially focused on the development of organic materials for applications in photonics and optoelectronics; the main topic is the design and synthesis of semiconducting materials for alternative energy applications.

Organic solar cells (both bulk heterojunction solar cells and crystalline organic solar cells) are the main target and the research activity involves two different kinds of applications.

Bulk heterojunction solar cells (BHJSCs) are experiencing an impressive growth, both for the continuous increase of photoconversion efficiency (PCE) and for the increasing numbers of research groups and industrial players involved in this subject. The still increasing values of PCE are the result of a careful design of the active materials composing the core of BHJSC. The third generation of semiconducting materials for BHJSC is give by internal donor-acceptor conjugated polymers. The design of new electron-acceptors and the correct synthesis of donor-acceptor polymers based on them are currently undertaken exploiting the know-how in the field of fluorinated materials and also exploring alternative synthons. The fabrication of solar cells and their analysis is carried out in collaboration with Italian and European research centres and companies.

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

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



Synthesis and characterization of novel polymeric nanostructures





ROBERTO SIMONUTTI

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

NEW MATERIALS BASED ON BLOCK COPOLYMERS

Block copolymers are constituted by two or three different types of polymer chains connected at the ends with a covalent bond. They display self-organization on the nanometre scale modulated by the external environment. For example, the interaction between block copolymer and solvent produces a diversity of self assembled shapes, including vescicles, spheres, cylinders, that can be tuned by concentration, solvent polarity, temperature and other external stimuli. The morphology in the solid state can also be very complex and is finely tuned by the conditions and the method of solid formation (melt cooling, casting from solvent).

Recently, by implementing advanced polymerization techniques like RAFT (Reversible Addition-Fragmentation chain Transfer polymerization) we synthesized several samples of highly controlled amphiphilic block copolymers. Our interest is currently focused on innovative techniques for their characterization in liquid and solid state, as well as the almost unexplored intermediate soft matter states: highly concentrated solutions, gels and sponge-like materials.

NANOPARTICLE POLYMER NANOCOMPOSITES

The mixing of polymers and inorganic nanoparticles, like oxides, semiconductors (usually defined as quantum dots) or noble metals, is opening pathways for engineering flexible composites that exhibit advantageous electrical, optical, or mechanical properties. In particular, the nanocomposite optical characteristics, as the refractive index, absorption of UV light, birefringence or scattering properties, can be modulated by carefully choosing the particle size and electronic structure of the nanoparticle used for its preparation.

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

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

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



Nanostructured materials and magic angle spinning NMR







SILVIA BRACCO, PIERO SOZZANI

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

CURRENT RESEARCH PROJECTS

Composite materials based on ceramics and polymers and characterization of heterogeneous interfaces (elastomeric materials reinforced with silica, in-situ formation of silica by gelification in polymer matrices). Confinement of molecules and macromolecules to cylindrical nano- and mesotubes (cross section of 0.5, 1 and over 30 nm). Some matrices, showing extended interactive areas (>1200 m²/g), form supramolecular adducts endowed with unusual properties (liquid-crystalline behaviour, anomalous glass-transition, conformational solitons propagating along the polymer-chains even at very low temperature). The study of reactivity and interactions among included species in molecular vessels is also addressed (gamma ray initiated polymerization). Preparation of end-functionalized polymers to be reactive onto heterogeneous materials. Crystal morphology, defects and mesomorphysm of polymeric materials (ethylene-propylene copolymers). Diffusion processes of gases into materials and exploitation of spin-active gases (¹²⁹Xe) diffusing into solids, for microphases determination and nanoporosity by NMR.

FACILITIES

NMR Bruker Avance with wide bore 7.05 Tesla superconduction magnets fully equipped for high power output, 7kHz and 15kHz magic angle spinning probes and several heads for wide-line spectroscopy, including deuterium. High vacuum (10⁻⁹ torr) pump and equipment for hyperpolarized Xenon spectroscopy -laser excited NMR). Dynamic Mechanical Analyzer, Differential Scanning Calorimetry Gel Permeation Cromatography and access to large NMR facilities.



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





MARCO BERNASCONI

PHASE CHANGE MATERIALS FOR DATA STORAGE

Phase change materials ($Ge_2Sb_2Te_5$ and related telluride alloys) are attracting an increasing interest worldwide for applications in optical disks (DVDs) and in a novel non volatile electronic memory, the phase change memory cell. Both applications rely on a fast (10-100 ns) and reversible transformation between the crystalline and amorphous phases induced by heating. The two states of the memory can be discriminated thanks to the large contrast in electronic conductivity and optical reflectivity between the two phases.

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

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

SURFACE PHONONS AND TOPOLOGICAL INSULATORS

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





Optical spectroscopy and fabrication of semiconductors and semiconductor quantum structures





EMILIANO BONERA, EMANUELE GRILLI, STEFANO SANGUINETTI

Our research is mainly devoted to the experimental study of the optical properties of both group IV and group III-V semiconductors and quantum structures of interest for micro- and opto-electronics. Most of our research is carried out in within the L-NESS interuniversity Centre.

SiGe HETEROSTRUCTURES

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

1. Using Raman and photoluminescence we study the correlations between growth conditions and system properties. We analyse the effects of strain, composition and dimensionality on the vibrational and electronic properties of the heterostructures.

2. The vibrational properties of SiGe nanostructures, mainly quantum dots, are currently under study by Raman and micro-Raman measurements.

3. The electronic properties of Ge/SiGe multiple quantum wells are studied by transmission and photoluminescence measurements in a wide temperature range.

4. Electron spin sensitive measurements on Ge/SiGe structures are performed; the photoluminescence with light polarization control is studied.

QUANTUM STRUCTURES BASED ON III-V SEMICONDUCTORS

Amongst the nanoscience advancements, relevant place is taken by quantum confinement effects that take place in semiconductor quantum dots (QDs). Like the natural atoms QDs show discrete energy levels. Laser, infrared photodetectors, as well as third generation photovoltaic cells show can be improved by the use of QDs in the active layer. The study of QD-based devices has provided new ways for the understanding of strongly correlated few electrons/excitons systems and their possible applications, such as single-electron devices and single photon emitters for quantum cryptography and computation.

1. We develop innovative growth procedures for the fabrication quantum nanostructures with ad-hoc designed electronic properties;

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

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

FACILITIES

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







Optics and Optometry





SILVIA TAVAZZI

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

MATERIALS FOR CONTACT LENSES

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

OPTICAL SYSTEMS

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

FACILITIES

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



Organic molecular films and heterostructures





Adele Sassella

Thin film growth. Films of organic molecular semiconductors are grown by organic molecular beam epitaxy (OMBE) under different conditions, such as pressure, substrate type and temperature, absence or presence of external fields. The study of the OMBE growth process itself is carried out by detecting in situ and in real time the properties of the growing samples. The main interest rests in the intrinsic properties of 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. 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. In the frame of well established collaborations, the structure of the thin films is checked by X-ray diffraction and, for some materials, the transport properties determined

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

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

FACILITIES

The OMBE apparatus consists of several ultra-high vacuum chambers where up to six sources can be installed for depositing different compounds; during OMBE growth, the film thickness is monitored insitu by a quartz microbalance and its optical behavior by RAS. Optical spectroscopies, such as absorption, reflection, photoluminescence and ellipsometry, are used for the study of thin films and multilayers ex-situ, also in comparison with the properties detected in-situ by RAS. Optical measurements can be carried out as a function of temperature, down to few K, under polarized light and at different incidence angles. Atomic force microscopy is used ex-situ for the morphology characterization of all the samples and for the study of the film growth process; morphology is usually checked over sereval μm^2 wide regions, while on crystalline samples molecular resolution is also achievable.



Photophysics of molecular semiconductors







SERGIO BROVELLI, FRANCO MEINARDI

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

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

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

FACILITIES

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



Oxide nanostructures and silica-based materials for optical technology











NORBERTO CHIODINI, MAURO FASOLI, ALBERTO PALEARI, ANNA VEDDA

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

RESEARCH LINES

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

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

FACILITIES

SPECTROSCOPY LABORATORY: optical absorption, photo- thermo- and radio-luminescence spectroscopy, micro-Raman scattering, refractive index and film thickness measurements, thermostimulated currents and complex impedance spectroscopy. Micro-ATR-FTIR analysis, micro-profilometryr, pulsed luminescence spectroscopy and SHG by Nd-YAG laser with second and fourth harmonics.

SYNTHESIS LABORATORY: inorganic chemistry laboratory for sol-gel preparations in controlled conditions, comprising hoods and dry-boxes for the synthesis of bulk samples and films. Film deposition by spin-coating. Samples from aerogel can also be obtained by hypercritical drying process. Furnaces for densification processes in controlled temperature and atmosphere, as well as instrumentation for optical finishing.


Materials and Spectroscopies for Nanoelectronics and Spintronics





MARCO FANCIULLI

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

RESEARCH LINES

Si and Ge nanostructures

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

Semiconductor/oxide interfaces

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

Point defects in semiconductors and oxides

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

FACILITIES

Growth and processing

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

Characterization

- Three CW X-band systems for electron spin resonance (ESR) spectroscopy, electrically detected spin resonance spectroscopy (EDMR) and electron nuclear double resonance spectroscopy (ENDOR). Variable temperature measurements (4-600 K).
- Multi-frequency (0.1-40 GHz) EDMR.
- Set-up for inelastic electron tunneling spectroscopy (IETS) working in the temperature range 4-300 K.
- Electrical measurements: I-V, C-V, C-t



Modeling and simulations of epitaxial semiconductor depositions and nanostructures





LEO MIGLIO, FRANCESCO MONTALENTI

Deposition of Ge (or SiGe alloys) on Si leads to a wealth of different phenomena, mostly caused by the elastic energy unavoidably accumulated when trying to epitaxially grow one material (Ge) on a substrate (Si) with a different lattice parameter. In our group, we investigate such phenomena by formulating interpretative models based on computer simulations.



For example, we are interested in understanding strain-release triggered formation, stability, morphological evolution, and ordering of Ge nanostructures (islands), including the effect of Si/Ge intermixing. A combination of different methods is needed to achieve this goal. If atomistic Kinetic Monte Carlo and/or continuum models are needed to describe growth kinetics, thermodynamic aspects can be tackled by a synergic use of Density Functional Theory, providing surface energies, and classical molecular dynamics simulations or elasticity theory (numerically solved by Finite Element Methods), used to establish the volumetric elastic energy.

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

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

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



Photovoltaics and Thermoelectrics











NANOTECHNOLOGY FOR THERMOELECTRICITY

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

SILICON FOR SOLAR CELLS

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

INORGANIC SEMICONDUCTOR THIN FILMS FOR PHOTOVOLTAICS

In collaboration with a small company we have recently developed a new, original method for chalcogenide thin film (CIGS) deposition on glass and flexible substrates, like plastic foils. This system is based on an innovative hybrid sputtering-evaporation approach combining the advantages of both growth techniques. First of all, such a growth apparatus allows to effectively controlling the metal compositional ratios also in an industrial process on large area substrates, as they only depend on the amount of metals deposited during the sputtering step. Furthermore, the implementation of an evaporation step allows the achievement of metal ratio in-depth profiles typical of three-stage grown CIGS layers. Last but not least, both the use of single metal targets and the extremely controlled nature of the sputtering deposition (which occurs in a Se vapours-free zone) allow a reduction of the costs. In the last few years, a possible alternative to CIGS PV thin film where more abundant and less expensive elements like Zn and Sn are used in place of In and Ga, namely Cu₂ZnSnS₄ (CZTS), was considered, too. Two main growth methods are under investigation and testing: sputtering process and chemical methods (i.e. dip coating, spray pyrolysis).



Theory and computations of low dimensional materials





GIAN PAOLO BRIVIO

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

EFFECTS OF THERMAL FLUCTUATIONS IN ABSORPTION OF DYE MOLECULES ON TITANIUM OXIDES.

The adsorption of catechol and isonicotinic acid on the TiO_2 anatase (101) and rutile (110) surfaces has been tackled at room temperature by means of first-principles molecular dynamics simulations and time-dependent DFT calculations. Our results on the absorption coefficient explain how thermal fluctuations induce dye sensitization depending on the hybridization between the dye and the TiO_2 states.

FEMTOMAGNETISM OF CORE EXCITED FUNCTIONALIZED GRAPHENE

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

COMPLEX STOCHIOMETRY OF POTASSIUM DOPED PTCDA ON METALS

Alkali metal atoms are a simple yet efficient n-type dopant of organic semiconductors. With a joint theoretical effort between this Group and that of E. Zojer (TU Graz) following the experiments performed at the Group of T. Fritz (Jena Univ.), we found that that potassium intercalation into PTCDA monolayer domains on a Ag(111) induces distinct stoichiometry-dependent structural reordering processes, resulting in highly ordered and large K_xPTCDA domains and large stable monolayer domains are found for x=2,4.



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





Michele Catti

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

EXPERIMENTAL

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

COMPUTATIONAL

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

RESULTS

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

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



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





ANGIOLINA COMOTTI

The research activity deals with the generation of frameworks containing one-, two- and three-dimensional confined spaces with uniform and precisely engineered geometries to create new environments for storage of chemical entities. The study is focused on new materials with nanoscale architectures for storage of important gases such as methane and hydrogen considered as clean fuels, carbon dioxide that is an intermediate product in the hydrogen production processes, and pollutant vapours, especially benzene. The construction of stable and robust ionic, inorganic and hybrid frameworks with 3D periodic motifs can increase separation, capture and storage of small gases. These frameworks can arrange sites and receptors into arrays for controlling and interacting with gas species. The advantages of the novel materials will be compared with the conventional material properties for obtaining the basis of patent applications.

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







Theory of oxide surfaces, interfaces, supported clusters





CRISTIANA DI VALENTIN, LIVIA GIORDANO, GIANFRANCO PACCHIONI

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

OXIDE SURFACE AND THIN OXIDE FILMS

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



SUPPORTED CLUSTERS

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

DEFECTS AND DOPANTS IN OXIDES

Nature of point defects in oxide materials for photocatalysis, photoelectrochemistry, microelectronics, fiber optics etc., in particular amorphous and crystalline TiO₂, ZnO, WO₃, SiO₂, alkaline earth oxides. The activity is directed toward the determination of stability, structure, and spectral properties of intrinsic and extrinsic point defects (vacancies, metal and non-metal dopants, codopants, hydroxyl groups, trapped electrons, etc.) and their interplay through charge transfer processes. Particular attention is devoted to the study of optical absorption for activation in the visible region and of electron spin resonance spectra for identification of paramagnetic centres.

CHEMICALLY MODIFIED GRAPHENE AND CARBON BASED NANOSTRUCTURES

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



Electrochemical activities





CLAUDIO MARI, RICCARDO RUFFO

Since the birth of the Department, the group is active in fields of Energy Storage and Production, Gas Sensing, and characterization of Organic Molecular or Polymeric Materials. Group facilities comprise a fully equipped electrochemical lab with several potentiostats-galvanostats, two multichannel systems for long time testing, two semi-automatic glove boxes at N₂ or Ar, a climatic chamber to control temperature and humidity, optical fibers coupled with UV-visible spectrophotometer for *in-situ* spectroelectrochemistry, and a quartz crystal electrochemical microbalance. Furnaces, thick/thin film applicators, and standard chemical equipments are available for chemical synthesis and electrode formulations.



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

MATERIAL FOR GAS SENSORS

Potentiometric or amperometric solid state electrochemical gas sensor are investigated and realized to determine the composition of CO/CO_2 or H_2/H_2O gas mixtures and the concentration of CO or H_2O or SO_2 in air as well as CI_2 or O_2 or CO_2 in nitrogen and air. Moreover, nanostructured thin film semiconductor gas sensors of pure or noble metal doped semiconductors prepared via sol gel or dip coating technique, were used as sensing elements to determine low concentration of reducing gas (CO). The experimental measurements pointed out the strong correlation among the electrical properties, the point defects, the amount of doping level, and the morphology.

MATERIAL FOR ORGANIC OPTOELECTRONICS

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



Chemistry of inorganic and organometallic materials







NANOSTRUCTURED OXIDES AND ORGANIC-INORGANIC HYBRID MATERIALS FOR PHOTOCATALYTIC APPLICATIONS

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

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

SHAPE CONTROLLED INORGANIC FILLERS FOR AUTOMOTIVE RUBBER NANOCOMPOSITES

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

EQUIPMENTS

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

LINK: NanoMat-Lab Unimib - Facebook



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







THE ARCHAEOMETRY LAB

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

For what concerns the dating techniques, thermoluminescence (TL) and optically stimulated luminescence (OSL) are used to determine the event of ceramics firing and sediment deposition respectively. Other available techniques are dendrochronology (dating of wood) and radiocarbon (preparation of samples for Accelerator Mass Spectrometry, AMS, to evaluate the concentration of ¹⁴C atoms in organic remains). The laboratory is member of the CUDAM (Centro Universitario Datazioni e Archeometria Università di Milano Bicocca, http://cudam.mater.unimib.it).

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



MAIN ACTIVITIES

Fundamental study of the low temperature TL peak in quartz and of the Pre-dose effect **S**tudy of the optical properties of mosaic glasses **S**tudy of charge transfer phenomena in guartz and feldspars luminescence.

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

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

Surface dating

Study and characterisation of natural materials for accident dosimetry

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



PUBLICATIONS TALKS THESIS

Distribution of articles by impact factor (IF)



PUBLICATIONS ON INTERNATIONAL JOURNALS

#	Authors.	IF
#	Title. CITATION.	(ISI)
	Abatangelo, L; Felli, V.	
1	Sharp asymptotic estimates for eigenvalues of Aharonov-Bohm operators with varying poles.	1,5
	CALCULUS OF VARIATIONS AND PARTIAL DIFFERENTIAL EQUATIONS 54, 3857.	
	Albanese, E; Di Valentin, C; Pacchioni, G; Sauvage, F; Livraghi, S; Giamello, E.	
2	Nature of Paramagnetic Species in Nitrogen-Doped SnO2: A Combined Electron Paramagnetic	4,8
	Resonance and Density Functional Theory Study. JOURNAL OF PHYSICAL CHEMISTRY C 119, 26895.	
2	Baby, A; Fratesi, G; Vaidya, S; Patera, L; Africh, C; Floreano, L; Brivio, G.	1.8
5	Anchoring and bending of pentacene on aluminum (001). J OURNAL OF PHYSICAL CHEMISTRY C 119.	4,0
	Baby, A; Lin, H; Brivio, G; Floreano, L; Fratesi, G.	
4	Core-level spectra and molecular deformation in adsorption: V-shaped pentacene on Al(001).	2,7
	BEILSTEIN JOURNAL OF NANOTECHNOLOGY 2015, 2242	
	Baldoli, C; Bertuolo, S; Licandro, E; Viglianti, L; Mussini, P; Marotta, G; Salvatori, P; De Angelis, F;	
5	Manca, P; Manfredi, N; Abbotto, A.	4.0
	Benzodithiophene based organic dyes for DSSC: Effect of alkyl chain substitution on dye efficiency.	7,0
	DYES AND PIGMENTS 121, 351.	
	Baroncini, M; D'Agostino, S; Bergamini, G; Ceroni, P; Comotti, A ; Sozzani, P ; Bassanetti, I; Grepioni, F;	
6	Hernandez, T; Silvi, S; Venturi, M; Credi, A.	25.3
	Photoinduced reversible switching of porosity in molecular crystals based on star-shaped azobenzene	23,5
	tetramers. NATURE CHEMISTRY 7, 634.	
	Basagni, A; Ferrighi, L ; Cattelan, M; Nicolas, L; Handrup, K; Vaghi, L; Papagni, A ; Sedona, F; Di	
7	Valentin, C; Agnoli, S; Sambi, M.	6.8
	On-surface photo-dissociation of C-Br bonds: Towards room temperature Ullmann coupling.	0,0
	CHEMICAL COMMUNICATIONS 51, 12593.	
	Basiricò, L; Ciavatti,A; Sibilia,M; Fraleoni-Morgera, A; Trabattoni, S; Sassella, A ; Fraboni, B.	
8	Solid state organic X-ray detectors based on rubrene single crystals.	1,3
	IEEE TRANSACTIONS ON NUCLEAR SCIENCE 62, 1791.	
	Bietti, S; Bocquel, J; Adorno, S; Mano, T; Keizer, J; Koenraad, P; Sanguinetti, S.	
9	Precise shape engineering of epitaxial quantum dots by growth kinetics.	3,7
	PHYSICAL REVIEW B 92, 75425.	
	Bietti, S; Esposito, L; Fedorov, A; Ballabio, A; Martinelli, A; Sanguinetti, S.	
10	Characterization and Effect of Thermal Annealing on InAs Quantum Dots Grown by Droplet Epitaxy on	2,7
	GaAs(111)A Substrates. NANOSCALE RESEARCH LETTERS 10, 247.	

	Binetti, S; Garattini, P; Mereu, R; Le Donne, A; Marchionna, S; Gasparotto, A; Meschia, M; Pinus, I;	
11	Acciarri, M.	2.2
11	Fabricating Cu(In,Ga)Se ₂ solar cells on flexible substrates by a new roll-to-roll deposition system	2,2
	suitable for industrial applications. SEMICONDUCTOR SCIENCE AND TECHNOLOGY 30, 105006.	
4.2	Binetti, S; Gonik, M; Le Donne, A; Croel, A.	47
12	Silicon samples grown under reduced melt convection. JOURNAL OF CRYSTAL GROWTH 417, 9.	1,7
-	Bollani, M; Chrastina, D; Gagliano, L; Rossetto, L; Scopece, D; Barget, M; Mondiali, V; Frigerio, J;	
12	Lodari, M; Pezzoli, F; Montalenti, F; Bonera, E.	2.2
13	Local uniaxial tensile strain in germanium of up to 4% induced by SiGe epitaxial nanostructures.	3,3
	APPLIED PHYSICS LETTERS 107, 083101.	
	Bongi, M;; Fasoli, M; Gregorio, A;; Vedda, A; Zampa, G; Zampa, N; Zerbo, B.	
14	CALOCUBE: An approach to high-granularity and homogenous calorimetry for space based detectors.	
	JOURNAL OF PHYSICS, CONFERENCE SERIES 587, 012029.	
4 5	Bouzid, A; Gabardi, S; Massobrio, C; Boero, M; Bernasconi, M.	2.7
15	First-principles study of amorphous Ga_4Sb6Te_3 phase-change alloys. PHYSICAL REVIEW B 91, 184201.	3,7
	Bracco, S; Beretta, M; Cattaneo, A; Comotti, A; Falqui, A; Zhao, K; Rogers, C; Sozzani, P.	
16	Dipolar Rotors Orderly Aligned in Mesoporous Fluorinated Organosilica Architectures.	11,3
	ANGEWANDTE CHEMIE 54m 4773.	
	Bussetti, G; Campione, M; Sassella, A; Duò, L.	
17	Optical and morphological properties of ultra-thin H_2 TPP, H_4 TPP, and ZnTPP films.	1,5
	PHYSICA STATUS SOLIDI B 252, 100.	
	Campi, D; Baldi, E; Graceffa, G; Sosso, G; Bernasconi, M.	
18	Electron-phonon interaction and thermal boundary resistance at the interfaces of Ge ₂ Sb ₂ Te ₅ with	2,3
	metals and dielectrics. JOURNAL OF PHYSICS.: CONDENSED MATTER 27, 175009.	
10	Campi, D; Bernasconi, M; Benedek, G; Toennies, J.	4.0
19	Surface Dynamics of Xe(111): An Ambiguous Nobility. JOURNAL OF PHYSICAL CHEMISTRY C 119.	4,8
	Campi, D; Donadio, D; Sosso, G; Behler, J; Bernasconi, M.	
20	Electron-phonon interaction and thermal boundary resistance at the crystal-amorphous interface of	2,2
	the phase change compound GeTe. JOURNAL OF APPLIED PHYSICS 117, 015304.	
	Campione, M; Capitani, G; Raimondo, L; Sassella, A.	
21	Porphyrin Nanowires with Epitaxially Locked Uniaxial Orientation. JOURNAL OF PHYSICAL CHEMISTRY	4,8
	C, 119, 18210.	
	Canevali, C; Alia, M; Fanciulli, M; Longo, M; Ruffo, R; Mari, C.	
22	Influence of doping elements on the formation rate of silicon nanowires by silver-assisted chemical	2,0
	etching. SURFACE & COATINGS TECHNOLOGY 280, 37.	
	Caravati, S; Bernasconi, M.	
23	Influence of the exchange and correlation functional on the structure of amorphous $\text{Ge}_2\text{Sb}_2\text{Te}_5$.	1,5
	PHYSICA STATUS SOLIDI B 252, 260.	

		T
	Cargnello, M; Sala, D; Chen, C; D'Arienzo, M ; Gorte, R; Murray, C.	
24	Structure, morphology and catalytic properties of pure and alloyed Au-ZnO hierarchical	3,8
	nanostructures. RSC ADVANCES 5, 41920.	
	Castelli, A; Meinardi, F; Pasini, M; Galeotti, F; Pinchetti, V; Lorenzon, M; Manna, L; Moreels, I;	
25	Giovanella, U; Brovelli, S.	13.6
	High-Efficiency All-Solution-Processed Light-Emitting Diodes Based on Anisotropic Colloidal	13,0
	Heterostructures with Polar Polymer Injecting Layers. NANO LETTERS 15, 5455.	
	Catti, M; Pinus, I; Knight, K.	
26	Lithium insertion properties of $Li_x TiNb_2O_7$ investigated by neutron diffraction and first-principles	2,1
	modelling. JOURNAL OF SOLID STATE CHEMISTRY 229, 19.	
	Cecconi, B; Manfredi, N; Ruffo, R; Montini, T; Romero-Ocaña, I; Fornasiero, P; Abbotto, A.	
27	Tuning thiophene-based phenothiazines for stable photocatalytic H_2 production. CHEMSUSCHEM 8.	7,7
	Celebrano, M; Baselli, M; Bollani, M; Frigerio, J; Bahgat Shehata, A; Della Frera, A; Tosi, A; Farina, A;	
28	Pezzoli, F; Osmond, J; Wu, X; Hecht, B; Sordan, R; Chrastina, D; Isella, G; Duò, L; Finazzi, M; Biagion, P.	
	Emission engineering in germanium nanoresonators. ACS PHOTONICS 2, 53.	
	Chen, H; Tosoni, S; Pacchioni, G.	
29	Hydrogen Adsorption, Dissociation, and Spillover on Ru-10 Clusters Supported on Anatase TiO ₂ and	9,3
	Tetragonal ZrO ₂ (101) Surfaces. ACS CATALYSIS 5, 5486	,
	Chen, H; Tosoni, S; Pacchioni, G.	
30	Adsorption of Ruthenium Atoms and Clusters on Anatase TiO ₂ and Tetragonal $ZrO_2(101)$ Surfaces: A	4,8
	Comparative DFT Study. JOURNAL OF PHYSICAL CHEMISTRY C 119, 10856.	
	Christodoulou, S; Rajadell, F; Casu, A; Vaccaro, G; Grim, J; Genovese, A; Manna, L; Climente, J;	
24	Meinardi, F; Rainò, G; Stöferle, T; Mahrt, R; Planelles, J; Brovelli, S; Moreels, I.	44 5
31	Band structure engineering via piezoelectric fields in strained anisotropic CdSe/CdS nanocrystals.	11,5
	NATURE COMMUNICATIONS 6, 7905.	
	Ciriello, F; Gualtieri, M; Longhin, E; Ruffo, R; Camatini, M; Parenti, P.	
32	A new method and tool for detection and quantification of PM oxidative potential.	2,8
	ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH 22, 12469.	
	Coghi, P; Papagni, A ; Pò, C; Calabrese, A; Tacca, A; Aavoini, A; Stuknyte, M.	
33	Reactivity of decafluorobenzophenone and decafluoroazobenzene towards aromatic diamines: A	3,1
	practical entry to donor-acceptor systems. NEW JOURNAL OF CHEMISTRY 39, 3615.	
	Comotti, A; Bracco, S; Beretta, M; Perego, J; Gemmi, M; Sozzani, P.	
34	Confined Polymerization in Highly Ordered Mesoporous Organosilicas. CHEMISTRY-A EUROPEAN	5,7
	JOURNAL 21, 18209.	
	Crippa, A; Tagliaferri, M; Rotta, D; De Michielis, M; Mazzeo, G; Fanciulli, M; Wacquez, R; Vinet, M;	
35	Prati, E.	3,7
	Valley blockade and multielectron spin-valley Kondo effect in silicon. PHYSICAL REVIEW B 82, 035424.	
36	Cui, Y; Tosoni, S; Schneider, W; Pacchioni, G ; Nilius, N; Freund, H.	75
	Phonon-Mediated Electron Transport through CaO Thin Films. PHYSICAL REVIEW LETTERS 114.	,,,

	D'Arienzo, M; Dozzi, M; Redaelli, M;Di Credico, B; Morazzoni, F; Scotti, R; Polizzi, S.	
37	Crystal Surfaces and Fate of Photogenerated Defects in Shape-Controlled Anatase Nanocrystals:	
	Drawing Useful Relations to Improve the H ₂ Yield in Methanol Photosteam Reforming.	4,8
	JOURNAL OF PHYSICAL CHEMISTRY C 119, 12385.	
	Di Credico, B; Bellobono, I; D'Arienzo, M; Fumagalli, D; Redaelli, M;Scotti, R; Morazzoni, F.	
38	Efficacy of the Reactive Oxygen Species Generated by Immobilized TiO ₂ in the Photocatalytic	1,6
	Degradation of Diclofenac, INTERNATIONAL JOURNAL OF PHOTOFNERGY 2015, 919217.	,
	Di Valentin. C: Fittipaldi. D: Pacchioni. G.	
39	Methanol Oxidation Reaction on α -Tunasten Carbide Versus Platinum (1 1 1) Surfaces: A DFT	4.6
	Electrochemical Study. CHEMCATCHEM 7. 3533.	<i>y</i> -
	Dotti, N; Sarti, F; Bietti, S; Azarov, A; Kuznetsov, A; Biccari, F; Vinattieri, A; Sanguinetti, S; Abbarchi,	
	M; Gurioli, M.	
40	Germanium-based quantum emitters towards a time-reordering entanglement scheme with	3,7
	degenerate exciton and biexciton states. PHYSICAL REVIEW B 91, 205316.	
	Etacheri, V; Di Valentin, C ; Schneider, J; Bahnemann, D; Pillai, S.	
41	Visible-light activation of TiO ₂ photocatalysts: Advances in theory and experiments.	16,1
	IOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY C: PHOTOCHEMISTRY REVIEWS 25, 1	- /
	Etzelstorfer, T: Ahmadpor Monazam, M: Cecchi, S: Kriegner, D: Chrastina, D: Gatti, E: Grilli, E :	
	Rosemann, N: Chatteriee, S: Holý, V: Pezzoli, F: Isella, G: Stangl, J.	
42	Structural investigations of the α 12 Si-Ge superstructure. JOURNAL OF APPLIED CRYSTALLOGRAPHY	4,0
	48, 262.	
	Fall, M; Felli, V.	
43	Unique continuation properties for relativistic Schrödinger operators with a singular potential.	1,0
	DISCRETE AND CONTINUOUS DYNAMICAL SYSTEMS 35, 5827.	
	Fanciulli, M; Belli, M; Paleari, S; Lamperti, A; Molle, A; Sironi, M; Pizio, A.	
44	Defects and Dopants in Silicon and Germanium Nanowires. ECS TRANSACTIONS 5, 3138	
	Fanelli, L; Felli, V ; Fontelos, M; Primo, A.	
45	Time Decay of Scaling Invariant Electromagnetic Schrödinger Equations on the Plane.	2,1
	COMMUNICATIONS IN MATHEMATICAL PHYSICS 337, 1515.	
	Favaro, M; Ferrighi, L; Fazio, G; Colazzo, L; Di Valentin, C; Durante, C; Sedona, F; Gennaro, A; Agnoli,	
16	S; Granozzi, G.	93
40	Single and Multiple Doping in Graphene Quantum Dots: Unraveling the Origin of Selectivity in the	5,5
	Oxygen Reduction Reaction. ACS CATALYSIS 5, 129.	
	Fazio, G; Ferrighi, L; Di Valentin, C.	
47	Spherical versus Faceted Anatase TiO ₂ Nanoparticles: A Model Study of Structural and Electronic	4,8
	Properties. JOURNAL OF PHYSICAL CHEMISTRY C 119, 20735.	
	Ferraro, E; De Michielis, M; Fanciulli, M; Prati, E.	
48	Effective Hamiltonian for two interacting double-dot exchange-only qubits and their controlled-NOT	1,9
	operations. QUANTUM INFORMATION PROCESSING 14, 47.	

 49 Oxygen reactivity on pure and B-doped graphene over crystalline Cu(111). Effects of the dopant and of the metal support. SURFACE SCIENCE 634, 68. Ferrighi, L; PS, I, Nguyen, T; Cattelan, M; Nappini, S; Basagni, A; Parravicini, M; Papagni, A; Sedona, F; Magnano, E; Bondino, F; Di Valentin, C; Agnoli, S. Control of the intermolecular coupling of dibromatetracene on Cu(110) by the sequential activation of C-Br and C-H bands. CHEMISTRY-A EUROPEAN JOURNAL 21, 5826. Ferrighi, L; PK, I, Trioni, M; Di Valentin, C Baron-doped, nitrogen-doped, and codoped graphene on Cu(111): A DFT + vdW study. JOURNAL OF PHYSICAL CHEMISTRY C 119, 6056. Gabardi, S; Caravati, S; Sosso, G; Behler, J; Bernasconi, M Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. PHYSICAL REVIEW B, 92, 54201. Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. ADVANCED OPTICAL MATERIALS 3, 1164. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Pacchioni, G. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Pacchioni, G. Gerosa, M; Butani, C; Caramella, L; Onida, G; Pacchioni, G. Goronz, C, Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. Goronz, M; Buttani, C; Dindan, G; Pacchioni, S, Di Valentin, C; Pacchioni, G. Goronz, M; Du Valentin, C; Battani, C; Onida, G; Pacchioni, S, Di v		Ferrighi, L; Di Valentin, C.	
the metal support. SURFACE SCIENCE 634, 68. Ferrighi, L; PIS, I; Nguyen, T; Cattelan, W; Nappini, S; Basagni, A; Parravicini, M; Papagni, A; Sedona, F; Magnano, E; Bondino, F; Di Valentin, C; Agnoli, S. 50 Control of the intermolecular coupling of dibromotetracene on Cu(110) by the sequential activation of C-Br and C-H bonds. CHEMISTRY-A EUROPEAN JOURNAL 21, 5826. 5.7 Ferrighi, L; Trioni, M; Di Valentin, C Boron-doped, nitrogen-doped, and codoped graphene on Cu(111): A DFT + vdW study. 4.8 JOURNAL OF PHYSICAL CHEMISTRY 119, 6056. Gabardi, S; Caravati, S; Sosso, G; Behler, J; Bernasconi, M 3.7 Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. PHYSICAL REVIEW B, 92, 54201. 3.7 Sa Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. ADVANCED OPTICAL MATERIALS 3, 1164. 4.1 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3.7 PHYSICAL REVIEW B 91, 15S201. 9.1 9.2 9.2 9.3 </td <td>49</td> <td>Oxygen reactivity on pure and B-doped graphene over crystalline Cu(111). Effects of the dopant and of</td> <td>1,9</td>	49	Oxygen reactivity on pure and B-doped graphene over crystalline Cu(111). Effects of the dopant and of	1,9
Ferrighi, L; Píš, I; Nguyen, T; Cattelan, M; Nappini, S; Basagni, A; Parravicini, M; Papagni, A; Sedona, F; Magnano, E; Bondino, F; Di Valentin, C; Agnoli, S. 5.7 50 Control of the intermolecular coupling of dibromotetracene on Cu(110) by the sequential activation of C-Br and C-H bonds. CHEMISTRY-A EUROPEAN JOURNAL 21, 5826. 5.7 51 Boron-doped, nitrogen-doped, and codoped graphene on Cu(111): A DFT + vdW study. JOURNAL OF PHYSICAL CHEMISTRY C 119, 6056. 4.8 52 Gabardi, S; Caravati, S; Sosso, G; Behler, J; Bernasconi, M Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. PHYSICAL REVLEW B, 92, 54201. 3.7 53 Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. ADVANCED OPTICAL MATERIALS 3, 1164. 4.1 54 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3.7 55 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3.0 56 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3.0 57 Al- and Ga-Doped TiO ₂ . ZrO ₂ and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. <td< td=""><td></td><td>the metal support. SURFACE SCIENCE 634, 68.</td><td></td></td<>		the metal support. SURFACE SCIENCE 634, 68.	
Magnano, E; Bondino, F; Di Valentin, C; Agnoli, S. 5,7 Control of the intermolecular coupling of dibromatetracene on Cu(110) by the sequential activation of C-Br and C-H bonds. CHEMISTRY-A EUROPEAN JOURNAL 21, 5826. 5,7 Ferrighi, L; Trioni, M; Di Valentin, C 8000-doped, nitrogen-doped, and codoped graphene on Cu(111): A DFT + vdW study. 4,8 JOURNAL OF PHYSICAL CHEMISTRY C 119, 6056. 3,7 Gabardi, S; Caravati, S; Sosso, G; Behler, J; Bernasconi, M 3,7 Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. 3,7 PHYSICAL REVIEW B, 92, 54201. Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. 4,1 ADVANCED OPTICAL MATERIALS 3, 1164. 4,1 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,7 FHYSICAL REVIEW B 91, 155201. 3,7 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 Gerosa, M; Bottani, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 3,0 Go		Ferrighi, L; Píš, I; Nguyen, T; Cattelan, M; Nappini, S; Basagni, A; Parravicini, M; Papagni, A; Sedona, F;	
S0 Control of the intermolecular coupling of dibromotetracene on Cu(110) by the sequential activation of C-Br and C-H bonds. CHEMISTRY-A EUROPEAN JOURNAL 21, 5826. 5,7 Ferrighi, L; Trioni, M; Di Valentin, C 8 S1 Boron-doped, nitrogen-doped, and codoped graphene on Cu(111): A DFT + vdW study. 4,8 JOURNAL OF PHYSICAL CHEMISTRY C 119, 6056. 3,7 S2 Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. 3,7 PHYSICAL REVIEW B, 92, 54201. 3,7 Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. 3,7 Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. 4,1 ADVANCED OPTICAL MATERIALS 3, 1164. 4,1 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,7 PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 Gonco, C; Livradi, S; Ma	50	Magnano, E; Bondino, F; Di Valentin, C ; Agnoli, S.	F 7
C-Br and C-H bonds. CHEMISTRY-A EUROPEAN JOURNAL 21, 5826. Ferrighi, L; Trioni, M; Di Valentin, C Boron-doped, nitrogen-doped, and codoped graphene on Cu(111): A DFT + vdW study. 4,8 JOURNAL OF PHYSICAL CHEMISTRY C 119, 6056. 4,8 Gabardi, S; Caravati, S; Sosso, G; Behler, J; Bernasconi, M 3,7 PHYSICAL REVIEW B, 92, 54201. 3,7 Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. 4,1 ADVANCED OPTICAL MATERIALS 3, 1164. 4,1 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 4,1 Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. 3,7 PHYSICAL REVIEW B 91, 155201. 3,0 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 SD Efect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 So foxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 3,0	50	Control of the intermolecular coupling of dibromotetracene on Cu(110) by the sequential activation of	5,7
Ferrighi, L; Trioni, M; Di Valentin, C 4,8 JOURNAL OF PHYSICAL CHEMISTRY C 119, 6056. 4,8 Gabardi, S; Caravati, S; Soso, G; Behler, J; Bernasconi, M 3,7 PHYSICAL REVIEW B, 92, 54201. 3,7 Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. 3,7 Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. 4,1 ADVANCED OPTICAL MATERIALS 3, 1164. 4,1 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 5 Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. 3,7 PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 Gionco, C; Ilvraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 3,0 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 8,4 Mucleation: Hole localization in Al-doped quartz SIO ₂ within ab initio hybrid-functional DFT. 3,0 Golubev, N		C-Br and C-H bonds. CHEMISTRY-A EUROPEAN JOURNAL 21, 5826.	
51 Boron-doped, nitrogen-doped, and codoped graphene on Cu(111): A DFT + vdW study. 4,8 JOURNAL OF PHYSICAL CHEMISTRY C 119, 6056. Gabardi, S; Caravati, S; Sosso, G; Behler, J; Bernasconi, M 3,7 52 Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. 3,7 PHYSICAL REVIEW B, 92, 54201. Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. 3,7 53 Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. 4,1 ADVANCED OPTICAL MATERIALS 3, 1164. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 4,1 54 Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. 3,7 94 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Pacchioni, G. 3,0 3,0 55 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional DFT. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 57 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio		Ferrighi, L; Trioni, M; Di Valentin, C	
JOURNAL OF PHYSICAL CHEMISTRY C 119, 6056. Gabardi, S; Caravati, S; Sosso, G; Behler, J; Bernasconi, M Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. PHYSICAL REVIEW B, 92, 54201. 3,7 Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. ADVANCED OPTICAL MATERIALS 3, 1164. 4,1 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. PHYSICAL REVIEW B 91, 155201. 3,7 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Pacchioni, G. 3,0 Gerosa, M; Bottani, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 Goroco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 3,0 Al- and Ga-Doped TiO ₂ : ZrO ₂ , and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. 8,4 Solubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. Nucleation-controlled vacancy formation in light-emitting wide-b	51	Boron-doped, nitrogen-doped, and codoped graphene on Cu(111): A DFT + vdW study.	4,8
Gabardi, S; Caravati, S; Sosso, G; Behler, J; Bernasconi, M 3,7 Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. 3,7 PHYSICAL REVIEW B, 92, 54201. 3,7 Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. 4 Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. 4,1 ADVANCED OPTICAL MATERIALS 3, 1164. 4,1 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 5 Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. 3,7 PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 55 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 57 Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF 8,4 58 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,7		JOURNAL OF PHYSICAL CHEMISTRY C 119, 6056.	
 Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. PHYSICAL REVIEW B, 92, 54201. Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. ADVANCED OPTICAL MATERIALS 3, 1164. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. Al- and Ga-Doped TiO₂. ZrO₂. and HfO₂: The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. DUFINAL OF MATERIALS CHEMISTRY C 3, 4380. Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 5141. Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. Characterization of OCenters on Single Crystallinge MOV(00		Gabardi, S; Caravati, S; Sosso, G; Behler, J; Bernasconi, M	
PHYSICAL REVIEW B, 92, 54201. Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. ADVANCED OPTICAL MATERIALS 3, 1164. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. Al- and Ga-Doped TiO ₂ ZrO ₂ , and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. Golubev, N; Ignat'E	52	Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe.	3,7
Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L. 4,1 Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. 4,1 ADVANCED OPTICAL MATERIALS 3, 1164. 6 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 8,7 Flectronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. 3,7 PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 55 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 56 Goinco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 8,4 57 Al- and Ga-Doped TiO ₂ . ZrO ₂ and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF 8,4 58 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,7 59 Diffusion-controlled vacancy formation in light-emitting wi		PHYSICAL REVIEW B, 92, 54201.	
53 Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods. 4,1 ADVANCED OPTICAL MATERIALS 3, 1164. 4,1 6 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 54 54 Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. 3,7 54 FHYSICAL REVIEW B 91, 155201. 3,7 55 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 57 THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. 3 56 Goinco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 8,4 57 Al- and Ga-Doped TiO ₂ . ZrO ₂ and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. 8,4 58 Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. 4,7 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy		Galliani, D; Mascheroni, L; Sassi, M; Turrisi, R; Lorenzi, R; Scaccabarozzi, A; Stingelin, N; Beverina, L.	
ADVANCED OPTICAL MATERIALS 3, 1164. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. 3,7 PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 55 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 6 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 57 THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. 3,0 57 Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 8,4 58 MatteriaLS 27, 3936. 8,4 58 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,7 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in glass. 4,7 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 <t< td=""><td>53</td><td>Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods.</td><td>4,1</td></t<>	53	Thermochromic Latent-Pigment-Based Time-Temperature Indicators for Perishable Goods.	4,1
Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,7 S4 Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. 3,7 S4 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,7 S5 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 S5 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 S6 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 4.1 A1- and Ga-Doped TiO ₂ ZrO ₂ , and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF 8,4 S8 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,7 S9 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,5 S9 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. <td< td=""><td></td><td>ADVANCED OPTICAL MATERIALS 3, 1164.</td><td></td></td<>		ADVANCED OPTICAL MATERIALS 3, 1164.	
54 Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments. PHYSICAL REVIEW B 91, 155201. 3,7 55 Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 57 THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. 3,0 57 Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. Al- and Ga-Doped TiO ₂ . ZrO ₂ , and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. 8,4 58 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. 4,7 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. PHYSICAL CHEMISTRY CHMICAL PHYSICS 17, 5141. 4,5 60 Gonchar, A; Lian, J; Risse, T;		Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G.	
 hybrid functional DFT, benchmarked against GW band structure calculations and experiments. PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. Communication: Hole localization in Al-doped quartz SiO₂ within ab initio hybrid-functional DFT. Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. Al- and Ga-Doped TiO₂. ZrO₂, and HfO₂: The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 5141. Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. Characterization of OCenters on Single Crystalline MaQ(001)-Eilms TOPICS IN CATALYSIS 58, 811 	F 4	Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent	2 7
PHYSICAL REVIEW B 91, 155201. Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 55 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 56 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 57 THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 8,4 57 Gionco, V; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 8,4 58 MatterilaLS 27, 3936. 8,4 58 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,7 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in glass. 4,5 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 60 Conchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4	54	hybrid functional DFT, benchmarked against GW band structure calculations and experiments.	3,7
Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G. 3,0 55 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. 3,0 56 Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 57 THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. 3,0 57 Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 8,4 57 Al- and Ga-Doped TiO ₂ ZrO ₂ , and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF 8,4 58 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,7 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 4,5 60 Conchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4		PHYSICAL REVIEW B 91, 155201.	
 Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. Communication: Hole localization in Al-doped quartz SiO₂ within ab initio hybrid-functional DFT. Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. Al- and Ga-Doped TiO₂. ZrO₂, and HfO₂: The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 5141. Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. Characterization of O₂-centers on Single Crystalline MaQ(001)-Ellms, TOPICS IN CATALYSIS 58, 811 		Gerosa, M; Bottani, C; Caramella, L; Onida, G; Di Valentin, C; Pacchioni, G.	
of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702. Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G. 56 Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT. 3,0 THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. Al- and Ga-Doped TiO ₂ , ZrO ₂ , and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. JUERNAL OF MATERIALS CHEMISTRY C 3, 4380. Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. JUFfusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 5141. 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 60 Characterization	55	Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case	3,0
Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G.3,056Communication: Hole localization in Al-doped quartz SiO2 within ab initio hybrid-functional DFT.3,056THE JOURNAL OF CHEMICAL PHYSICS 143, 111103.3,0Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G.57Al- and Ga-Doped TiO2, ZrO2, and HfO2: The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936.8,458Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. JOURNAL OF MATERIALS CHEMISTRY C 3, 4380.4,759Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 5141.4,560Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. Characterization of OCenters on Single Crystalline MaQ(001)-Films TOPICS IN CATALYSIS 58, 8112,4		of oxygen vacancies in metal oxides. THE JOURNAL OF CHEMICAL PHYSICS 143, 134702.	
56Communication: Hole localization in Al-doped quartz SiO2 within ab initio hybrid-functional DFT.3,0THE JOURNAL OF CHEMICAL PHYSICS 143, 111103.Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G.8,457Al- and Ga-Doped TiO2, ZrO2, and HfO2: The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF8,458Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R.4,759JOURNAL OF MATERIALS CHEMISTRY C 3, 4380.4,759Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 5141.4,560Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. Characterization of OCenters on Single Crystalline MaQ(001)-Films TOPICS IN CATALYSIS 58, 8112,4		Gerosa, M; Di Valentin, C; Bottani, C; Onida, G; Pacchioni, G.	
THE JOURNAL OF CHEMICAL PHYSICS 143, 111103. Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 8,4 57 Al- and Ga-Doped TiO2, ZrO2, and HfO2: The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF 8,4 57 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 8,4 58 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,7 59 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,5 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4	56	Communication: Hole localization in Al-doped quartz SiO ₂ within ab initio hybrid-functional DFT.	3,0
Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G. 8,4 57 Al- and Ga-Doped TiO ₂ , ZrO ₂ , and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron 8,4 57 Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF 8,4 58 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,7 58 Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. 4,7 59 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,5 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4		THE JOURNAL OF CHEMICAL PHYSICS 143, 111103.	
Al- and Ga-Doped TiO2, ZrO2, and HfO2: The Nature of O 2p Trapped Holes from a Combined Electron 8,4 57 Al- and Ga-Doped TiO2, ZrO2, and HfO2: The Nature of O 2p Trapped Holes from a Combined Electron 8,4 57 Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF 8,4 58 Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,7 58 Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. 4,7 JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. 4,7 59 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,5 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4		Gionco, C; Livraghi, S; Maurelli, S; Giamello, E; Tosoni, S; Di Valentin, C; Pacchioni, G.	
 ⁵⁷ Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. CHEMISTRY OF MATERIALS 27, 3936. ^{8,4} ^{8,4} Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. ⁵⁸ Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. ⁶⁰ Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. ⁶⁰ Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. ⁶⁰ Characterization of OCenters on Single Crystalline MaQ(001)-Films, TOPICS IN CATALYSIS 58, 811 		Al- and Ga-Doped TiO ₂ , ZrO ₂ , and HfO ₂ : The Nature of O 2p Trapped Holes from a Combined Electron	
MATERIALS 27, 3936. Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 58 Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. 4,7 JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. 4,7 S9 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,5 PHYSICAL CHEMISTRY C HEMICAL PHYSICS 17, 5141. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4	57	Paramagnetic Resonance (FPR) and Density Functional Theory (DET) Study, CHEMISTRY OF	8,4
Golubev, N; Ignat'Eva, E; Sigaev, V; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 58 Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. 4,7 58 JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. 4,7 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 59 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,5 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4		MATERIALS 27, 3936.	
58 Nucleation-controlled vacancy formation in light-emitting wide-band-gap oxide nanocrystals in glass. 4,7 58 JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. 4,7 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4		Golubey, N. Ignat'Eva, F. Sigaey, V. De Trizio, I.: Azarbod, A.: Paleari, A. : Lorenzi, R	
50 Mathematical vacuum y formation in right chineling what bank gup owner hander ystals in glass. 4,7 JOURNAL OF MATERIALS CHEMISTRY C 3, 4380. 50 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,5 59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4 60 Characterization of OCenters on Single Crystalline MaQ(001)-Films, TOPICS IN CATALYSIS 58, 811 2,4	58	Nucleation-controlled vacancy formation in light-emitting wide-hand-gap oxide nanocrystals in glass	47
60 Golubev, N; Ignat'Eva, E; Sigaev, V; Lauria, A; De Trizio, L; Azarbod, A; Paleari, A; Lorenzi, R. 4,5 79 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 9 PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 5141. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4	50	IOURNAL OF MATERIALS CHEMISTRY C. 3, 4380	.,,
59 Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host. 4,5 60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4 60 Characterization of OCenters on Single Crystalline MaQ(001)-Films, TOPICS IN CATALYSIS 58, 811 2,4		Golubey N: Ignat'Eva E: Sigaey V: Lauria A: De Trizio I: Azarbod A: Paleari A : Lorenzi R	
60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4 60 Characterization of OCenters on Single Crystalline MaQ(001)-Films, TOPICS IN CATALYSIS 58, 811 2,4	59	Diffusion-driven and size-dependent phase changes of gallium oxide nanocrystals in a glassy host	45
60 Gonchar, A; Lian, J; Risse, T; Freund, H; Di Valentin, C; Pacchioni, G. 2,4 60 Characterization of OCenters on Single Crystalline MaQ(001)-Films, TOPICS IN CATALYSIS 58, 811 2,4		PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 5141	.,.
60 Characterization of Ω Centers on Single Crystalline Ma Ω (Ω 01)-Films TOPICS IN CATALYSIS 58 811 2,4	60	Gonchar, A: Lian, I: Risse, T: Freund, H: Di Valentin, C: Pacchioni, G .	
		Characterization of O Centers on Single Crystalline Ma $O(001)$ -Films, TOPICS IN CATALYSIS 58, 811	2,4

	Gregori, M: Bertani, D: Cazzaniga, E: Orlando, A: Mauri, M: Bianchi, A: Re, F: Sesana, S: Minniti, S:	
61	Francolini, M: Cagnotto, A: Salmona, M: Nardo, L: Salerno, D: Mantegazza, F: Masserini, M:	
	Simonutti. R.	
	Investigation of Functionalized Polv(N.N-dimethylacrylamide)-block-polystyrene Nanoparticles As	3,9
	Novel Drug Deliverv System to Overcome the Blood-Brain Barrier in Vitro.	
	MACROMOLECULAR BIOSCIENCE 15, 1687.	
	Ha, N: Mano, T: Kuroda, T: Mitsuishi, K: Ohtake, A: Castellano, A: Sanguinetti, S: Noda, T: Sakuma, Y:	
	Sakoda, K.	
62	Droplet epitaxy arowth of telecom InAs augustum dots on metamorphic InAlAs/GgAs(111)A.	1,1
	JAPANESE JOURNAL OF APPLIED PHYSICS 54, 04DH07.	
	Hevn, C: Bartsch, T: Sanguinetti, S: Jesson, D: Hansen, W.	
63	Dynamics of mass transport during nanohole drilling by local droplet etching.	
	NANOSCALE RESEARCH LETTERS 10, 67.	
	Hoseinkhani, S; Tubino, R; Meinardi, F ; Monguzzi, A.	
64	Achieving the photon up-conversion thermodynamic yield upper limit by sensitized triplet-triplet	4,5
	annihilation. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 4020.	
-	Hu, C; Liu, S; Fasoli, M; Vedda, A; Nikl, M; Feng, X; Pan, Y.	
65	ESR and TSL study of hole and electron traps in LuAG:Ce,Mg ceramic scintillator. OPTICAL MATERIALS	2,0
	45, 252.	
66	Hu, C; S. Liu, S; Fasoli, M; Vedda, A ; Nikl, M; Feng X; Pan, Y.	2.1
00	O- centers in LuAG:Ce,Mg ceramics. PHYSICA STATUS SOLIDI. RAPID RESEARCH LETTERS 9, 245.	2,1
	Hund, Z; Nihill, K; Campi, D; Wong, K; Lewis, N; Bernasconi, M; Benedek, G; Sibener, S.	
67	Atomic Surface Structure of CH ₃ Ge(111) Characterized by Helium Atom Diffraction and Density	4,8
	Functional Theory. JOURNAL OF PHYSICAL CHEMISTRY C 119, 18458.	
	Hund, Z; Nihill, K; Campi, D; Wong, K; Lewis, N; Bernasconi, M; Benedek, G; Sibener, S.	
68	Vibrational dynamics and band structure of methyl-terminated Ge(111).	3,0
	THE JOURNAL OF CHEMICAL PHYSICS 143, 124705.	
	Illas, F; Pacchioni, G.	
	Surfaces are different: A perspective on structural, energetic and electronic properties of (001)	
69	surfaces of alkaline earth metal oxides as calculated with hybrid density functional theory by Andrew	1,9
	J. Logsdail, David Mora-Fonz, David O. Scanlon, C. Richard A. Catlow, Alexey A. Sokol.	
	SURFACE SCIENCE 642, 66.	
	Isa, F; Cheze, C; Siekacz, M; Hauswald, C; Lahnemann, J; Fernandez-Garrido, S; Kreiliger, T;	
70	Ramsteiner, M; Dasilva, YAR; Brandt, O; Isella, G; Erni, R; Calarco, R; Riechert, H; Miglio, L.	4.0
70	Integration of GaN Crystals on Micropatterned Si(001) Substrates by Plasma-Assisted Molecular Beam	4,9
	Epitaxy. CRYSTAL GROWTH & DESIGN 15, 4886.	
	Isa, F; Pezzoli, F; Isella, G; Meduňa, M; Falub, C; Müller, E; Kreiliger, T; Taboada, A; Känel, H; Miglio, L.	
71	Three-dimensional Ge/SiGe multiple quantum wells deposited on Si(001) and Si(111) patterned	2,2
	substrates. SEMICONDUCTOR SCIENCE AND TECHNOLOGY 30, 105001.	

	Kanaki, A; Zianni, X; Narducci, D.	
72	Boron Diffusion in Silicon in the Presence of Grain Boundaries and Voids.	
	MATERIALS TODAY: PROCEEDINGS 2, 583.	
	Khalil, M; Bernasconi, R; leffa, S; Lucotti, A; Le Donne, A; Binetti, S; Magagnin, L.	
73	Effect of Co-Electrodeposited Cu-Zn-Sn Precursor Compositions on Sulfurized CZTS Thin Films for Solar	
	Cell. ECS TRANSACTIONS 64, 33.	
	Khung, YL; Ngalim, SH; Scaccabarozzi, A; Narducci, D.	
74	Thermal and UV Hydrosilylation of Alcohol-Based Bifunctional Alkynes on Si (111) surfaces: How	5,6
	surface radicals influence surface bond formation. SCIENTIFIC REPORTS 5, 11299.	
	Khung, Y-L; Ngalim, SH; Scaccabarozzi, A; Narducci, D.	
75	Formation of stable Si–O–C submonolayers on hydrogen-terminated silicon(111) under low-	2,7
	temperature conditions. BEILSTEIN JOURNAL OF NANOTECHNOLOGY 6, 19.	
	Kitao, T; Bracco, S; Comotti, A; Sozzani, P; Naito, M; Seki, S; Uemura, T; Kitagawa, S.	
76	Confinement of Single Polysilane Chains in Coordination Nanospaces.	12,1
	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 137, 5231.	
	Lanzilotto, V; Lovat, G; Fratesi, G; Bavdek, G; Brivio, G ; Floreano, L.	
77	TiO ₂ Charge Donation to an Extended pi-Conjugated Molecule.	7,5
	THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS 6, 308.	
	Le Donne, A; Marchionna, S; Garattini, P; Mereu, R; Acciarri, M; Binetti, S.	
78	Effects of CdS buffer layers on photoluminescence properties of Cu ₂ ZnSnS ₄ solar cells.	1,6
	INTERNATIONAL JOURNAL OF PHOTOENERGY 2015, 583058.	-
	Li, Z; Chen, H; Schouteden, K; Janssens, E; Van Haesendonck, C; Lievens, P; Pacchioni, G.	
79	Spontaneous doping of two-dimensional NaCl films with Cr atoms: aggregation and electronic	7,4
	structure. NANOSCALE 7, 2366.	
	Li, Z; Chen, H; Schouteden, K; Lauwaet, K; Janssens, E; Van Haesendonck, C; Pacchioni, G; Lievens, P.	
80	Lateral manipulation of atomic vacancies in ultrathin insulating films. ACS NANO 9, 5318.	12,9
	Longoni, G; Wang, J; Jung, Y; Kim, D; Mari, C; Ruffo, R.	
81	The Na ₂ FeP ₂ O ₇ -carbon nanotubes composite as high rate cathode material for sodium ion batteries.	6,2
	JOURNAL OF POWER SOURCES 302. 61.	
	Lorenzi, B: Acciarri, M: Narducci, D.	
82	Analysis of Thermal Losses for a Variety of Single-Junction Photovoltaic Cells: An Interesting Means of	1,8
	Thermoelectric Heat Recovery. JOURNAL OF ELECTRONIC MATERIALS 44, 1809.	,
	Lorenzi, B; Acciarri, M; Narducci, D.	
83	Conditions for beneficial coupling of thermoelectric and photovoltaic devices.	1,6
	JOURNAL OF MATERIALS RESEARCH 30, 2663.	
	Lorenzon, M; Christodoulou, S; Vaccaro, G; Pedrini, J; Meinardi, F; Moreels, I; Brovelli, S.	
84	Reversed oxygen sensing using colloidal quantum wells towards highly emissive photoresponsive	11,5
	varnishes. NATURE COMMUNICATIONS 6, 6434.	

	Luches, P; Giordano, L; Grillo, V; Gazzadi, G; Prada, S; Campanini, M; Bertoni, G; Magen, C; Pagliuca,	
85	F; Pacchioni, G; Valeri, S.	
	Atomic Scale Structure and Reduction of Cerium Oxide at the Interface with Platinum.	
	Maccariello D: Campi D: Al Taleb A: Benedek G: Farías D: Bernasconi M: Miranda B	
86	Low-energy excitations of araphene on Ru(0 0 0 1). CARBON 93. 1.	6,2
	Mahato, P: Monguzzi, A : Yanai, N: Yamada, T: Kimizuka, N.	
87	Fast and long-range triplet exciton diffusion in metal-organic frameworks for photon upconversion at	36,5
	ultralow excitation power. NATURE MATERIALS 14, 924.	,
	Mauri, M; Farina, M; Patriarca, G; Simonutti, R; Klasson, K; Cheng, H.	
88	¹²⁹ Xe NMR Studies of Pecan Shell-Based Biochar and Structure-Process Correlations.	1,3
	INTERNATIONAL JOURNAL OF POLYMER ANALYSIS AND CHARACTERIZATION 20, 119.	
	Meinardi, F; Mcdaniel, H; Carulli, F; Colombo, A; Velizhanin, K; Makarov, N; Simonutti, R; Klimov, V;	
89	Brovelli, S.	34.0
0.5	Highly efficient large-area colourless luminescent solar concentrators using heavy-metal-free colloidal	34,0
	quantum dots. NATURE NANOTECHNOLOGY 10, 878.	
	Mereu, R; Le Donne, A; Trabattoni, S; Acciarri, M; Binetti, S.	
00	Comparative study on structural, morphological and optical properties of Zn ₂ SnO ₄ thin films prepared	2.0
90	by r.f. sputtering using Zn and Sn metal targets and ZnO–SnO ₂ ceramic target.	3,0
	JOURNAL OF ALLOYS AND COMPOUNDS 626, 112.	
	Mondiali, V; Lodari, M; Chrastina, D; Barget, M; Bonera, E; Bollani, M.	
91	Micro and nanofabrication of SiGe/Ge bridges and membranes by wet-anisotropic etching.	1,2
	MICROELECTRONIC ENGINEERING 141, 256.	
	Monguzzi, A; Borisov, S; Pedrini, J; Klimant, I; Salvalaggio, M; Biagini, P; Melchiorre, F; Lelii, C;	
92	Meinardi, F.	11.8
52	Efficient Broadband Triplet-Triplet Annihilation-Assisted Photon Upconversion at Subsolar Irradiance	11,0
	in Fully Organic Systems. ADVANCED FUNCTIONAL MATERIALS 25, 5617.	
	Narducci, D.	
93	Explicitly Accounting for the Heat Sink Strengths in the Thermal Matching of Thermoelectric Devices. A	
	Unified Practical Approach. MATERIALS TODAY: PROCEEDINGS 2, 474.	
	Narducci, D; Frabboni, S; Zianni, X.	
94	Silicon de novo: Energy filtering and enhanced thermoelectric performances of nanocrystalline silicon	4,7
	and silicon alloys. JOURNAL OF MATERIALS CHEMISTRY C 3, 12176.	
	Ogawa, T; Yanai, N; Monguzzi, A; Kimizuka, N.	
95	Highly Efficient Photon Upconversion in Self-Assembled Light-Harvesting Molecular Systems.	5,6
	SCIENTIFIC REPORTS 5, 10882.	
96	Pacchioni, G.	2.2
	First Principles Calculations on Oxide-Based Heterogeneous Catalysts and Photocatalysts: Problems	2,3
	and Advances. CATALYSIS LETTERS 145, 80.	

97	Palla, L; Castelli, L; Czelusniak, C; Fedi, M; Giuntini, L; Liccioli, L; Mandò, P; Martini, M ; Mazzinghi, A; Ruberto, C; Schiavulli, L; Sibilia, E ; Taccetti, F. <i>Preliminary measurements on the new TOF system installed at the AMS beamline of INFN-LABEC.</i> NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH B 361, 222.	1,1
98	Pan, Q; Weng, X; Chen, M; Giordano, L; Pacchioni, G ; Noguera, C; Goniakowski, J; Shaikhutdinov, S; Freund, H. <i>Enhanced CO Oxidation on the Oxide/Metal Interface: From Ultra-High Vacuum to Near-Atmospheric</i> <i>Pressures</i> .CHEMCATCHEM 7, 2620.	4,6
99	Pastori, V; Tavazzi, S ; Lecchi, M. Lactoferrin-loaded contact lenses: Eye protection against oxidative stress. CORNEA 34, 693.	2,0
100	Petretto, G; Masse, A; Fanciulli, M ; Debernardi, A. <i>Analysis of hyperfine structure in chalcogen-doped silicon and germanium nanowires.</i> PHYSICAL REVIEW B 91, 125430.	3,7
101	Pezzoli, F ; Balocchi, A; Vitiello, E; Amand, T; Marie, X. <i>Optical orientation of electron spins and valence-band spectroscopy in germanium.</i> PHYSICAL REVIEW B 91, 201201.	3,7
102	Robledo, M; Pacchioni, G ; Martïn, F; Alcamï, M; Dïaz-Tendero, S. Adsorption of benzene on Cu(100) and on Cu(100) covered with an ultrathin NaCl film: Molecule- substrate interaction and decoupling. JOURNAL OF PHYSICAL CHEMISTRY C 119, 4062.	4,8
103	Rocchetti, M; Abbotto, A ; Perna, F; Salomone, A; Florio, S; Capriati, V. Regio- and stereochemical aspects in the functionalisation of a lithiated 2-(3-chloro-2-methyl-1- propenyl)-2-oxazoline: electrophile and temperature effects. TETRAHEDRON 71, 7451.	2,6
104	Rotunno, E; Longo, M; Wiemer, C; Fallica, R; Campi, D; Bernasconi, M ; Lupini, A; Pennycook, S; Lazzarini, L. <i>A Novel Sb₂Te₃ Polymorph Stable at the Nanoscale.</i> CHEMISTRY OF MATERIALS 27, 4368.	8,4
105	Salvalaglio, M; Backofen, R; Bergamaschini, R; Montalenti, F ; Voigt, A. Faceting of equilibrium and metastable nanostructures: A phase-field model of surface diffusion tackling realistic shapes. CRYSTAL GROWTH & DESIGN 15, 2787.	4,9
106	Salvalaglio, M; Bergamaschini, R; Isa, F; Scaccabarozzi, A; Isella, G; Backofen, R; Voigt, A; Montalenti, F; Capellini, G; Schroeder, T; Von Känel, H; Miglio, L. Engineered Coalescence by Annealing 3D Ge Microstructures into HQ Suspended Layers on Si. ACS APPLIED MATERIALS & INTERFACES 7, 19219.	6,7
107	Scarpellini, D; Somaschini, C; Fedorov, A; Bietti, S; Frigeri, C; Grillo, V; Esposito, L; Salvalaglio, M; Marzegalli, A; Montalenti, F; Bonera, E ; Medaglia, P; Sanguinetti, S. <i>InAs/GaAs Sharply Defined Axial Heterostructures in Self-Assisted Nanowires.</i> NANO LETTERS 15, 3677.	13,6
108	Schlexer, P; Ruiz Puigdollers, A; Pacchioni, G. <i>Tuning the charge state of Ag and Au atoms and clusters deposited on oxide surfaces by doping: A</i> <i>DFT study of the adsorption properties of nitrogen- and niobium-doped TiO</i> ₂ <i>and ZrO</i> ₂ PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 22342.	4,5

	Sidletskiy, O; Vedda, A; Fasoli, M; Neicheva, S; Gektin, A.	
109	Crystal Composition and Afterglow in Mixed Silicates: The Role of Melting Temperature.	
	PHYSICAL REVIEW APPLIED 4, 024009.	
	Sighinolfi, GP; Sibilia, E; Contini, G; Martini, M.	
110	Thermoluminescence dating of the Kamil impact crater (Egypt).	3,1
	METEORITICS & PLANETARY SCIENCE 50, 204.	
	Smerieri, M; Pal, J; Savio, L; Vattuone, L; Ferrando, R; Tosoni, S; Giordano, L; Pacchioni, G; Rocca, M.	
111	Spontaneous Oxidation of Ni Nanoclusters on MgO Monolayers Induced by Segregation of Interfacial	7,5
	Oxygen. THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS 6, 3104.	
	Smolentsev, G; Cecconi, B ; Guda, A; Chavarot-Kerlidou, M; van Bokhoven, J; Nachtegaal, M; Artero, V.	
112	Microsecond X-ray Absorption Spectroscopy Identification of Co(I) Intermediates in Cobaloxime-	5,7
	Catalyzed Hydrogen Evolution. CHEMISTRY-A EUROPEAN JOURNAL 21, 15158.	
	Sosso, G; Salvalaglio, M; Behler, J; Bernasconi, M; Parrinello, M.	
113	Heterogeneous crystallization of the phase change material GeTe via atomistic simulations.	4,8
	JOURNAL OF PHYSICAL CHEMISTRY C 119, 6428.	
	Stirling, A; Rozgonyi, T; Krack, M; Bernasconi, M.	
114	Pyrite in contact with supercritical water: the desolation of steam.	4,5
	PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17, 17375.	
	Stoerzinger, K; Hong, W; Azimi, G; Giordano, L; Lee, Y; Crumlin, E; Biegalski, M; Bluhm, H; Varanasi, K;	
115	Shao-Horn, Y.	4.0
115	Reactivity of Perovskites with Water: Role of Hydroxylation in Wetting and Implications for Oxygen	4,8
	Electrocatalysis. JOURNAL OF PHYSICAL CHEMISTRY C 119, 18504.	
	Susanna, A; Armelao, L; Callone, E; Dirè, S; D'Arienzo, M; Di Credico, B; Giannini, L; Hanel, T;	
110	Morazzoni, F; Scotti, R.	4.2
110	ZnO nanoparticles anchored to silica filler. A curing accelerator for isoprene rubber composites.	4,3
	CHEMICAL ENGINEERING JOURNAL 275, 245.	
	Tadiello, L; D'Arienzo, M; Di Credico, B ; Hanel, T; Matejka, L; Mauri, M; Morazzoni, F ; Simonutti, R ;	
117	Spirkova, M; Scotti, R.	4.0
11/	The filler-rubber interface in styrene butadiene nanocomposites with anisotropic silica particles:	4,0
	Morphology and dynamic properties. SOFT MATTER 11, 4022.	
110	Tao, L; Cinquanta, E; Chiappe, D; Grazianetti, C; Fanciulli, M ; Dubey, M; Molle, A; Akinwande, D.	34.0
110	Silicene field-effect transistors operating at room temperature. NATURE NANOTECHNOLOGY 10, 227.	54,0
110	Tavazzi, S; Ferraro, L; Fagnola, M; Cozza, F; Farris, F; Bonetti, S; Simonutti, R; Borghesi, A.	4.2
119	Mechanically triggered solute uptake in soft contact lenses. COLLOIDS AND SURFACES B, 130, 16.	4,2
	Toma, O; Mercier, N; Allain, M; Forni, A; Meinardi, F ; Botta, C.	
120	Aggregation induced phosphorescent N-oxyde-2,2'-bipyridine bismuth complexes and polymorphism-	4,2
	dependent emission. DALTON TRANSACTIONS 44, 14589.	
	Tombolato, S; Berner, U; Colombara, D; Chrastina, D; Widenmeyer, M; Binetti, S; Dale, P.	
121	Cu ₂ ZnSnSe ₄ device obtained by formate chemistry for metallic precursor layer fabrication.	3,5
	SOLAR ENERGY 116, 287.	

	Tosoni, S; Chen, H; Pacchioni, G.	
122	A DFT Study of the Reactivity of Anatase TiO ₂ and Tetragonal ZrO ₂ Stepped Surfaces Compared to the	3,4
	Regular (101) Terraces. CHEMPHYSCHEM 16, 3642.	
	Tosoni, S; Spinnato, D; Pacchioni, G.	
123	DFT Study of CO ₂ Activation on Doped and Ultrathin MgO Films.	4,8
	JOURNAL OF PHYSICAL CHEMISTRY C 119, 27594.	
	Trabattoni, S; Raimondo, L; Campione, M; Braga, D; Holmberg, V; Norris, D; Moret, M; Ciavatti, A;	
124	Fraboni, B; Sassella, A.	
124	Substrate Selection for Full Exploitation of Organic Semiconductor Films: Epitaxial Rubrene on β-	
	Alanine Single Crystals. ADVANCED MATERIALS INTERFACES 2, 1500423.	
	Tumino, F; Carrozzo, P; Mascaretti, L; Casari, C; Passoni, M; Tosoni, S; Bottani, C; Bassi, A.	
125	Two-dimensional TiO _x nanostructures on Au(111): a scanning tunneling microscopy and spectroscopy	
	investigation. 2D MATERIALS 2, 045011.	
	Turrisi, R; Sanguineti, A; Sassi, M; Savoie, B; Takai, A; Patriarca, G; Salamone, M;Ruffo, R; Vaccaro, G;	
176	Meinardi, F; Marks, T; Facchetti, A; Beverina, L.	7 4
120	Stokes shift/emission efficiency trade-off in donor-acceptor perylenemonoimides for luminescent	7,4
	solar concentrators. JOURNAL OF MATERIALS CHEMISTRY A 3, 8045.	
	Uddin, M; Babot, O; Thomas, L; Olivier, C; Redaelli, M;D'Arienzo, M ; Morazzoni, F ; Jaegermann, W;	
	Rockstroh, N; Junge, H; Toupance, T.	
127	New insights into the photocatalytic properties of RuO_2/TiO_2 mesoporous heterostructures for	4,8
	hydrogen production and organic pollutant photodecomposition.	
	JOURNAL OF PHYSICAL CHEMISTRY C 119, 7006.	
	Vanacore, G; Nicotra, G; Zani, M; Bollani, M; Bonera, E; Montalenti, F; Capellini, G; Isella, G; Osmond,	
128	J; Picco, A; Boioli, F; Tagliaferri, A.	22
120	Delayed plastic relaxation limit in SiGe islands grown by Ge diffusion from a local source.	2,2
	JOURNAL OF APPLIED PHYSICS 117, 104309.	
	Veronese, I; De Mattia, C; Fasoli, M; Chiodini, N; Cantone, M; Moretti, F; Dujardin, C; Vedda, A.	
129	Role of Optical Fiber Drawing in Radioluminescence Hysteresis of Yb-Doped Silica.	4,8
	JOURNAL OF PHYSICAL CHEMISTRY C 119, 15572.	
	Villa, I; Vedda, A; Cantarelli, I; Pedroni, M; Piccinelli, F; Bettinelli, M; Speghini, A; Quintanilla, M;	
	Vetrone, F; Rocha, U; Jacinto, C; Carrasco, E; Rodriguez, F; Juarranz, A; del Rosal, B; Ortgies, D;	
130	Gonzalez, P; Sole, J; Garcia, D.	7,0
	1.3 μ m emitting SrF ₂ :Nd ^{2*} nanoparticles for high contrast in vivo imaging in the second biological	
	window. NANO RESEARCH 8, 649.	
	Vitiello, E;Virgilio, M; Giorgioni, A;Frigerio, J; Gatti, E; De Cesari, S; Bonera, E; Grilli, E; Isella, G;	
131	Pezzoli, F.	3,7
	Spin-dependent direct gap emission in tensile-strained Ge films on Si substrates.	,
	PHYSICAL REVIEW B 92, 201203.	

132	Yadav, V; Comotti, A ; Sozzani, P ; Bracco, S ; Bonge-Hansen, T; Hennum, M; Görbitz, C. <i>Microporous Molecular Materials from Dipeptides Containing Non-proteinogenic Residues.</i> ANGEWANDTE CHEMIE 54, 15684.	11,3
133	Zhang, R; Santangelo, S; Fazio, E; Neri, F; D'Arienzo, M; Morazzoni, F ; Zhang, Y; Pinna, N; Russo, P. Stabilization of Titanium Dioxide Nanoparticles at the Surface of Carbon Nanomaterials Promoted by Microwave Heating. CHEMISTRY-A EUROPEAN JOURNAL 21, 14901.	5,7
134	Zianni, X; Narducci, D. <i>Parametric modeling of energy filtering by energy barriers in thermoelectric nanocomposites.</i> JOURNAL OF APPLIED PHYSICS 117, 035102.	2,2
135	Zianni, X; Neophytou, N; Narducci, D. Compact Model for Thermoelectric Power Factor Enhancement by Energy Barriers in a Two-phase Composite Semiconductor. MATERIALS TODAY: PROCEEDINGS 2, 497.	
136	Zoellner, M; Richard, M; Chahine, G; Zaumseil, P; Reich, C; Capellini, G; Montalenti, F ; Marzegalli, A ; Xie, Y; Schülli, T; Häberlen, M; Storck, P; Schroeder, T. <i>Imaging structure and composition homogeneity of 300 mm SiGe virtual substrates for advanced</i> <i>CMOS applications by scanning X-ray diffraction microscopy.</i> ACS APPLIED MATERIALS & INTERFACES 7, 9031.	6,7



COMMUNICATIONS AT CONFERENCES & SEMINARS

1	Albanese, E; Leccese, M; Di Valentin, C; Pacchioni, G.
	Electronic and Magnetic Properties of Nitrogen Doped ZrO ₂ : An ab-initio Study. III Congresso Nazionale
	Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana (DCTC2016). Roma, Italy.
2	Albanese, E; Di Valentin, C; Pacchioni, G; Sauvage, F; Livraghi, S; Giamello, E.
	Nature of Paramagnetic Species in Nitrogen-doped SnO ₂ : a A Combined Electron Paramagnetic Resonance
	and Density Functional Theory Study. COST Action CM1104. Osnabrück, Germany.
3	Albinati, A; Moret, M; Rizzato, S.
	Crystal Growth of Coordination Polymers by Gel Diffusion16. Oesterreichische Chemietage Joint Meeting
	of the Italian & Austrian Chemical Societies. Innsbruck (Austria).
4	Baby, A; Fratesi, G; Brivio, GP.
	Anchoring and bending of pentacene on Al(001). 7th School on Organic Electronics. Como, Italy.
5	Baby, A; Fratesi, G; Floreano, L; Brivio, GP.
	Molecular adsorption of pentacene on Al(001).
	Summer school on emerging renewable energy conversion and storage.Como, Italy.
6	Bergamaschini, R; Salvalaglio, M; Isa, F; Scaccabarozzi, A; Isella, G; Backofen, A; Voigt, A; Marzegalli, A;
	Capellini, G; Skibitzki, O; Yamamoto, Y; Schroeder, T; von Känel, H; Montalenti, F; Miglio, L.
	Engineered coalescence of three-dimensional Ge microcrystals into high-quality suspended layers on Si
	pillars. EMRS Fall Meeting 2015. Warsaw (Poland).
7	Bernasconi, M.
	Atomistic simulations of phase change materials for data storage (invited).
	Spring Meeting of the Swiss Association of Computational Chemistry. Zurich (Switzerland).
8	Bernasconi, M.
	Atomistic simulations of phase change materials for non-volatile memories (invited).
	FISIMAT2015. Cagliari (Italy)
9	Bernasconi, Ni.
	Large scale molecular dynamics simulations of materials for phase change memories (invited).
10	Porpassoni M
10	Structural Palayations and Pasistance Drift in Amorphous CaTa from Atomistic Simulations (invited)
	EVECOS European and Phase Change Ovenics Symposium 2015 Amsterdam (NL)
11	Bracco S: Comotti A: Castiglioni E: Asnaghi D: Sozzani P
11	Adelandar Datara in Darana Constant Frameworks and Constant alecular Architectures
1	1 Molecular Ratars in Paralls Lavalent Frameworks and Subramolecular $\Delta renue cures$

12	Brivio, GP.
	PCAM stategies (invited). Meeting on European Universities of the 21 century. Oldenburg (Germany).
13	Brivio, GP; Fratesi, G; Lin, H; Ravikumar, A; Adak, O; Venkataraman, L; Kladnik, G; Cvetko, D; Morgante, A.
	Lifetimes for fast charge transfer of core excited molecules on gold and graphene.
	APS March Meeting 2015. San Antonio (TX,USA.)
14	Brivio, GP.
	Career, CV and Networking (invited). Winter school on soft skills. Miraflores de la Sierra (Spain).
15	Comotti, A.; Bracco, S.; Marchio', L.; Ienco, A.; Sozzani, P.
	Discrete cyclic supramolecules and nanotubes self-assembled to form porous materials. (invited).
	The International Chemical Congress of Pacific Basin Societies 2015, PACIFICHEM. Honolulu, Hawaii, US.
16	Comotti, A; Bracco, S; Asnaghi, D; Castiglioni, F.; Sozzani, P.
	Regulation of dipolar rotor dynamics by gas adsorption and photoinduced gas uptake-release in porous
	materials. ICSU/IUPAC Workshop on Crystal Engineering. Como, Italy.
17	Comotti, A; Bracco, S; Asnaghi, D; Sozzani, P.
	Molecular Rotors in Nanoporous Periodic Architectures. European crystallographic meeting Rovinj, HR.
18	Comotti, A; Bracco, S; Castiglioni, F; Sozzani, P.
	Porosity and molecular rotor dynamics in covalent frameworks and supramolecular
	.architectureInternational. School of Crystallography: from Molecule to Crystal to Functional. Erice, Italy.
19	De Cesari, S; Giorgioni, A;Vitiello, E;Grilli, E; Guzzi, M; Pezzoli, F.
	All-Optical Switching of Photon Helicity at Direct-gap Transition in Germanium.
	E-MRS Spring Meeting, Lille (France).
20	De Mattia, C; Veronese, I; Fasoli, M; Chiodini, N; Mones, E; Cantone, M; Cialdi, S; Gargano, M; Ludwig, N;
	Bonizzoni, L; Vedda, A.
	Ionizing radiation detection by Yb-doped silica optical fibers.
	Hard X-Ray, Gamma-Ray, and Neutron Detector Physics .San Diego, (CA, USA).
21	Di Martino, D; Perelli Cippo, E; Uda, I; Riccardi, M; Paleari, A; Lorenzi, R; Scherillo, A; Gorini, G.
	Study of ancient metal samples from Valle delle Forme.
	TechnArt 2015.Catania (Italy).
22	Di Valentin, C.
	Charge Carriers Separation at the Graphene/TiO2 Interface (invited).
	Winter Modeling 2015. Scuola Normale Superiore, Pisa (Italy).
23	Di Valentin, C.
	Computational Electrocatalysis: Novel Material for Oxygen Reduction Reaction (ORR) and Methanol
	Oxidation Reaction (MOR) (invited).
	7th Topical Meeting of the International Society of Electrochemistry: "Multiscale Analysis of
	Electrochemical Systems".Saint-Malo, France.
24	Di Valentin, C.
	Oxygen at Graphene/Cu(111) and Graphene/TiO2(101) Interfaces: a Van Der Waals DFT Study (invited).
	Workshop ECSCD-12. Trieste, Italy.

25	Fanciulli, M; Belli, M; Paleari, S; Lamperti, A; Molle, A; Sironi, M; Pizio, A.
	Defects and Dopants in Silicon and Germanium Nanowires (invited).
	ECS Meeting.Phoenix, (AZ, USA).
26	Fratesi, G; Baby, A; Vaidya, SR; Patera, LL; Africh, C; Floreano, L; Brivio, GP.
	Anchoring and Bending of Pentacene on Aluminum (001).
	APS March Meeting 2015.San Antonio (TX,USA.)
27	Gabardi, S; Sosso, G; Caravati, S; Colombo, J; Del Gado, E; Behelr, J; Bernasconi, M.
	Fragility of the supercooled liquid and structural relaxation in the glass from large scale molecular
	dynamics simulations of phase change compounds (invited).
	Materials Research Society Spring Meeting .San Francisco, (CA, USA).
28	Giorgioni, A.; Paleari, S.; Cecchi, S.; Grilli, E.; Isella, G.; Jantsch, W. ; Fanciulli, M.; Pezzoli, F.
	Electron Spin Resonance of conduction electrons in Ge/SiGe quantum wells.
	Spin Physics, Spin Chemistry, and Spin Technology. St. Petersubrg (Russia).
29	Lorenzi, R; Azarbod, A; De Trizio, L; Ignat'Eva, E; Sigaev, V; Golubev, N; Paleari, A.
	Phase separation and optical properties of nanostructured oxide-in-oxide Ga2O3-containing
	germanosilicate glasses.
	E-MRS 2015 – European Materials Research Society Fall Meeting. Warsaw (Poland).
30	Lorenzi, R; Azarbod, A; De Trizio, L; Ignat'Eva, E; Sigaev, V; Golubev, N; Paleari, A.
	γ-Ga2O3 nanocrystals in germano-silicate glass as multipurpose photonic material.
	FISMAT 2015 - Italian National Conference on Condensed Matter Physics.Palermo (Italy).
31	Lorenzi, R; Azarbod, A; De Trizio, L; Ignat'Eva, E; Sigaev, V; Paleari, A; Golubev, N.
	Energy transfer process between γ -Ga2O3 nanocrystals and Gd3+ ions in nanostructured germano-silicate
	glassceramic. LUMDETR 2015, Tartu (Estonia)
32	Maspero, F; Sibilia, E; Martini, M.
	Bayesian analysis and the way to look at absolute dating.
	International Conference on Metrology for Archaeology.Benevento, Italy.
33	Meinardi, F ; Klimov, V I; Brovelli, S.
	Large-area luminescent solar concentrators based on 'Stokes-shift-engineered' nanocrystals (invited).
	Italian National Conference on Condensed Matter Physics (FisMA12015).Palermo, Italy.
34	Montalenti, F.
	Towards a realistic, continuum modeling of neteroepitaxial growth: elastic relaxation, surface-energy
	minimization, misjit dislocations, and intermixing (invited)
25	Simorow 2015 Workshop, Schloss Rauschholzhausen, Germany.
35	Wontalenti, F; Bergamaschini, R; Salvalagilo, W; Backolen, R; Rovaris, F; Albani, W; Warzegalli, A; Volgt,
	A, IVIIGIIU, L.
	dislocations and intermixing EISMAT 2015. Delarmo, theke
	uisiocutions unu intermixing. FISIVIAT 2015. Palemio, italy.
36	Montalenti, F; Bergamaschini, R; Salvalaglio, M; Backofen, R; Rovaris, F; Albani, M; Marzegalli, A; Voigt,
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	A; Miglio, L.
	Continuum modeling of heteroepitaxial growth on silicon: elastic relaxation, surface-energy minimization,
	misfit dislocations and intermixing. (invited). E-MRS Fall Meeting, Warsaw, Poland.
37	Pacchioni, G.
	Adsorption on two-dimensional insulators3rd FIRB Meeting Oxides at the nanoscale: multifunctionality
	and applications. Montelibretti CNR, Roma (Italy).
38	Pacchioni, G.
	"Laudatio" Laurea Honoris Causa in ScieLaurea Honoris Causa in Scienza dei Materiali a Enrico Albizzati.
	University of Milano-Bicocca, Milano (Italy).nza dei Materiali a Enrico Albizzati (invited).
39	Pacchioni, G.
	Adsorption and reactivity of doped insulators: chlorides versus oxides (invited).
	International SFB FOXSI Symposium .Vienna, Austria.
40	Pacchioni, G.
	Adsorption and reactivity of two-dimensional insulators (invited). Rideal conference .Berlin, Germany
41	Pacchioni, G.
	Adsorption on two-dimensional insulators (invited).
	FIRB Meeting Oxides at the nanoscale: multifunctionality and applications. Torino, Italy.
42	Pacchioni, G.
	Deposition of metal atoms and clusters on two-dimensional insulators (invited). ELETTRA Trieste, Italy.
43	Pacchioni, G.
	From reduction to reaction. TiO2 and ZrO2 catalytic materials in bio-mass conversion: hints from DFT
	(invited). The Technical Committee Meeting of CASCATBEL .Bled, Slovenia
44	Pacchioni, G.
	Gold nanostructures on pure and doped oxide thin films (invited).
	International Symposium on Relations between Homogenous and Heterogeneous Catalysis. Utrecht,
	Netherlands.
45	Pacchioni, G.
	Metal atoms and clusters on two-dimensional insulators: reactive adsorption, incorporation and doping
	effects (invited). University of Graz, Austria.
46	Pacchioni, G.
	Modellistica computazionale di bio e nano-sistemi. Un approccio razionale alla catalisi (invited.)
	Scuola Superiore Università di Catania.
47	Pacchioni, G.
	Modern electronic structure theory and catalysis: towards the simulation of complex problems in chemistry
	(invited). Summer school on Physics and chemistry of nanoclusters. Bruges, Belgium.
48	Pacchioni, G.
	Nanocatalysis: from size-selected clusters, to defects engineering and two-dimensional oxides (invited)
	CRC Summer School: Strategies for the Synthesis and the Characterization of Metal Oxides. Berlin-Erkner.

49	Pacchioni, G.
	Nanocatalysis: from size-selected clusters, to defects engineering and two-dimensional oxides (invited).
	E-WISPOC 2015 Chemistry and Chemical Processes in Confined Spaces.Bressanone, Italy.
50	Pacchioni, G.
	Nanocatalysis: from supported clusters to two-dimensional oxides (invited).
	Scientific Meetings Symposium on Catalysis.Prague, Czech Republic.
51	Pacchioni, G.
	The unusual properties of two-dimensional oxides supported on metals (invited).
	International Conference Nanomeeting 2015. Minsk, Belarus.
52	Pacchioni, G.
	Theory of magnetic impurities in oxides. A pragmatic approach to a complex problem (invited).
	GIRSE Workshop & NIS Colloquium - EPR in catalysis: from models to real systems. Torino, Italy.
53	Pacchioni, G.
	Theory of magnetic impurities in oxides. Problems (and solutions?) (invited).
	Workshop Nothing is perfect: the quantum mechanics of defects .Ascona, Switzerland
54	Pacchioni, G.
	Titania in cement and construction industry: the contribution of modeling (invited).
	New trends in computational chemistry for industry applications.Barcelona, Spain.
55	Pacchioni, G.
	Two-dimensional oxides: from microelectronics to nanocatalyis (invited).
	Trendoxides 2015: new trends in correlated oxides and interfaces. Brescia, Italy.
56	Pacchioni, G.
	Two-dimensional oxides: from microelectronics to nanocatalysis (invited).
	Thomas Young Centre - The London centre for the theory and simulation of materials (UCL). London, UK.
57	Pacchioni, G.
	Unusual properties of two-dimensional insulators: transition metals on NaCl and MgO ultrathin films
	(invited).
	CECAM Workshop Emergent structural and electronic phenomena of nanoscale oxides .Lausanne,
	Switzerland.
58	Paleari, S; Molle, A; Lamperti, A; Fanciulli, M.
	Negative-U trapping centers evidenced by admittance spectroscopy at the Ge/GeO ₂ interface.
	E-MRS spring meeting. Grand Palais, Lille (France).
59	Palomba, M; Coscia, U; Ambrosone, G; Binetti, S; Le Donne, A; Carotenuto, G.
	Nanosized Tellurium Preparation by Vibration Milling.
	XI Convegno Nazionale Materiali Nanofasici. Roma, Italy.
60	Panzeri, L; Martini, M; Sibilia, E.
	OSL single grain dating: comparison of different statistical age models applied to renaissance mortars.
	International Conference on Metrology for Archaeology. Benevento, Italy.

61	Pellegrino, S; Longoni, L; Scorticati, D; Binetti, S; Le Donne, A; Rolfi, A; Grilli, E; Busto, C; Neuenschwander,
	B; Jäggi, B.
	Random surface texturing of mc-Silicon for solar cells with picosecond lasers; a comparison between 1064
	nm, 532 nm and 355 nm laser emission wavelengths. CLEO-AT 2015.San Jose (CA, USA)
62	Pezzoli, F; Balocchi, A; Amand, T; Marie X.
	Optical orientation and electron spin dynamics in Germanium (invited).
	International Conference on Silicon Epitaxy and Heterostructures – ICSI. Montréal, Québec, Canada
63	Ravikumar, A; Lin, H; Baby, A; Fratesi, G; Brivio, G.
	Adsorption of Organic Molecules on Graphene School on Organic Electronics. Como, Italy.
64	Rizzato, S; Moret, M ; Merlini, M; Albinati, A; Beghi, F.
	Morphological and Structural Effects of Gels on Coordination Polymers Crystallization.
	XLIV Annual Meeting of the Italian Crystallographic Association (AIC). Vercelli (Italy
65	Ruffo, R; Brazzo, P; Salamone, MM; Mari, CM; Beverina, L.
	Cheap and abundant organic perylene diimmide based pigment as electrode material for rechargeable
	batteries. ICAE 2015 The 3rd International Conference on Advanced Electromaterials. Jeju (Korea)
66	Ruffo, R; Longoni, G; Mari, CM.
	Na2FeP2O7/MWCNT composite as cathode for sodium ion batteries. GEI 2015. Bertinoro (FC), Italy.
67	Salvalaglio, M; Bergamaschini, R; Backofen, R; Albani, M; Rovaris, F; Montalenti, F; Voigt, A; Miglio, L.
	Faceting of Equilibrium and Metastable Nano- and Micro- structures: A Phase-Field Model of Surface
	Diffusion Tackling Realistic Shapes. ECOSS-31. Barcellona, Spain.
68	Sozzani, P; Bracco, S; Comotti, A; Piga, D; Forani, M; Perego, J.
	Porous materials for in situ polymerization and morphological transcription.
	ICSU/IUPAC Workshop on Crystal Engineering. Como, Italy
69	Sozzani, P; Bracco, S; Forani, M ; Piga, D; Comotti, A
	Nanoporous materials for confined polymerization and molecular rotor dynamics. (invited).
	The International Chemical Congress of Pacific Basin Societies 2015, PACIFICHEM. Honolulu, Hawaii, USA.
70	Sozzani, P; Comotti, A; Bracco, S.
	Rotor Dynamics and Photoinduced Porosity Switch in Supramolecular Architectures and Covalent
	Frameworks (invited).
	The International Chemical Congress of Pacific Basin Societies 2015, PACIFICHEM. Honolulu, Hawaii, USA.
71	Sozzani, P; Comotti, A; Bracco, S; Castiglioni, F.
	Regulation of dipolar rotor dynamics by gas adsorption and photoinduced gas uptake/release.
	The 29th European Crystallographic Meeting. Rovinj, Croatia.
72	Vedda, A.
	Medical Applications of Nanomaterials. International School of Atomic and Molecular Spectroscopy -
	Nano-Optics: Principles Enabling Basic Research and Applications. Erice (Italy).

73	Vedda, A.
	Spectroscopic techniques for imaging (invited).
	International School of Cardiac Surgery and International School of Solid State Physics - 6th and 67th
	Course: Scientific and Technological Advances in Cardiac and Vascular Surgery: a Translational Approach.
	Erice (Italy)
74	Vedda, A.
	Controlling, reducing, and exploiting defects in scintillators (invited). Shanghai Institute of Ceramics.
75	Vedda, A.
	Role of defects in the scintillation process (invited). Shanghai Institute of Ceramics.
76	Vitiello, E; Giorgioni, A; Frigerio, J; Gatti, E; De Cesari, S; Grilli, E; Isella, G; Pezzoli, F.
	Spin-dependent direct gap emission in tensile-strained Ge-on-Si heterostructures.
	SpinTechVIII International School and Conference . Basilea, Switzerland.
77	Zolotarev, P N; Moret, M ; Proserpio, D M; Blatov, V A.
	Search for the cleavable organic crystals: topological and energetic aspects.
	Joint British-Russian workshop "Molecular crystals: from fundamentals to applications". Novosibirsk,
	Russia.

PHD THESIS

Murali Krishna DIBBANTI	Study of polymer crosslink density by time domain NMR spectroscopy
Reza FATHI	Investigation of Alkaline Ion Rocking Chair Batteries
Silvia GABARDI	First principles simulations of phase change materials for data storage
Svitlana KARAMSHUK	Organic sensitizers for application in photonic and photovoltaic devices
Bruno LORENZI	Polycrystalline Silicon as Thermoelectric Material -Bringing the nanotechnological advantage into bulk-
Federica PARRAVICINI	Characterization of enzymes from desulfurizing bacterial strains
Jesus PENARANDA	Biomedical applications of inorganic nanoparticles: Magnetic Resonance Imaging and Hyperthermia
Davide ROTTA	Emerging devices and materials for nanoelectronics. Silicon spin qubits and MoS2 thin-film transistors
Luciano TADIELLO	Role of the silica nanoparticle anisotropy on morphological and mechanical properties of Styrene Butadiene Rubber nanocomposites
Riccardo TURRISI	Novel approaches to solution-processable organic electronics
Irene VILLA	Structural and Morphological Tuning of Inorganic Luminescent Nanophosphors. Towards Applications in Sensing and Lighting

ERC Consolidator Grant awarded to Prof. Cristiana Di Valentin

(BIOINOHYB: Smart bioinorganic hybrids for nanomedicine)

The use of bioinorganic nanohybrids (nanoscaled systems based on an inorganic and a biological component) has already resulted in several innovative medical breakthroughs for drug delivery, therapeutics, imaging, diagnosis and biocompatibility. However, researchers still know relatively little about the structure, function and mechanism of these nanodevices.



Theoretical investigations of bioinorganic interfaces are mostly limited to force-field approaches which cannot grasp the details of the physicochemical mechanisms.

The BIOINOHYB project proposes to capitalize on recent massively parallelized codes to investigate bioinorganic nanohybrids by advanced quantum chemical methods.

This approach will allow to master the chemical and electronic interplay between the bio and the inorganic components in the first part of the project, and the interaction of the hybrid systems with light in the second part.

The ultimate goal is to provide the design principles for novel, unconventional assemblies with unprecedented functionalities and strong impact potential in nanomedicine. More specifically, in this project the traditional metallic nanoparticle will be substituted by emerging semiconducting metal oxide nanostructures with photocatalytic or magnetic properties capable of opening totally new horizons in nanomedicine (e.g. photocatalytic therapy, a new class of contrast agents, magnetically guided drug delivery).

Potentially efficient linkers will be screened regarding their ability both to anchor surfaces and to bind biomolecules. Different kinds of biomolecules (from oligopeptides and oligonucleotides to small drugs) will be tethered to the activated surface according to the desired functionality.

The key computational challenge, requiring the recourse to more sophisticated methods, will be the investigation of the photo-response to light of the assembled bioinorganic systems, also with specific reference to their labelling with fluorescent markers and contrast agents.

Project cost: 1.75M€ EU Contribution: 1.75M€ Duration: 5 years

P. Mahato, **A. Monguzzi**, N. Yanai, T. Yamada, N. Kimizuka, *Fast and long-range triplet exciton diffusion in metal–organic frameworks for photon upconversion at ultralow excitation power*. Nature Materials **14**, 924–930 (2015).

By exploiting metal-organic frameworks (MOF) crystalline systems, we maximized the efficiency of sensitized upconversion under very weak excitation intensities. This breakthrough was based on combining donor/acceptor dves integration into a solid upconverter and precise control of the acceptor spatial organization in crystalline MOFs, which led to fast and longrange triplet exciton diffusion. By taking advantage of the enhanced exciton migration among fluorophores that are regularly aligned with spatially controlled reciprocal orientations, quantitative triplet-triplet we achieved а



annihilation in the solid state, producing high energy up-converted photons even under excitation intensities much lower than solar irradiance.

F. Meinardi, H. McDaniel, **F. Carulli**, **A. Colombo**, K. A. Velizhanin, N. S. Makarov, **R. Simonutti**, V. I. Klimov and **S. Brovelli**, *Highly efficient large-area colourless luminescent solar concentrators using heavy-metal-free colloidal quantum dots.* Nature Nanotechnology **10**, 178, (2015).

Luminescent solar concentrators (LSCs) servina as semitransparent photovoltaic windows could become an important element in net zero energy consumption buildings of the future. Colloidal quantum dots are promising materials for LSCs as they can be engineered to provide the large Stokes shift necessary for suppressing reabsorption losses in large-area devices. Here, we use quantum dots of ternary I-III-VI₂ semiconductors to realize the first largearea LSC free of toxic elements- By incorporating photo-polymerized CuInSe_vS_{2-v} auantum dots into poly(lauryl methacrylate), we obtain freestanding, colorless slabs that introduce no distortion to perceived colors and are thus well suited for the realization of photovoltaic windows. We achieve a record optical power efficiency of 3.2%.



Z. Li, **H-Y T. Chen**, K. Schouteden, K. Lauwaet, E. Janssens, C. Van Haesendonck, **G. Pacchioni**, and P. Lievens, *Lateral Manipulation of Atomic Vacancies in Ultrathin Insulating Films*. ACS Nano **9**, 5318 (2015).

During the last 20 years, using scanning tunneling microscopy and atomic force (STM) microscopy, scientists have achieved vertical and lateral repositioning of individual atoms on and in different types of surfaces. It is therefore surprising that controlled repositioning of virtual atoms,



i.e., atomic vacancies, across atomic lattices has not yet been achieved experimentally. Here we use STM at liquid helium temperature (4.5 K) to create individual Cl vacancies and subsequently to laterally manipulate them across the surface of ultrathin sodium chloride films. Our findings are corroborated by density functional theory calculations and STM image simulations.

M. Baroncini, S. d'Agostino, G. Bergamini, P. Ceroni, **A. Comotti, P. Sozzani, I. Bassanetti,** F. Grepioni, T. M. Hernandez, S. Silvi, M. Venturi, A. Credi, *Photoinduced reversible phase change in porous molecular crystals based on star-shaped azobenzene tetramers.* Nature Chem. **7**, 634 (2015).

Shape-persistent azobenzene tetramers form porous molecular crystals in their *E*-configuration and their porosity can be tuned by changing the peripheral substitutents on the molecule. Efficient $E \rightarrow Z$ photoisomerization of the azobenzene units takes place in the solid state and converts the crystals into a non-porous amorphous phase. Crystallinity and porosity are restored upon $Z \rightarrow E$ isomerization promoted by visible light irradiation or heating. We demonstrate that the photoisomerization enables reversible on/off switching of optical properties, such as birefringence, and of the capture of carbon dioxide from the gas phase. The linear design, the structural versatility and the synthetic accessibility make this new family of materials extremely interesting for technological applications.



A. Castelli, F. Meinardi, M. Pasini, F. Galeotti, **V. Pinchetti, M. Lorenzon**, L. Manna, I. Moreels, U. Giovanella, and **S. Brovelli**, *High-Efficiency All-Solution-Processed Light-Emitting Diodes Based on Anisotropic Colloidal Heterostructures with Polar Polymer Injecting Layers*. *Nano Lett.* **15**, 5455 (2015) - **ACS Editors' Choice, Most read article**

in 2015

Despite over twenty years of research since the initial demonstration of QD-LEDs in 1994, the external quantum efficiency (EQE) of LEDs based on colloidal nanostructures sandwiched between semiconducting polymers has never surpassed ~0.3-0.4%, and record devices embedding vacuum-deposited small organic molecules have reached EQEs just above 3%.

Here, we outperform all previous approaches using both solution-based *and* thermally evaporated organic interlayers by synthesizing polyelectrolytic conjugated polymers soluble in non-solvents for the QD emitters, that can be spin-coated without causing damage to the active underlayers. Using this approach, in combination with anisotropic CdSe/CdS heteronanostructures, we obtain all-solution-based, roll-off-free QD-LEDs with high brightness (>1200 cd/m²) and

EQE=6,1%, which is about *twenty times* higher than the previous record QD-LEDs with polymer interlayers and exceeds by ~200% top performing QD-LEDs embedding vacuum deposited organic molecules

D. Scarpellini, C. Somaschini, A. Fedorov, **S. Bietti**, C. Frigeri, V. Grillo, L. Esposito, **M. Salvalaglio, A. Marzegalli, F. Montalenti, E. Bonera**, P.G. Medaglia, and **S. Sanguinetti**, *InAs/GaAs Sharply Defined Axial Heterostructures in Self-Assisted Nanowires*. Nano Lett. **15**, 3677 (2015).

We present the fabrication of axial InAs/GaAs nanowire heterostructures on silicon with atomically sharp interfaces by molecular beam epitaxy. Our method exploits the crystallization at low temperature, by As supply, of In droplets deposited on the top of GaAs NWs grown by the selfassisted (self-catalyzed) mode. Extensive characterization based on transmission electron microscopy sets an upper limit for the InAs/GaAs interface thickness within few bilayers (\leq 1.5 nm).

Importantly, we obtained such a result in a fully catalyst-free growth mode, therefore eliminating the longstanding problem of gold incorporation into the wires. Hence, the proposed procedure first gives the possibility to produce high-quality wires for laser or transport devices, whose performances are presently degraded by unwanted metal incorporation caused by Au-seeded VLS at high concentrations.





Highlights

A. Monguzzi, S. M. Borisov, **J. Pedrini**, I. Klimant, M. Salvalaggio, P. Biagini, F. Melchiorre, C. Lelii, **F. Meinardi**, *Efficient Broadband Triplet–Triplet Annihilation-Assisted Photon Upconversion at Subsolar Irradiance in Fully Organic Systems*. Advanced Functional Materials **25**, 5617–5624 (2015).

The latest trend in solar cell technology is to develop photon managing processes that adapt the solar emission to the spectral range at which the devices show the largest intrinsic efficiency. Triplet-triplet annihilation assisted photon upconversion (sTTA-UC) is currently the most promising process to blue-shift sub-bandgap photons at solar irradiance. Here we demonstrate how to obtain broadband sTTA-UC at sub-solar irradiance, by enhancing the system's light-harvesting ability by way of an ad-hoc synthesized family of chromophores with complementary absorption properties. The overall absorptance is boosted, doubling the number of upconverted photons and reducing the irradiance required to achieve the maximum upconversion yield. An unprecedented yield of $\approx 10\%$ is obtained under broadband air mass 1.5 conditions.





S. Bracco, M. Beretta, A. Cattaneo, A. Comotti, A. Falqui, K. Zhao, C. Rogers, **P. Sozzani**, Dipolar *Rotors Orderly Aligned in Mesoporous Fluoro-organosilica Architectures*. Angew. Chem. Int. Ed. **54**, 4681 (2015). VIP article and Cover Picture of the Issue.



New mesoporous covalent frameworks, based on hybrid fluoroorganosilicas, were prepared to realize a periodic architecture of fast molecular rotors containing dynamic dipoles in their structure. The mobile elements, designed on the basis of fluorinated *p*-divinylbenzene moieties, were integrated into the robust covalent structure through siloxane bonds, and showed not only the rapid dynamics of the aromatic rings (ca. 10^8 Hz at 325 K), as detected by solid-state NMR, but also a dielectric response typical of a fast dipole reorientation under the stimuli of an applied electric field. Furthermore, the mesochannels are open and accessible to diffusing-in gas molecules, and rotor mobility could be individually regulated by I₂ vapors. The iodine enters the channels of the periodic structure and reacts with the pivotal double bonds of the divinyl-fluoro-phenylene rotors, affecting their motion and the dielectric properties.

FUNDED PROJECTS

Coordinator	⁻ dinator Project	
A. ABBOTTO	Dispositivi Solari a Coloranti di Nuova Generazione: Sensibilizzatori e Conduttori Nano-Ingegnerizzati (DSSCX).	MIUR
MACCIADDI	SOLARDESIGN-On-the-fly alterable thin-film solar modules for design driven Applications.	EU
M. ACCIARRI	New materials with low environmental impact for thin film solar cells fabrication.	MAE
M. BERNASCONI	SYNAPSE-SYnthesis and functionality of chalcogenide NAnostructures for PhaSE change memories.	EU
L. BEVERINA	Exploitation of self-assembly and photochemistry for the straightforward, low cost production of nanostructured organic photovoltaic devices.	Cariplo
S. BINETTI	CHEETAH-Cost-reduction through material optimisation and Hight EnErgy outpuT of solAr pHotovoltaic modules-joining Europe's research and Development efforts in support of its PV industry.	EU
	Caratterizzazione di silicio multicristallino cresciuto in condizione di microgravità, a partire da silicio metallurgico.	ASI
G.P. BRIVIO	THINFACE-Thin-film Hybrid Interfaces: a training initiative for the design of next-generation energy devices.	EU
S. BROVELLI	Electronic Doped Colloidal Nanocrystal Heterostructures for transformational Breakthrought in solid-state lighting.	EU
A. COMOTTI	Meccanismi di attivazione della CO2 per la progettazione di nuovi materiali per l'efficienza dell'energia e delle risorse.	MIUR
	BIOINOHYB-Smart Bioinorganic Hybrids for Nanomedicine	EU-ERC
	Nuovi materiali fotocatalitici per la conversione di energia solare basati su eterogiunzioni.	Cariplo
C. DI VALENTIN	Oltre il grafene: strati di carbonio nanostrutturati disegnati su misura per ottenere nuovi materiali per la catalisi e la chimica sostenibile.	MIUR
	DECORE-Direct ElectroChemical Oxidation Reaction of Ethanol: optimization of the catalyst/support assembly for high temperature operation.	EU

R. LORENZI	LORENZI Nanostructured oxide-in-oxide glasses for solar-blind UV- monitoring of work-safety and energy-saving in electric power distribution.	
	Giotto, l'Italia: oltre l'immagine.	Cariplo
	Sliding Doors: 600 anni di eccellenza tecnologica lombarda.	Regione Lombardia
M. MARTINI	Studio e sviluppo applicativo di ossicarbonati e ossidi misti contenenti ioni lantanidi con proprietà luminescenti per applicazioni nel bio-imaging e nell'optoelettronica.	MIUR
	Nuove nanostrutture colloidali con molteplici funzionalità ottiche e magnetiche per applicazioni avanzate in elettronica, fotonica e diagnostica biomedica.	Fondazione CRTortona
F. MLINARDI	Electronic Doped colloidal Nanocrystal Heterostructures with designed Interfacial composition: towards the development of new nano-device concepts for lighting and Energy Technologies.	EU
D. NARDUCCI	Silicon Friendly Materials and device solutions for microenergy applications.	EU
	ERC starting grants: una proposta per colmare il gap dei giovani ricercatori italiani.	Cariplo
G. PACCHIONI	Cascade deoxygenation process using tailored nanocatalysts for the production of biofuels from lignocellulosic biomass.	EU
	CATSENSE.	EU
	Ossidi Nanostrutturati: multi-funzionalità e applicazioni	MIUR
F. PEZZOLI	Spin optoElectronics ARCHitectures based on group IV compounds – SEARCH IV.	Cariplo
R.RUFFO	Give Sodium a Chance!Investigation of nanostructured mixed Na oxides as electrode materials for energy storage.	Cariplo
S. SANGUINETTI	FemToTera- Plasmon-enhanced Tera-Hertz emission by Femtosecond laser pulses of nanostructured semiconductor - metal surfaces	Regione Lombardia
	COSMOS	Cariplo
R. SCOTTI	Rational design of hybrid organic-inorganic interfaces: the next step towards advanced functional materials – Action MP1202.	EU
F. COZZA S. TAVAZZI	Augmented Environment for Control in amyotrophic lateral sclerosis	Ricerca SLA
	AIDA 2020-Advanced European Infrastructures for Detectors at Accelerators.	EU
A. VEDDA	INTELUM-International and intersectoral mobility to develop advanced scintillating fibres and Cerenkov fibres for new hadron and jet calorimeters for future colliders.	EU
	EIT KIC Raw Materials.	EU

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Administration and technical staff

Administration and didactics



Laboratories



Luisa RAIMONDO

Enterprise Services/Conto terzi

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

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

- Materials characterization
- Research projects
- Consultancy
- Training

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

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

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

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



Research Facilities

Spin off





www.cudam.mater.unimib.it

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

four participating departments:

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



Aims of the CUDAM are:

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

Dating techniques:

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

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

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

Applications: Geological and geoarchaeological dating of sediments.

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

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



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

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

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

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

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



Laboratory of Scanning Electron Microscopy and Microanalysis

www.mater.unimib.it/utenti/sem/SEMWEB/

The Scanning Electron Microscope (SEM) allows to obtain three-dimensional images at high resolution (~ 5 nm) by scanning an electron beam in a small area of the test sample. All the effects that are produced in the point of impact of the beam can be used, with appropriate detectors, to produce a contrast, and then the image. Furthermore, the analysis of the producedX-rays allows to perform compositional analysis with high spatial resolution (microanalysis). The sample to be examined must be conductive.

In case the sample is not conductive it is possible to deposit a thin gold film in order to make possible the vision. The microscope available in our laboratory allows the viewing of non-conductive samples even in the absence the gold film. Our SEM offers the opportunity to work in conditions of variable pressure of argon using an exclusive detector for low vacuum LVSTD.

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

FIB/SEM BOMBAY LABORATORY. SOFT AND BIOLOGICAL MATERIALS MICROMANIPULATION AND MICROSCOPY

Following a joint application of the Department of Materials Science and Department of Physics, a FEI Quanta 3-D DualBeam[™] system was installed at Milano-Bicocca University in the mid of 2006.

This important system (hosted by the Center of Excellence Plasma Prometeo) is devoted to studies on soft materials and biological specimens, that hopefully could invade the field of nanomedicine. Actually nanotechnology has led to a remarkable convergence of disparate fields including biology, applied physics, optics, computational analysis, modeling, and materials science.

The DualBeam system combines a Scanning Electron Microscope (SEM) with a Focused Ion Beam (FIB). The SEM is based on a tungsten electron column, able to operate as a

conventional, high vacuum SEM or as an Environmental SEM, which allows working pressures up to 3000 Pa during electron microscopy by means of special gaseous detectors.

The Focused ion beam (FIB) is a tool that performs basically three functions: ion imaging (from secondary electrons or ions), milling (precision down to 10 nm) and deposition (with the insertion of a small needle delivering special gases).

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

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

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

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

- Charge neutralization of the sample with electron beam during FIB milling;
- Two gas injector systems (GIS) for selective carbon milling (SCM) and Pt deposition;
- Alternative use of the electron beam induce deposition instead of the ion beam induced deposition in order to deposit films and growth nanostructures in a *milder* way.





e- column

Solid State BSE Detector (SS-BSED)

Electron Multiplier (CDEM)

Ga⁺ column



www.mibsolar.mater.unimib.it

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

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

Main objectives of MIB-SOLAR are:

- Study and research of new materials and devices related to solar energy in its various forms;
- The aggregation and coordination of researchers in the field of solar energy;
- Training of young researchers in the field of materials science and technology for solar energy;

- The development of intellectual property of the University of Milano-Bicocca in the field of solar energy;

- Cooperation with institutions, public and private research centers, and Fondazioni in the field of solar energy;

- Support and technology transfer to companies operating in the field of solar energy;

- Promotion of seminars, conferences, meetings and discussions for the study and exchange of information and knowledge in the field of solar energy.

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

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

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

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

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

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

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

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

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

IRELLI CORIMAV - CONSORZIO PER LA RICERCA SUI MATERIALI AVANZATI

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



ETSF -European Theoretical Spectroscopy Facility www.etsf.eu

The University of MIlano Bicocca is member of the European Theoretical Spectroscopy Facility, a research network and e-infrastructure dedicated to providing support and services for ongoing research in academic, government and industrial laboratories. Comprised of 68 research teams across Europe and the United States, the ETSF carries out state-of-the-art research on theoretical and computational methods for studying electronic and optical properties of materials. All fields in need of knowledge about electronic excitations, transport and spectroscopy will benefit from the ETSF, such as condensed matter physics and chemistry, biology, materials and nano science. The ETSF gathers the experience and know-how of more than 200 researchers in Europe and the United States, facilitating innovation and rapid knowledge transfer. The ETSF is headquartered in Louvain-la-Neuve, Belgium.





DeltaTi Research

http://www.universita.it/brevetto-universita-bicocca-ricupero-energia/

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

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

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



PILEGROWTH TECH S.R.L.

http://www.pilegrowth.com

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

Galaleabiolech 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 applciations.

The technological processes developed by Galatea biotech build molecules with a low carbon footprint, which is typical of products of plant origin and which contributes to the reduction of greenhouse gas emissions, achieving thus Kyoto's Protocol targets.



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

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

MATERIALS SCIENCE GOES TO TOWN



MEETmeTONIGHT, the Researchers' Night in Lombardy, is an annual event that aims to spread scientific culture and knowledge of the research professions among citizens of all ages through events and fun and challenging initiatives. In the 2015 edition, we were present with two stands: ARCHEO-LAB, an interactive laboratory to present the Radiocarbon dating technique and LEGO-LIGHT to discover the magic of colours



Science Corner was an event organized by the Universities of Lombardy for Expo 2015. The Department's Archaeometry group proposed the exhibit ArcheoFOOD, an interactive time travel to discover how our ancestors nourished, cooked and assembled food.



La sapienza è figliola della sperienzia (Wisdom derives from experience, Leonardo, cod. Forster III)

Exibition of ancient scientific instruments

Milano Bicocca, Ponte U1-U2, 26/11/2015-10/1/2016

About 60 instruments were on display: the exhibition, organized in collaboration with the University of Pavia, was in the honor of prof. Borghesi and regarded *Electricity and magnetism* and *Optics and spectroscopy*. The exhibition, opened on November 27, in about two months was visited by over 3000 people, including students and professors from both Universities, high school students and common people.



TEACHING



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

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

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

Elaborati finali e Tesi Magistrali Lauree Triennali in Scienza dei Materiali

F.ARCADI	Distribuzioni periodiche di dislocazioni in film di Ge su Si(100)
A. BARZANI	Dislocazioni di misfit in film di GexSi(1-x) su Si(001)
D. BESGHINI	Nuove frontiere per l'impiego di copolimeri a blocchi in nanomedicina: produzione di scaffolds per tissue engineering
L. BETTAMIN	Dispositivi semiconduttori applicati alla microelettronica, transistors a corpo ultra sottile: mosfets e finfets.
F. BOCCARDO	Studio e implementazione del modello di crescita "Diffusion Limited Aggregation".
V. BONERA	Realizzazione di quantum dots mediante crescita "droplet epitaxy"
C. CAPITANI	Nanomateriali per sensing raziometrico di gas
F. COLOMBO	Batterie con catodi a base di radicali stabili
L.DEI CAS	Diamanti funzionalizzati-sintesi e proprietà
S.DISTASO	Ottimizzazione delle performance in impianti fotovoltaici
M.DITERLIZZI	Materiali nanoporosi per il confinamento di molecole volatili usate in polimerizzazione e in biomedicina
S.ERBA	Fotosintesi artificiale: splitting di acqua indotta da radiazione solare. Sensibilizzatori.
L.KACANI	Proprietà e struttura di nanoclusters metallici utilizzati per bioimaging e biosensing
E.MAHAJNEH	Proprietà elettroniche e strutturali delle leghe a cambiamento di fase in GeTe
M.MARINI	Ricerca e Sviluppo di nuove leghe di oro a 22 carati per il mercato indiano
A.MARZO	Crescita di nanowires di semiconduttori III-V
D.PARINI	Sensori di gas a base di ossidi nanostrutturati
A.ROCCO	Matrici polimeriche per upconversion basata sull'annichilazione tripletto-tripletto: sviluppi e prospettive nel fotovoltaico
A.ROLFI	Studio mediante tecniche spettroscopiche di celle fotovoltaiche
M.ROSSI	Applicazioni del germanio nella plasmonica
J.ERRAGNI	Modelli di diffusione con anisotropia nel termine di energia di superficie
L.VACCARI	Polimeri e rapid prototyping. Modelli per il training neurochirurgico
A.VARIN	Sviluppo di una schiuma di polietilene reversibilmente termoformabile
M.ZAFFALON	Diodo ad emissione di luce basato su GaN
F.ZANENGA	Auto-assemblaggio di copolimeri a blocchi PS-b-PMMA a basso peso molecolare
G.ZUCCA	Self-healing polymers: polimeri autoriparanti quali additivi innovativi per vernici

Lauree Magistrali in Scienza dei Materiali

		Growth, fabrication and characterization of strain-free quantum dot infrared
G.	BENEDETTI	photodetector.
Μ.	CAPUTO	Sintesi colloidale di cluster bimetallici luminescenti per biosensoristica e bioimaging
		Materials based on metal-organic frameworks built with new polyazotated ligands:
F.	CASTIGLIONI	synthesis, properties and charaterization.
	CONTI	Optical emission and energy transfer processes in Gd3+ doped gallium oxide
υ.	CONTI	nanocrystals embedded in titanium-doped germano-silicate amorphous matrices
Α.	CORNA	Development of electrolyte/oxide/metal devices for neuron interfacing
		Caratterizzazione e messa a punto di protocolli di stabilità per prodotti cosmetici
F.	CORSO	per capelli.
		Characterization of ring shape defects in n-type Czochralski silicon wafers for
V.	FOLEGATTI	photovoltaic application
		Sintesi di nanocompositi polimerici a base di materiali porosi ad elevata area
Μ.	FORANI	superficiale
		Studio della dinamica segmentale in miscele polimeriche e polimeri iper-reticolati
Μ.	MAURI	attraverso risonanza magnetica nucleare risolta in tempo
		Difetti di punto in quarzo cristallino in relazione alle caratteristiche luminescenti e
Μ.	PERRON	paramagnetiche
		Materiali microporosi covalenti per l'adsorbimento di gas di interesse energetico e
D.	PIGA	ambientale
		Studio delle proprietà ottiche di ioni ni2+ e di nanocristalli di ga2o3 dispersi in
Μ.	PROIETTI	vetri germanosilicati
S.	SALVIATI	Decorazione di nanoparticelle di titania con polimeri mediante reazione tiolo-ene
		Ruolo degli stati superficiali nel decadimento radiativo e non radiativo in
L.	SORTINO	nanocristalli colloidali di perovskite CsPbBr3.
		Sviluppo di dielettrici polimerici di nuova generazione per applicazioni nel campo
Μ.	TAWFILAS	delle microonde.
R.	ZAGHENO	Sintesi di nanocapsule polimeriche per applicazioni in fotonica

Lauree Triennali in Ottica e Optometria

Α.	BAGLIVI	Valutazione delle abilità visive nei giocatori di pallacanestro
N.	BIANCOFIORE	Gli effetti dell'ortocheratologia sulla qualità dell'immagine retinica e sulle attività visive
C.	BRACCHI	Valutazione clinica e caratterizzazione ottica di una nuova lente a contatto multifocale commerciale a ricambio giornaliero
C.	BRAIA	Miopia e suo controllo
G.	BRAMBILLA	Sensibilità di due test di disparità di fissazione verificata con stereoacuità e velocità di lettura
F.	BREMBILLA	Confronto tra il sistema accomodativo e delle vergenze attraverso training visivo optometrico modificato
V.	BRIVIO	Confronto tra tecniche diverse per l'analisi dell'endotelio corneale
Μ.	BUSI	Analisi visiva tramite l'utilizzo di filtri colorati su soggetti affetti da visual stress.
E.	CASAZZA	Analisi morfometriche dell'endotelio corneale in lampada a fessura.
E.	CHEKURKOVA	Valutazione della visione stereoscopica con lente oftalmica multifocale
Α.	CHIERICATI	Metodo per la valutazione della capacità antiossidante delle lacrime umane
S.	CHIERICATI	Influenza della manutenzione sulle aberrazioni delle lac
I.	CUTER	Progettazione e realizzazione di un test per la valutazione della Sensibilità al Contrasto su tablet
E.	DE MARTINO	Trattamento di mgd e dryeye tramite l'applicazione di eyebag e relativa valutazione della loro efficacia
R.	DE NARDI	Valutazione delle performance visive legate all'equilibrio e alla visualizzazione nella ginnastica artistica
V.	DI SANTO	Valutazione degli effetti di integratori alimentari sulle performance visive
J.	FACCHETTI	Gestione clinica della cornea irregolare con lenti a contatto.
V.	FALANGA	Studio dell'influenza del colore sulla disparità di fissazione
I.	FIORILLO	Caratterizzazione delle proprietà superficiali di diversi materiali per lenti a contatto rigide.
Α.	GALDI	Recidiva dell'occhio secco marginale post trattamento con integratore lacrimale a base di acido ialuronico
V.	GRECO	Validità dei test di accomodazione e vergenza al forottero
D.	ISIMBALDI	Accomodazione e videoterminale: analisi delle variazioni del sistema accomodativo in relazione all'utilizzo di un videoterminale
Α.	LEONE	Valutazione dell'efficacia di sostituti lacrimali alla carbossimetilcellulosa e acido ialuronico: uno studio comparativo
Υ.	MAHRI	Confronto tra reticoli di Amsler diversi testati su soggetti glaucomatosi
C.	MANGILI	Confronto tra test visivi optometrici e "Wachs Analysis of Congnitive Structures" in bambini di età prescolare
М.	MARTON	Realizzazione e caratterizzazione di materiali biopolimerici funzionalizzati per lenti a contatto
F.	MASSIRONI	La Stella di Van Orden: costruzione stereoscopio e procedure

М.	MATERA	Sensibilità al contrasto temporale . Test della funzionalità delle cellule ganglionari retiniche in soggetti sani e glaucomatosi
S.	MAURI	Valutazione delle abilità oculomotorie e visuo-percettive in bambini in età prescolare
В.	MOLTENI	Analisi visive di sensibilità e recupero all'abbagliamento in diversi intervalli spettrali su normovedenti e affetti da patologie retiniche.
М.	NAPOLI	Tonometria non invasiva a confronto
V.	OSSUZIO	Applicazione di lenti rigide gas-permeabili minisclerali e corneali su cornee irregolari
М.	PAGANONI	Effetti del Visual Training d'integrazione visiva multi-sensoriale su atleti e non atleti con palla di Marsden e Sherman numbers.
М.	PAINI	Effetti della dissociazione verticale sulla disparità laterale. Produzione di un test per la valutazione della stereo acuità su tablet.
E.	PALMISANO	Analisi visiva integrata: dalla valutazione della variazione astigmatica, all'utilizzo del metodo mkh.
Α.	PANCERA	Studio dell'endotelio corneale: microscopio speculare e Endoker a confronto
C.	PATRIA	Influenza ed effetti della visione periferica sulla visione binoculare
L.	PRISCIANTELLI	Effetto comportamentale di lenti e prismi sul Re.Vi.P.
C.	QUIESE	Confronto di tecniche cliniche per la valutazione della risposta accomodativa
М.	RONZONI	L'illuminazione negli ambienti di lavoro: effetti dell'attenuazione della luce blu sulle abilità visive.
E.	ROSSI	Studio sulla disparità di fissazione con "dark test" modificato
G.	ROSSINI	Effetti del training visuo-spaziale su atleti e non atleti con Prismi Gemellati e Life Saver.
S.	SEBAI	Studio della progressione miopica nei bambini
G.	SEVESO	Progettazione, produzione e applicazione di lenti a contatto RGP toriche su misura.
Α.	TAGLIABUE	Analisi e confronto di materiali in silicone idrogel per porto continuo
F.	TAMBURRELLI	Influenza dell'apporto idrico e di Omega-3 sul film lacrimale e sulla sensibilità al contrasto
L.	TRIVELLA	Valutazione della performance visiva in seguito a visual training
Μ.	TUVÈ	Valutazione della dimensione orizzontale dell'area fusionale di Panum utilizzando stereogrammi a disparità crescente su tablet
J.	VATTOLIL	Progettazione, produzione ed applicazione di lenti a contatto morbide toriche su misura.
Ρ.	VILLA	Valutazione delle abilità visive in condizioni di illuminazione ambientale a diversa emissione di luce blu
E.	ZANONI	Caratterizzazione di un sistema ottico di concentrazione della radiazione solare per celle fotovoltaiche.

Miriam Ferrari Award

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

The award consists of 2.000 Euro and is granted thanks to a donation of the family in memory of Miriam Ferrari, a former student of the Materials Science course.

This year, the awards were granted to Mattia Negroni and Elisa Lassi.


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

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

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

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

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

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

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

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

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

Chairman is prof.Gianfranco Pacchioni

DOCTORATE IN CHEMICAL SCIENCES http://www.scuoladottorato.scienze.unimib.it/

The doctorate in Chemical Science lasts three years and is divided into 3 curricula:

- Chemistry and environment
- Chemistry and materials
- Chemistry of bioactive compounds

Every year the following educational activities are required:

-Attendance to the courses of advanced chemistry offered at UNIMIB

-Research activity with the support of and internal tutor, professor of Chemistry at UNIMIB -Participation in schools and courses on subject inherent to the chosen curriculum. Training or research periods outside the University of Milano Bicocca are possible.

At the conclusion of the three years the student will present research in a written dissertation in English, which will be discussed before a specifically nominated commission. Following a positive result of the elaboration and presentation, the student will receive the diploma of Doctorate in Chemical Science.

Chairman is prof. Marco Vighi.

CREDITS

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Pictures









SEM MAG: 1.10 kx HV: 20.0 kV VAC: HiVac

DET: SE Detector DATE: 10/27/15 Device: TS5136XM

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