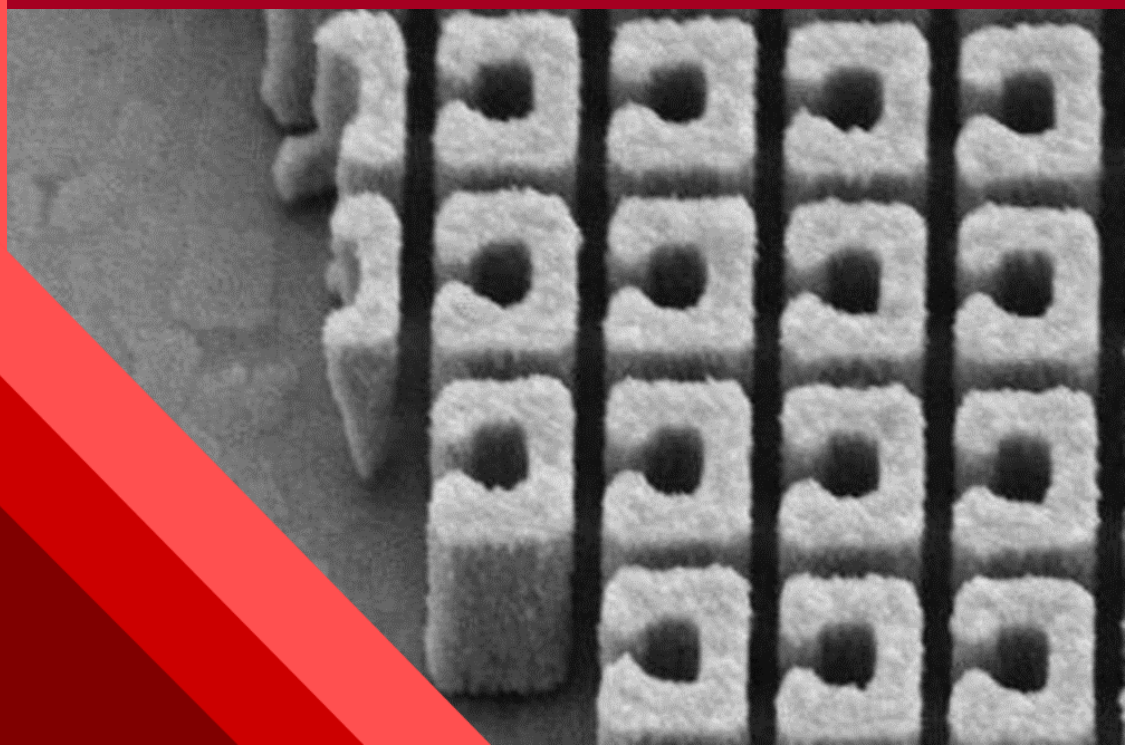
Istituto Officina dei Materiali

Scientific Report
2010 - 2012



Istituto Officina dei Materiali

Scientific Report
2010 - 2012

Cover image: Plasmonic materials

Foreword

The Institute of Materials (IOM, Istituto Officina dei Materiali) of the National Research Council (CNR) has been established in 2010 from former groups and laboratories of INFM (Istituto Nazionale di Fisica della Materia, National Institute for Condensed Matter Physics): the TASC National Laboratory in Trieste, the Operative Group in Grenoble (OGG), the Democritos Simulation Centre at Sissa in Trieste, the Sardinian Laboratory for computational materials science (SLACS) at the University of Cagliari, .and the Perugia Unit, at the Department of Physics of the Perugia University.

IOM pursues the objective of developing innovative materials and micro-, nano-devices. To this aim, it can rely on a set of tools and methodologies like theoretical modelling, atom-by-atom synthesis, fine analysis, materials and device functionalization. The scientific focus is on hybrid materials (inorganic, organic, biologic), superconductivity, spintronics (spin transport electronics, exploiting the magnetic moment of the electron), sub-microscopic energy transportation and storage, fundamental properties of structures like DNA or proteins, development of devices and sensors for biomedical applications.

The IOM manages a great share of CNR activities at the Italian and European large scale research infrastructures in the field of matter characterization. The Institute operates six beamlines at the Elettra laboratory as well as two neutron and a x-ray beamline at the ILL and the ESRF laboratories, respectively, inside the scientific hub of Grenoble, France. At these facilities the available beam time is assigned by international committees that select the most scientifically relevant proposals of international research groups. This procedure has a beneficial impact also on the in-house scientific output.

The Institute hosts laboratories for electronic microscopy (TEM and SEM) and scanning probe microscopy (STM and AFM) built in-house or adapted for specific applications to expand the range of available experimental techniques for materials and nanostructure analysis. Besides fine analysis of Matter, IOM activities include new materials synthesis based on growth technologies via atomic beam deposition, including extremely high-purity MBE deposition, and the manufacturing of devices based on nano- and micro-structuring through lithography.

IOM carries out atomic-level numerical modelling applied to materials, biologic systems and physics of highly correlated systems. Research activities are combined to a strong commitment to the development of new computational methodologies to be used by an enlarged international scientific community. The Institute played a relevant role in developing, disseminating and promoting training associated to the Quantum ESPRESSO project, a high-level software platform, which has been encountering great appreciation at national and international level.

In 2012, the IOM was crucial in having the CNR ranked among the world's top 100 scientific institutions by number of publications on journals affiliated to the Nature Publishing Group.

The IOM headquarters, located inside AREA Science Park, fosters shared use of premises and laboratories located in the vicinity of major research facilities and infrastructures, in initiatives such as Open-Lab and NFFA (Nanoscience Foundries and Fine Analysis), thus promoting a more successful involvement of the industrial sector in research and innovation projects at European level.

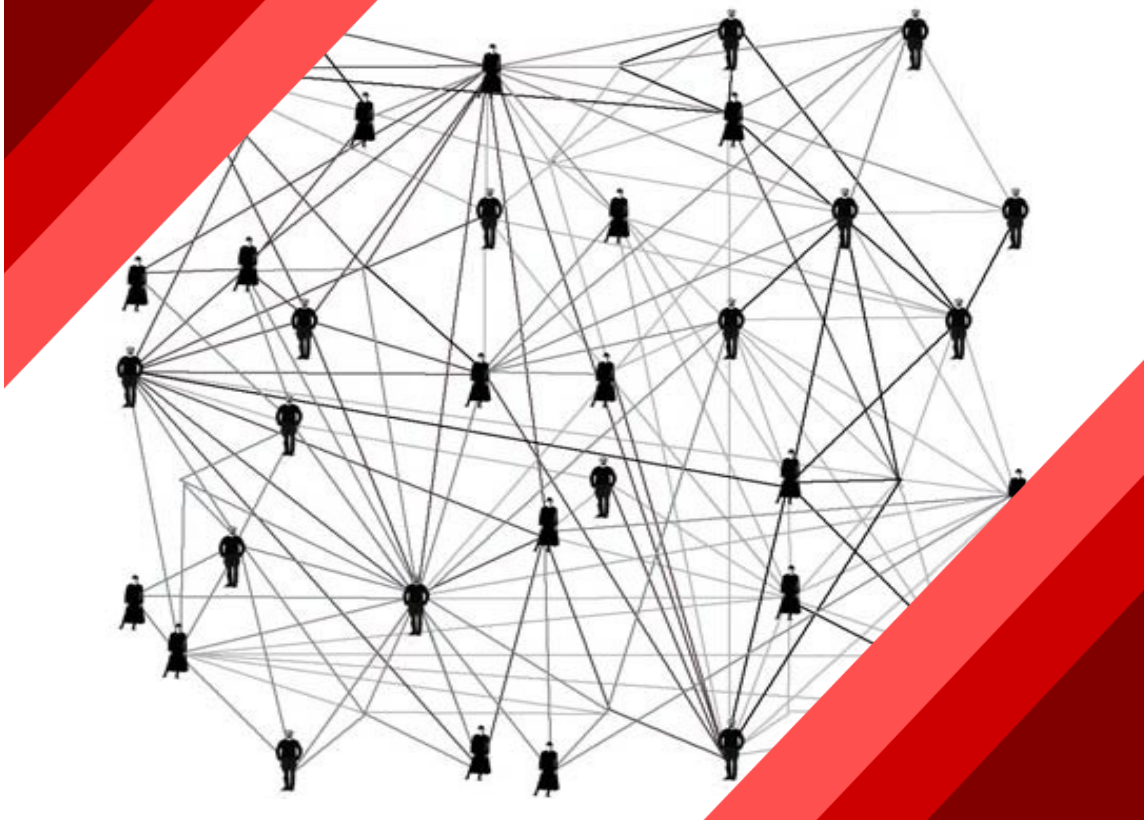
This report includes a description of the research activities of the institute and of the main scientific achievements of the 2010-2012 period, together with the illustration of the most relevant equipment.

Prof. Alberto Morgante
CNR-IOM Director

Istituto Officina dei Materiali

Table of contests

People



People

Researchers and Technologists

Africh Cristina (Ts-Tasc)
Alagia Michele (Ts-Tasc)
Becca Federico (Ts-Democritos)
Biasiol Giorgio (Ts-Tasc)
Bondino Federica (Ts-Tasc)
Businaro Luca (Ts)
Calzolari Arrigo (Ts)
Capogna Lucia (Grenoble)
Capone Massimo (Ts)
Caponi Silvia (Pg)
Carlino Elvio (Ts-Tasc)
Cepek Cinzia (Ts-Tasc)
Ciancio Regina (Ts-Tasc)
Cojoc Danut Adrian (Ts-Tasc)
Comez Lucia (Pg)
Cossaro Albano (Ts-Tasc)
Cozzini Stefano (Ts-Democritos)
D'acapito Francesco (Grenoble)
Davidson Bruce (Ts-Tasc)
De Francesco Alessio (Grenoble)
De Palo Stefania (Ts)
De Simone Monica (Ts-Tasc)
Delugas Pietro Davide (Ca)
Esch Friedrich (Ts-Tasc)
Fabris Stefano (Ts-Democritos)
Felici Roberto (Ts)
Filippetti Alessio (Ca)
Floreano Luca (Ts-Tasc)
Formisano Ferdinando (Grenoble)
Fujii Jun (Ts-Tasc)
Galasso Germano (Ts)
Giglia Angelo (Ts-Tasc)
Giovannetti Gianluca (Ts)
Gotter Roberto (Ts-Tasc)
Grenci Gianluca (Ts)
Gubbiotti Gianluca (Pg)
Kivimaki Antti Eerik (Ts-Tasc)
Krizmancic Damjan (Ts)
Lazzarino Marco (Ts-Tasc)
Lopez Giorgia Maria (Ca)
Magistrato Alessandra (Ts-Democrit)
Magnano Elena (Ts-Tasc)
Mahne Nicola (Ts-Tasc)
Marquestaut Nicolas (Ts)
Martin Samos Colomer Layla (Ts)
Mattoni Alessandro (Ca)
Mondelli Claudia (Grenoble)
Moroni Saverio (Ts-Democritos)
Natali Francesca (Grenoble)
Orani Daniela (Ts)
Panaccione Giancarlo (Ts-Tasc)
Pedio Maddalena (Ts-Tasc)
Piccinin Simone (Ts-Democritos)
Pinato Giulietta (Ts)
Prasciolu Mauro (Ts)
Romanato Filippo (Ts-Tasc)
Rubini Silvia (Ts-Tasc)
Russo Daniela (Grenoble)
Santucci Silvia (Ts)
Satta Alessandra (Ca)
Tacchi Silvia (Pg)
Torelli Piero (Ts)
Tormen Massimo (Ts-Tasc)
Trapananti Angela (Grenoble)
Umari Paolo (Ts-Democritos
Verdini Alberto (Ts-Tasc)
Vobornik Ivana (Ts-Tasc)
Zacchigna Michele (Ts-Tasc)
Zangrando Marco (Ts-Tasc)

Technician and Administrative staff

Aisa Simone (Pg)
Babic Claudia (Ts-Tasc)
Baricevic Moreno (Ts)
Benedetti Davide (Ts)
Bertoch Paolo (Ts)
Bigaran Stefano (Ts-Tasc)
Carpentiero Alessandro (Ts)
Centazzo Martina (Ts-Tasc)
Cociancich Ezio (Ts)
Cvelbar Vanja (Ts-Tasc)
De Luisa Aleksander (Ts-Tasc)
De Marco Massimiliano (Ts-Tasc)
Fanucchi Rossella (Ts-Tasc)
Ferranti Roberta (Ts-Tasc)
Gregori Iztok (Ts)
Gustin Sabrina (Ts)
La Manna Fabrizio (Grenoble)
Laloni Alessio (Grenoble)
Marinelli Giulia (Pg)
Martin Andrea (Ts)
Masala Giovanna (Ca)
Mistron Paola (Ts-Tasc)
Pertot Alessandro (Ts)
Rizzo Antonello (Grenoble)
Salvador Federico (Ts)
Suran Fabio (Ts)
Tonezzer Matteo (Ts)
Varas Stefano (Ts)

Research Associates

Ancilotto Francesco, Ass. Ts
Anselmi Claudio, Ass. Ts
Baldereschi Alfonso, Ass. Ts
Baraldi Alessandro (Ts-Tasc)
Baroni Stefano, Ass. Ts
Bernardini Fabio, Ass. Ca
Binggeli Nadia Arlette, Ass. Ts
Bongiovanni Giovanni, Ass. Ca
Boscherini Federico, Ass. Ts
Bussi Giovanni, Ass. Ts
Capotondi Flavio, Ass. Ts
Cappellini Giancarlo, Ass. Ca
Carloni Paolo, Ass. Ts
Castellarin Cudia Carla, Ass. Ts
Ceccarelli Matteo, Ass. Ca
Colombo Luciano, Ass. Ca
Comelli Giovanni, Ass. Ts-Tasc
Coslovich Giacomo, Ass. Ts
Cvetko Dean, Ass. Ts-Tasc
Dal Corso Andrea, Ass. Ts
De Franceschi Silvano, Ass. Ts
De Gironcoli Stefano, Ass. Ts
De Simone Antonio, Ass. Ts
De Vita Alessandro, Ass. Ts
Decleva Pietro, Ass. Ts
Decuzzi Paolo, Ass. Ts
Di Fabrizio Enzo, Ass. Ts-Tasc
Dri Carlo, Ass. Ts
Ercolessi Furio, Ass. Ts
Esch Friedrich, Ass. Ts
Fabrizio Michele, Ass. Ts
Fanetti Mattia, Ass. Ts
Fiorentini Vincenzo, Ass. Ca
Fornasini Paolo, Ass. Ts
Fragiacomo Massimo, Ass. Ca

People

Franciosi Alfonso, Ass. Ts-Tasc
Franz Silvio, Ass. Ts
Fronzoni Giovanna, Ass. Ts
Gallo Paola, Ass. Ts
Gavioli Luca, Ass. Ts
Gebauer Ralph, Ass. Ts
Giannozzi Paolo, Ass. Ts
Grazioli Cesare, Ass. Ts
Grenci Gianluca, Ass. Ts
Kokalj Anton, Ass. Ts
Laio Alessandro, Ass. Ts
Lupi Stefano, Ass. Ts
Malvestuto Marco, Ass. Ts
Manini Nicola, Ass. Ts
Marsili Matteo, Ass. Ts
Martucci Alessandro, Ass. Ts
Masia Marco, Ass. Ca
Massidda Sandro, Ass. Ca
Maurizio Chiara, Ass. Grenoble
Meneghini Carlo, Ass. Ts
Micheletti Cristian, Ass. Ts
Mobilio Settimio, Ass. Grenoble
Modesti Silvio, Ass. Ts-Tasc
Montecchi Monica, Ass. Ts
Morgante Alberto, Ass. Ts-Tasc
Nannarone Stefano, Ass. Ts-Tasc
Parmigiani Fulvio, Ass. Ts-Tasc
Paroni Roberto, Ass. Ca
Pasquali Luca, Ass. Ts
Pastore Giorgio, Ass. Ts
Pederiva Francesco, Ass. Ts
Peressi Maria, Ass. Ts
Peronio Angelo, Ass. Ts
Petrillo Caterina, Ass. Pg
Pinato Giulietta Ass. Ts
Postorino Paolo, Ass. Ca
Prince Kevin Charles, Ass. Ts-Tasc
Quochi Francesco, Ass. Ca
Resta Raffaele, Ass. Ts
Romanato Filippo, Ass. Ts-Tasc
Rosei Renzo, Ass. Ts
Rossi Giorgio, Ass. Ts-Tasc
Rovere Mauro, Ass. Ts
Ruggerone Paolo, Ass. Ts-Democritos
Saba Michele, Ass. Ca
Sacchetti Francesco, Ass. Pg
Santoro Giuseppe, Ass. Ts
Sauvage-Simkin Rose Michele, Ass. Ts-Tasc
Scandolo Sandro, Ass. Ts-Democritos
Scoles Giacinto, Ass. Ts-Democritos
Senatore Gaetano, Ass. Ts-Democritos
Silvestrelli Pierluigi, Ass. Ts
Smargiassi Enrico, Ass. Ts
Sorella Sandro, Ass. Ts-Democritos
Stener Mauro, Ass. Ts
Stranges Stefano, Ass. Ts-Tasc
Toigo Flavio, Ass. Ts
Tosatti Erio, Ass. Ts-Democritos
Vesselli Erik, Ass. Ts
Zecchina Riccardo, Ass. Ts-Democritos

Affiliated Fellowship

Ambrosini Stefano, Ass. Ts
Annese Emilia, Ass. Ts
Antonello Alessandro, Ass. Ts
Bagolini Luigi, Ass. Ca
Baranwal Vikas, Ass. Ts
Benassi Andrea, Ass. Ts
Bersani Marco, Ass. Ts
Bhardwaj Sunile, Ass. Ts
Biarnes Xavier, Ass. Ts
Birarda Giovanni, Ass. Ts
Borin Daniele, Ass. Ts
Calzia Vasco, Ass. Ca
Capogrosso Valentina, Ass. Tss
Carleo Giuseppe, Ass. Ts
Cassese Damiano, Ass. Ts
Chiodi Mirco, Ass. Ts
Cilento Federico, Ass. Ts
Coceano Giovanna, Ass. Ts
Colizzi Giuseppe, Ass. Ca
Dai Pre' Marta, Ass. Ts
Dal Zilio Simone, Ass. Ts
De Leo Federica, Ass. Ts
Denis Garola Denis, Ass. Ts
D'este Elisa, Ass. Ts
Fior Raffaella, Ass. Ts
Fortuna Sara, Ass. Ts
Franco Duvan, Ass. Ts
Ganbold Tamiraa, Ass. Ts
Gentile Francesco, Ass. Ts
Giorgis Valentina, Ass. Ts
Hu Xiaoliang, Ass. Ts
Hussain Sajid, Ass. Ts
Kucukbenli Emine, Ass. Ts
Kumar Manvendra, Ass. Ts
Lanzilotto Valeria, Ass. Ts
Lopez Giorgia Maria, Ass. Ca
Lovat Giacomo, Ass. Ts
Malloci Giuliano, Ass. Ca
Marchese Roberto, Ass. Ts
Mattioli Giuseppe, Ass. Ca
Melis Claudio, Ass. Ca
Melli Mauro, Ass. Ts
Migliorini Elisa, Ass. Ts
Mitri Elisa, Ass. Ts
Monni Marco, Ass. Ca
Mukherjee Subhrangsu, Ass. Ts
Novelli Fabio, Ass. Ts
Olivieri Giorgia, Ass. Ts
Hossein Pakdast Seid, Ass. Ts
Palla Pierluca, Ass. Ca
Pellegrini Franco, Ass. Ts
Petrov Aleksandr, Ass. Ts
Piantanida Luca, Ass. Ts
Pierro Elena, Ass. Ts
Pozzato Alessandro, Ass. Ts
Radivo Andrea, Ass. Ts
Ricci Francesco, Ass. Ca
Rizzi Michele, Ass. Ts
Rossetti Giulia, Ass. Ts
Saba Maria Ilenia, Ass. Ca
Salles Benjamin, Ass. Ts
Sammito Davide, Ass. Ts
Sgrignani Jacopo, Ass. Ts
Sovernigo Enrico, Ass. Ts
Tavano Federica, Ass. Ts
Toffoli Valeria, Ass. Ts
Torchio Raffaella, Ass. Ts
Uffato Gianluca, Ass. Ts
Vaidya Shital, Ass. Ts
Vargiu Attilio Vittorio, Ass. Ca
Venturelli Leonardo, Ass. Ts
Verna Adriano, Ass. Ts
Virgilio Francesca, Ass. Ts
Vitali Ettore, Ass. Ts
Zacco Gabriele, Ass. Ts
Zannier Valentina, Ass. Ts
Zilio Pierfrancesco, Ass. Ts

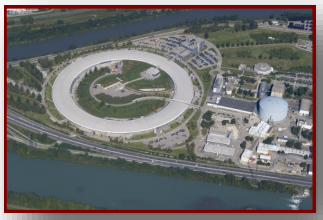
Locations and contacts

CNR-IOM (Trieste, TASC)
Area Science Park - Basovizza
Strada Statale 14 Km 163,5 - 34149 Trieste
ph. +39 040 3756411
www.iom.cnr.it
direttore@iom.cnr.it

Director: A. Morgante

CNR-IOM (Trieste, DEMOCRITOS)
c/o SISSA, Scuola Internazionale Superiore di Studi Avanzati
Via Bonomea 265, 34136 Trieste
ph. +39 040 3787443

Local contact: S. Fabris



CNR-IOM (Grenoble)
c/o ESRF, 71, Avenue des Martyrs
CS40220 F-38043 Grenoble Cedex 9, France
ph. +33 0476 882857

Local contact: F. D'Acapito

CNR-IOM (Cagliari)
c/o Dip.to di Fisica, Cittadella Universitaria,
09042 Monserrato, Cagliari
ph. +39 070 6754893

Local contact: A. Satta

CNR-IOM (Perugia)
c/o Dip.to di Fisica, Università di Perugia,
Via A. Pascoli, 06123 Perugia
ph. +39 075 5853060

Local contact: F. Sacchetti

Research activities

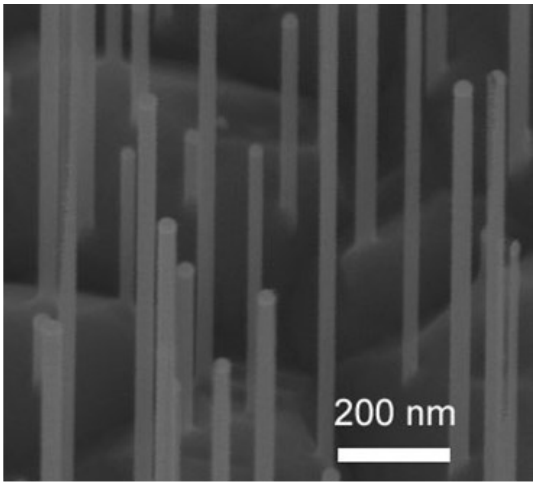
Istituto Officina dei Materiali

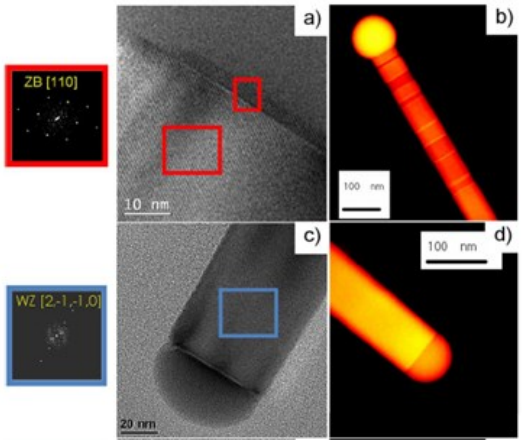
Semiconductor Nanowires Growth

Written by Silvia Rubini (rubini@iom.cnr.it)

Permanent staff: A. Franciosi, S. Rubini

Semiconductor nanowires are ideally 1-D nanostructures with diameter in the 1-100 nm range and in principle unconstrained length.
These systems are attracting increasing interest for the possibility they offer to exploit the properties related to their nano-scale size and their high surface to volume ratio in novel devices for electronics and optoelectronics.
NWs can be obtained by different growth methods and the anisotropic growth is typically induced by the presence of a metal nanoparticle that is found at the NW tip at the end of the process.
The activity of the molecular beam epitaxy (MBE) group has been devoted both to the study of the growth mechanism of III-V (GaAs, InAs, InGaAs) nanowires by MBE assisted by metal nanoparticles and to the investigation of the nanowire properties.
Concerning the growth mechanism, we developed novel Si-treated GaAs substrates suitable for the growth of Ga-assisted GaAs NWs and we studied the impact of As/Ga ratio on the morphology and on the structure of the nanowires, pointing out how As-rich growth conditions induce the collapse of the Ga nanoparticle at the NW tip and the formation of wurtzite GaAs. Moreover we studied the growth of InAs NWs assisted by different metals (Mn, Au) and self-assisted, pointing out how for this material system the suitable growth temperature range is very narrow and does not depend on the metal.
Concerning the characterisation of the NWs, we deeply investgated their morphological, structural, optical and electronic properties, via scanning and transmission electron microscopy, photoluminescence spectroscopy, optical reflectivity and spatially resolved syncrotron radiation photoemission spectroscopy, in by house activity and thanks to collaborations with CRN Institutes (IMM, IMEM, Nano) and ELETTRA Syncrotron radiation center.



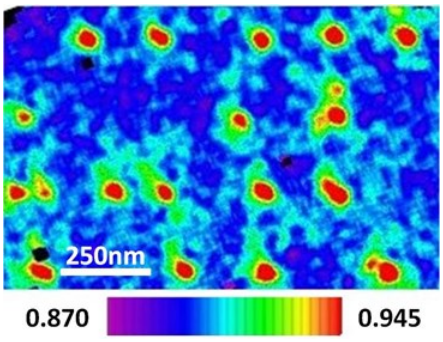


Top: as grown GaAs nanowires grown by Au-assisted MBE.
Bottom: TEM (a,c) and HAADF (b, d) images of Ga-assisted GaAs nanowires. On the left the FFT of the boxed areas evidencing the crystal structure.

Growth of High Purity Semiconductors and Site-Controlled Nanostructures

Written by Giorgio Biasiol (biasiol@iom.cnr.it)

Permanent staff: G. Biasiol, L. Sorba



2D In composition map of an InAs/GaAs QD array grown by MBE on a 250-nm period square hole array defined by electron beam lithography on a GaAs substrate

The HM MBE (High Mobility Molecular Beam Epitaxy) laboratory accomplishes the double function of facility for the synthesis of semiconductor materials with high quality and purity in external collaborations (in the fields of nanophotonics, coherent transport, biosensors, photon detectors), and of performing internal research activities devoted to the study of site-controlled, self-assembled quantum semiconductor nanostructures. The HM MBE system at TASC is the only one in Italy and one of the few in the world capable of synthesizing high-purity compound semiconductors, which allows to explore electronic transport regimes not attainable otherwise. We are able to synthesize 2D electron gases (2DEGs) in heterostructures based on both GaAs/AlGaAs materials, which allows the exploration of the more extreme regimes of coherent transport, on and InGaAs/InAlAs, with applications in spintronics and in hybrid superconductor-semiconductor devices. Several national and international collaborations are active, including a strong collaboration with the CNR-Nano Institute. Other collaborations are active in the field of nanophotonics. A collaboration with CNR-Nano, Scuola Normale Superiore, Pisa, and Konstanz and Paris Universities in the framework of cavity quantum electrodynamics, is dedicated to the implementation and control of ultra-strong light-matter interactions in the Terahertz regime, which open the possibility of observing of a whole new class of quantum phenomena and may find applications in next-generation optical information technologies. Within a collaboration with the Université Paris Diderot, we have synthesised multiple quantum well structures in planar waveguides, which allowed the observation of ultra-strong light-matter coupling. A collaboration with EPFL Lausanne is dedicated to the growth of GaAs membranes for the synthesis of ordered QD arrays coupled to photonic crystal defects in a microcavity. A collaboration the University of Padova and Veneto Nanotech, within the CaRiPaRo "Splendid" project, is dedicated to the realization of plasmonic devices based on GaAs/AlGaAs 2DEG patterned with gold gratings for the development of optical biosensors. We are also involved in the JRA HIZPAD2 project within the CALIPSO consortium; here our activity is devoted to the realization of an in-situ detector for the simultaneous monitoring of the position and intensity of the photon beam in Synchrotron Radiation and Free Electron Lasers. The more strictly internal research is aimed to the synthesis and the study of self-assembled quantum dots with full site control, through a hybrid top-down and bottom-up approach, by growth on nanoscale-size patterned substrates. This ensures a tight control over the dot location and properties, beneficial for today's devices, but also for a revolutionary new class of photonic devices. After the first tests on patterns defined by electron beam lithography, we have scaled the technique with use of nanoimprint lithography, which will open the way to a time- and cost-effective realization of broad-area devices based on site-controlled dots.

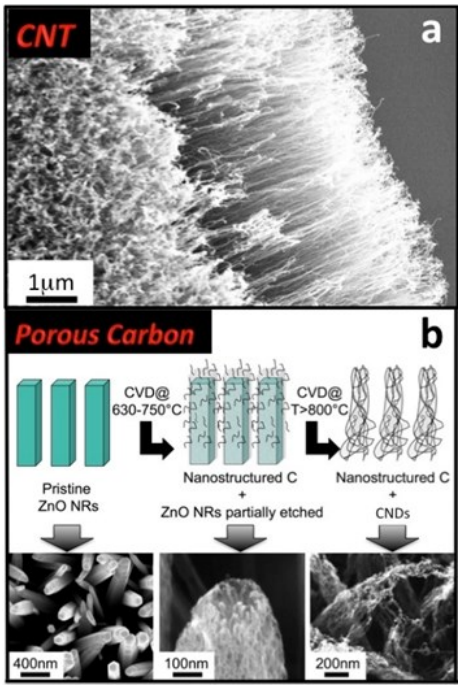
Istituto Officina dei Materiali

Nano Carbon Based Materials Growth and Characterization

Written by Cinzia Cepek (cepek@iom.cnr.it)

Permanent staff: C. Cepek

The growth of carbon-based materials by chemical vapour deposition (CVD) is of great scientific and technological interest, as CVD allows the direct growth on substrates at low temperature and may facilitate the integration of these materials into various technologies. Optimised catalytic CVD recipes yield the growth of well ordered graphene overlayers, as well as vertically-aligned forests of carbon nanotubes (CNTs) with controlled location, diameter, and density, properties which are required for many CNTs applications, including interconnects, supercapacitor electrodes, thermal management surfaces, or adhesive layers. The IOM Analytical division has several years of experience in the growth of carbon-based materials. In 2010 -2012 the work inside this research line was focused into the study of the growth mechanisms governing the synthesis via catalytic CVD of many carbon nanostructures, spanning from CNTs and nanofibers to graphene, up to porous nanostructured carbon. The growth processes were studied using *in-situ* spectroscopic and microscopy techniques, with the objective to find the best protocols allowing the controlled synthesis of *a priori* defined carbon nanostructures. In the available experimental apparatus it is possible to control the chemical state of the catalyst and precisely monitoring all the CVD parameters, such as: precursor gas purity (*via* residual gas analyser), pressure and its gradient, sample temperature, gas fluxes, etc.



a) SEM image of a CNTs forest grown on a conductive TiN film; b) Growth scheme and corresponding SEM images of C-nanostructures obtained after different CVD processes done on ZnO NRs templates.

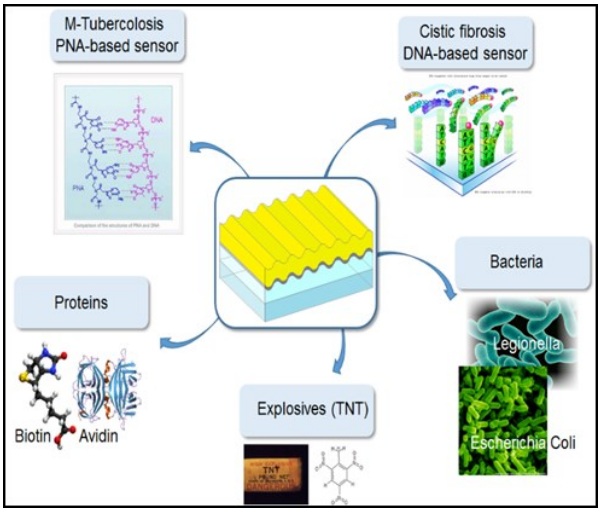
These characteristics allow understanding in detail the mechanisms driving the synthesis, and allowed us to determine the conditions necessary to obtain high-density CNT forests non only on oxide substrates, but also on metallic overlayers, fundamental requirement to use these material in interconnect and supercapacitors. We also showed that CVD on vertically aligned ZnO nanorods (NRs) can synthesize different carbon nanostructures, whose morphology is driven by the NRs and whose dimensions and structures change as a function of the process temperature. When used as a chemiresisitor, the so-obtained porous carbon has a higher sensitivity to ammonia compared to chemiresistors made by bare ZnO NRs, to other one-dimensional C-nanostructures. Inside these research topics, IOM-CNR was a partner of the FP7 project (large) *Technology for Wafer-Scale Carbon Nanotube Applications*, and in 2012 was approved the PRIN 2010 project *Hierarchical Photosynthetic Nano-Structures for Carbon-Neutral Renewable Energy* (HI-PHUTURE).

Plasmonics materials and nanodevices

Written by Filippo Romanato (romanato@iom.cnr.it)

Permanent staff: F. Romanato

In recent decades, surface plasmon resonance has known a growing interest in the realization of miniaturized devices for label-free sensing applications due to the need of increasing the sensitivity of the sensor and limiting the consumption of material. This research activity is aimed to the realization of plasmonic nanostructures that can be applied to different sensoristic fields in order to create a starting point for the realization of miniaturized sensors for a wide range of applications.
In this context a careful study of geometry and materials suitable for creating the starting plasmonic platforms (i.e. gold sinusoidal gratings) was performed and a characterization method has been optimized.
Subsequently a manufacturing strategy that would allow to obtain a large number of versatile substrates in a short time and in a cheap way was designed.
Thus by combining interference lithography and soft lithography the required plasmonic substrates were realized and characterized by varying the azimuthal rotation of the grating. The substrates were tested in different application fields: the detection of M. tuberculosis DNA using PNA probes, the detection of cystic fibrosis DNA using DNA probes, the detection of explosive trace and the detection of legionella bacteria.
The reached optimization and control of the sensing experiment and plasmonic surface preparation procedures, and the obtained results, have shown the extreme versatility of the sensors realized with respect to different applications.
One of the most important result of this thesis work is the demonstration of the applicability of our sinusoidal grating to a wide range of sensing application with results, in term of efficiency, sensitivity and resolution, at the state of the art or above. Starting from this result, the possibility of further develop our detection system and integrate the sensing platform here described into a final miniaturized device is now open and the transfer of our sensing prototype to commercial or medical field could be easily achieved in the future.



Sensors realized in this work starting from the same plasmonic sensing platform

Istituto Officina dei Materiali

Growth of complex oxide heterostructures with atomic control

Written by Bruce Davidson, davidson@iom.cnr.it

Permanent staff: B. A. Davidson, A. Giglia, N. Mahne, S. Nannarone, M. Pedio

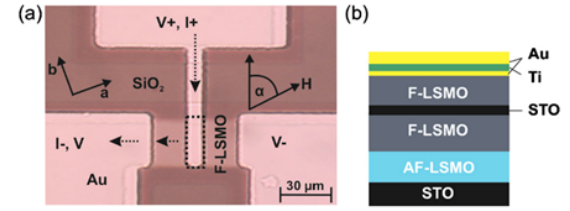


FIG. 1. (Color online) (a) Optical image of the MTJ. The arrows indicate the current flow while the junction area is indicated by the dashed rectangle. (b) The inset shows a cross section of the stacking sequence of the MTJ.

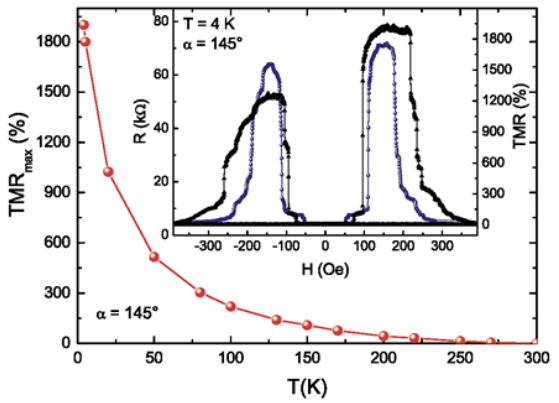


FIG. 2. (Color online) Maximum TMR ratio vs. temperature for $\alpha_{FC}=70°$, $\alpha=145°$. The inset shows two $R(H)$ sweeps measured at 4 K for the same field conditions after different cooling cycles.

The Oxide MBE (OxMBE) laboratory has the goal of atomic design of interfaces to probe new physical phenomena for future devices, that it realizes through three main research lines: 1) development of new growth methods to improve atomic–layer control during the growth of complex oxide films; 2) application of these methods to the atomic design of perovskite interfaces; and 3) study of these interfaces in devices. During the period 2010 –2012, we have focused on magnetic oxides based primarily manganites (e.g. $LaMnO_3$ and $SrMnO_3$) and ferrites ($LaFeO_3$ and $SrFeO_3$), and insulators and ferroelectrics based on titanates (e.g. $SrTiO_3$ and $BaTiO_3$). Initial work began as well on multiferroic films of $BiFeO_3$ possessing coupled ferroelectric and antiferromagnetic properties.

Our approach to the atomic design of interfaces culminated in its successful completion of the regional FVG "SPINOX" project (ending in 2011) with a series of important results on magnetic tunnel junction (MTJ) devices based on manganites [1, 2]. The key was the development of a new method to use *in situ* reflection high-energy electron diffraction (RHEED) to identify the surface termination layer at any point during the growth. Consequently, just prior to the tunnel barrier deposition during the growth of the MTJ heterostructure, the surface termination could be adjusted as desired. This level of control over the atomic stacking at the electrode/barrier interface resulted in unprecedented values of the tunneling magnetoresistance (TMR) over 1900%, the highest in the literature for any materials system including CoFeB/MgO. Unfortunately this high TMR persists only at low temperature, and drops to zero near room temperature. Advanced characterization of the electronic structure of these interfaces is currently being performed to understand the underlying causes for this temperature dependence of the interfacial spin polarization, and eventually bring the operating temperature up to room temperature.

[1] R. Werner, A. Yu. Petrov, L. Alvarez Miño, R. Kleiner, D. Koelle and B. A. Davidson, "*Improved tunneling magnetoresistance at low temperature in manganite junctions grown by molecular beam epitaxy*", Appl. Phys. Lett. 98, 162505 (2011).

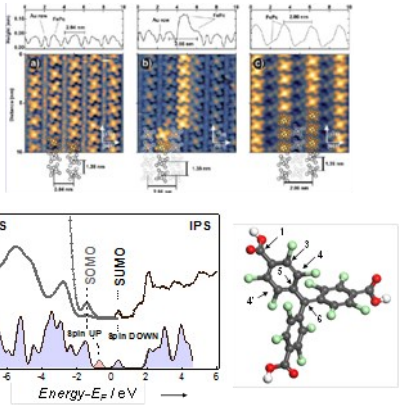
[2] R. Werner, M. Weiler, A. Yu. Petrov, B. A. Davidson, R. Gross, R. Kleiner, S. T. B. Goennenwein and D. Koelle, "*Local tunneling magnetoresistance probed by low-temperature scanning laser microscopy*", Appl. Phys. Lett. 99, 182513 (2011)..

Electronic and paramagnetic properties of open shell molecular thin films

Written by Maddalena Pedio (pedio@iom.cnr.it)

Permanent staff: M. Pedio

Single molecule magnets, and metal-organic molecules adsorbed on surfaces have been receiving much attention for their potentiality in the realization of spintronics devices. A key stage in their engineering is represented by controlling the molecular assembly into ordered networks. Two case systems are here reported: planar transition metal phthalocyanine (MPc) nanochains on Au(110) and Open Shell tri-para-carboxylic perchlorotriphenylmethyl Radical PTMTC on Au (111) and Ag(111) substrates. In the first case the magnetism is provides by the 3d empty states of the central metal atom, while in case of radical the open-shell electronic configuration corresponds to the unpaired electron of the central C atom. In all these cases our results reveal the effect on magnetic moment due to the electronic mixing of the interface states. For Transition Metal complexes the interconnection between the structural phases of ordered FePc-nanochains self-assembled on Au(110) and the paramagnetic properties has been enlighten. [1] The chain assembly is driven by the molecule–molecule interaction and the chains interact with the Au nanorails via the central metal atom, while the chain–chain distance in the different structural phases is primarily driven by the redistribution of the Au substrate.



Up: STM Nanochains of FePc on Au(110) as a function of coverage a) 0.5, b 0.7, c) 0.8 ML. Bottom Right: Molecular structure of radical PTMTC. C grey; Cl green; oxygen red; H white. Bottom Left: PES-IPS spectra of thin films of PTMTC the SOMO and SUMO respectively. Bottom: calculated Density of States (DOS) of the spin up (red shadow) and spin down (blue shadow) of the isolated molecule.

In case of FePc and CoPc this hybridization leads to a decreasing of the paramagnetic properties. The magnetic moment is recovered only for thin films aggregations.

Purely organic free radicals appear suitable candidates towards applications thanks to the small spin orbit-coupling and hyperfine interactions that allow for long spin relaxation times. In case of three dimensional radical PTMTC and the presence of a Single Occupied Molecular Orbital (SOMO) and its unoccupied counterpart (SUMO) are clearly detectable as frontier orbitals in combined Photoemission (PES) and Inverse Photoemission (IPS) data [2]. Recently we found that in case of PTMTC deposition on Au(111) the paramagnetism of the organic radical is preserved while it appears partially quenched on Ag(111). This antithetic behaviour is explained on the basis of a detailed study of the interfacial electronic properties: The spin loss and preservation for such organic radicals could not have been demonstrated without looking inside the interface.

1] M G Betti, P.Gargiani, Carlo Mariani, R. Biagi, J.Fujii, G.Rossi, A. Resta, S. Fabris, S. Fortuna, X. Torrelles, M. Kumar, M. Pedio Langmuir 2012 DOI: 10.1021/la302192n; P.Gargiani, G. Rossi, R. Biagi, V. Corradini, M. Pedio, S. Fortuna, A. Calzolari, S. Fabris, J. Criginski Cezar, N. Brookes, M. G. Betti Phys. Rev B, 87 165407 (2013).
[2] F. Grillo, V. Mugnaini, M. Oliveros, S. M. Francis, D-J. Choi, M. V. Rastei, L. Limot, C. Cepek, M. Pedio, S.T. Bromley, N.V. Richardson, J-P. Bucher, J. Veciana, J. Phys. Chem. Lett., 3 1559-1564 (2012).

Organic Interfaces and Charge Transfer

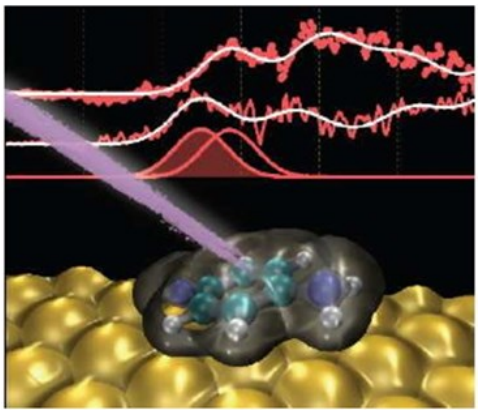
Written by Luca Floreano (floreano@iom.cnr.it)

Permanent staff: A. Cossaro, L. Floreano, A. Verdini, G. Bavdek, D. Cvetko, A. Morgante

This research line aims at improving our knowledge and modeling of the interfacial properties of small organic molecules at surfaces. The pivotal interest is centered on organic semiconductors, but much attention is also payed to the properties of the substrates as well as to there functionalization. With the goal of setting new directions for the fabrication/assembly of high performance devices, we aim at a self consistent description and tailoring of the dynamical processes of chemical interaction as well as charge transport at interfaces. Starting from the basic study of the single components, we follow the modification of the electronic structure at hybrid organic-inorganic and hetero-organic junction, which are representative of the full architecture of an archetypal device.

For a better control of the system degrees of freedom, the substrate interaction is studied starting from single crystal surfaces. The latter are eventually nanopatterned and/or functionalized with an intermediate self-assembled monolayer (alkanethiols, aminoacid derivatives) for specific linking to the substrate and suitable coupling to the next layer molecules.

Coinage metal surfaces are mostly employed as archetypal electrodes, while a growing interest is dedicated to specific transition metal oxides, which can display large conductivity upon reduction and/or doping. For a modeling purpose, most studies are focused on planar aromatic and heteroaromatic molecules (such as poly-conjugated aromatic hydrocarbons and phthalocyanines), that are eventually functionalized to trim their interaction with the substrate or with electronically/ chemically complementary organics. We employ a large suitcase of techniques spanning from Synchrotron radiation spectroscopy to scanning probe microscopy for achieving a chemical and structural characterization of the systems. We make use of advanced spectroscopic techniques, such as valence band resonant photoemission, to study the dynamics of charge transfer down to the femtosecond timescale, whereas the static charge transfer, which measure the degree of chemical interaction, is probed via conventional Synchrotron spectroscopy (both emission and absorption). This research line is pursued in collaboration with several research groups in Italy (Chem. Dep. Univ of Padova, Rif. Maurizio Casarin; Phys. Dep., Univ. MIBicocca, Rif: Gian Paolo Brivio) and abroad (ICMM-CSIC, Madrid, Rif. Jose', A. Martin-Gago; UPV/EHU-CSIC San Sebastian, Rif. Celia Rogero; Phys. Dep. Univ. Columbia, NY, Rif. Latha Venkataraman).



Top: valence band resonant photoemission spectra for a benzenediamine molecule adsorbed on Au (111) and Au(110), as shown in the 3D drawing on the bottom. At variance with conventional ultraviolet spectroscopy, only the VB states localized on the carbon atoms are singled out when the photon energy is tuned to the Carbon ionization threshold

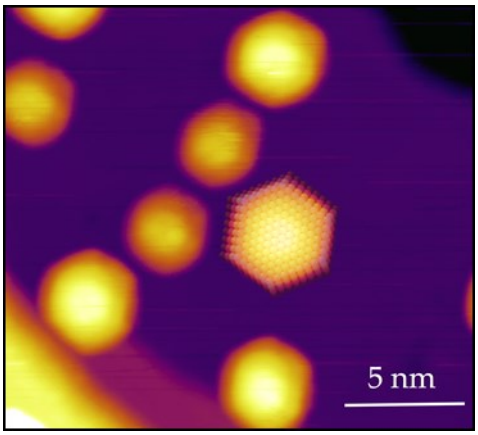
Catalytic processes at surfaces

Written by Cristina Africh (africh@iom.cnr.it)

Permanent staff: C. Africh, A. Baraldi, E. Vesselli, C. Dri, G. Comelli

This research line is focused on the determination of the geometric and electronic structure of solid surfaces, with specific interest in the characterization of their chemical activity. A variety of systems, including clean and adsorbate covered transition metal surfaces, ultra-thin oxide films, surface alloys, self-assembled organic monolayers and hetero-architectures, and epitaxial graphene are investigated. The main goal is the understanding of the interaction of adsorbates with surfaces, analyzing the induced structural modifications, the formation of bonds, the changes in the electronic structure at the interface, and the elementary steps involved in surface processes (e.g. atomic and molecular diffusion, segregation, growth, chemical reactions). Catalytic systems are investigated by both microscopy and spectroscopy techniques. In particular, Scanning Tunneling Microscopy is used for characterizing at the atomic scale the induced structural modifications.

Experiments are performed in a wide range of temperature regimes, from 4K to 900K, to explore different processes and enable complementary approaches. Both temperature- and gas-induced surface kinetics are monitored in-operando with variable frame rates, up to video-rate. At 4K, single molecule vibrational spectroscopy is also applied. X-ray Photoelectron Spectroscopy is often used for chemical characterization before, during and after surface processes; furthermore, Low Energy Electron Diffraction and Thermal Desorption Spectroscopy complement the experiments. In many cases catalytic surface processes are investigated also by synchrotron radiation at Elettra – in particular Super-Esca, Nanospectroscopy and ALOISA beamlines – or at other international facilities. Finally, experimental results are often corroborated with and compared to ab-initio calculations performed by collaborating groups at both local and International institutions. In order to continuously improve the experimental capabilities for the investigation of chemical surface processes, a thorough effort is dedicated to the constantly and progressive update, development, and realization of new instrumentation. In this context, a prototype of an add-on module for fast scanning was developed and implemented in collaboration with the Detectors and Instrumentation Lab of Elettra, and a method for driving a scanning probe microscope at elevated scan frequencies was recently patented. The latter innovation introduces the possibility to investigate a new range of surface process, with an imaging rate exceeding 100 frames/s. To reduce the surface science pressure gap, a novel experimental setup, dedicated to vis-IR sum frequency generation vibrational spectroscopy (SFG) has recently been designed and commissioned. It will allow investigation of surfaces from UHV up to ambient pressure and in liquid, in situ and in operando under (electro)-catalytic conditions.



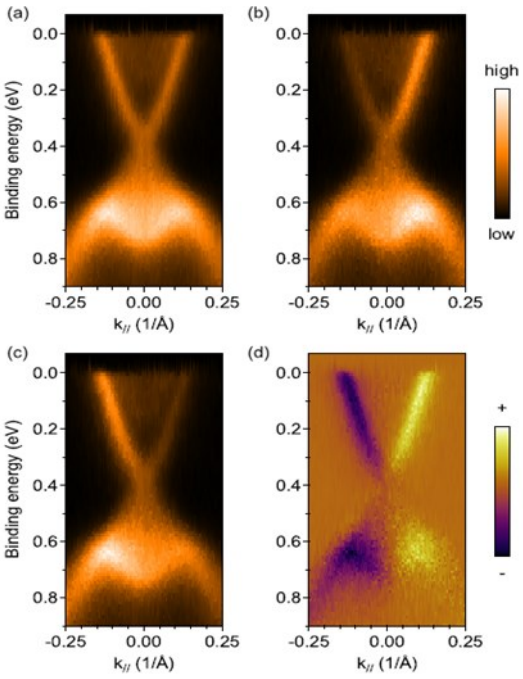
Rh clusters deposited on graphene/Ir(111)
[A. Cavallin *et al*, ACS Nano **6** (2012) 3034-3043]

Istituto Officina dei Materiali

Quantum phenomena in innovative materials

Written by Giancarlo Panaccione

Permanent staff: G. Panaccione, P. Torelli, I. Vobornik, J. Fujii, D. Krizmancic



(a) ARPES of a 50-QL-thick Bi2Se3 thin film (hv= 60 eV (b,c) Same as (a), with a circular left and right polarization, respectively (d) dichroic signal

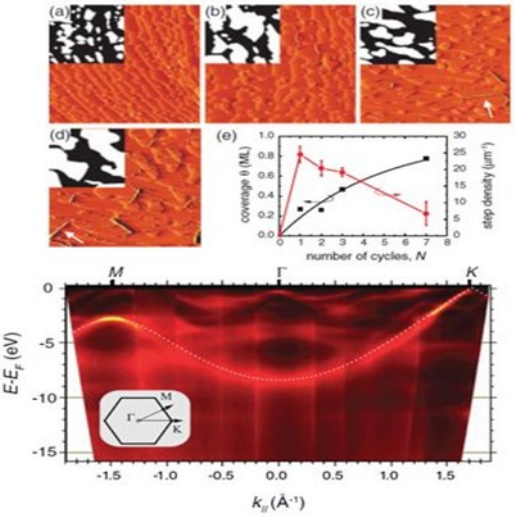
The collective behaviour of matter is one of the central topics of modern science and technology. Collective quantum phenomena in materials arise from the interplay between quantum mechanics and interactions in many-particle systems — i.e., materials for which the interactions between particles cannot be treated in a classical manner. The atomic environment provides a unique opportunity to understand the quantum nature of matter, and the search for fundamentally new states of matter is a central challenge at the intersection of basic and applied science, and a crucial crossroad for technological innovation. One of the next frontiers in the research of quantum effects will be the ability of understanding, designing, and controlling, i.e. 'building' systems with tailored structural, electronic and magnetic properties, directly connected with a whole new world of emergent new collective phenomena (to name but a few self-assembly and self-ordering, quantum size confinement, wave-like transport, orbitally/magnetically driven effects). To address such goal, advanced synthesis and growth capabilities (PLD, MBE) are coupled to analytical tools based on synchrotron radiation spectroscopies.The materials under investigation mainly address the search of new functionalities in systems where surface/interface effects and quantum confinement give rise to new collective phenomena, as unconventional superconductors, multiferroics, and topological insulators. Furthermore, a promising direction that goes beyond conventional methodologies is to tailor novel properties by exploiting heterostructures of complex oxides, anomalous metals and diluted systems. Recent examples of such research field are: i) the electric control of magnetization at the ferromagnet/ferroelectric interface, ii) the analysis of hybridization and phase separation in diluted magnetic semiconductor and iii) the magnetic proximity effect in ferromagnet/ topological insulators hybrid structures. In order to reach a step forward in the control of functionalities, a fundamental understanding of synthesis processes and functional behaviour must be gained. A significant effort has been devoted in recent year to the development and integration of In-operando experiments (applied magnetic and electric field) , where real time informations allow designing more effective and efficient synthesis routes.

Surfaces, films and interfaces

Written by Elena Magnano (magnano@iom.cnr.it)

Permanent staff: F. Bondino, L. Floreano, J. Fujii, E. Magnano, A. Verdini, I. Vobornik

A multitude of fundamental chemical and physical processes occurs at surfaces and interfaces that drives the behavior of catalysts, chemical sensors, and devices for optoelectronics, light harvesting/conversion, magnetic applications. Thin films of the order of a few nanometers in thickness have been shown to be useful analogues of bulk materials. At the same time, tailoring the film size at the nanoscale allows the fine tuning of the electronic properties due to the quantum confinement. The study of surfaces and thin films has driven the development of a number of technologically advanced experimental techniques in order to probe and modify such systems down to the scale of single atoms. The surface reactivity and conductivity of many transition metal oxides, TMO, is much relevant for the fabrication of efficient catalysts and photovoltaic cells (e.g. TiO_2). The electronic properties of TMOs depend on the possibility of locally inject charge, which is made available elsewhere by the surface for triggering chemical reaction or for being extracted. The atomic distribution of the charge in the surface and nearby layers can be probed by means of resonant photoemission, which allows one to achieve chemical sensitivity in the valence band. In particular, one can discriminate among atoms of the same species but with different ionization states. The corresponding intensity enhancement of the photoelectron yield can be valuably exploited also to study the distribution of dopants in highly diluted semiconductors (e.g. $Mn_xCd_{1-x}Te$). The magnetic ordering and coupling in diluted magnetic systems (e.g Fe/(Ga,Mn)As) or in ferromagnetic metal/semiconductors heterojunctions (e.g. Mn/Si, Mn/Ge) are very suitable to realize structures in which the magnetic properties of the semiconductors are controlled by designed magnetic ions or to combine silicon technology with the functionality of magnetic systems, making these systems promising for applications in the field of spintronics. The ferromagnetic ordering of these systems can be revealed by x-ray circular magnetic dichroism measurements , probing the magnetic properties of specific elements in thin films that cannot be explored with conventional magnetic tools due to the reduced layer thickness. The combination of scanning tunneling microscopy and high resolution angle resolved photoemission spectroscopy reveal the growth morphology and the peculiar electronic properties of graphene/metal interfaces (e.g. graphene/Ru, Ir, Pt) and the chemically modified (doped or functionalized) graphene or graphene oxide layers by self-assembling of on-purpose synthesized organic precursors with tailored features.



Scanning tunneling microscopy characterization of the graphene growth in Ir(111) and ARPES map showing the dispersion of the π band for the ΓK and ΓM directions *M. Kralj et al. Physical Review B, 84, 075427 (2011)* - Data collected at APE beamline, Elettra.

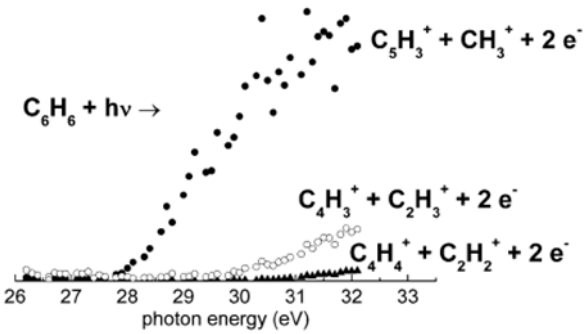
Istituto Officina dei Materiali

Electronic properties of gaseous phase systems

Written by Antti Kivimäki (kivimaki@iom.cnr.it)

Permanent staff: M. Alagia; M. de Simone; A. Kivimäki

The electronic structure of any matter determines its most physical and chemical properties. It can be studied with spectroscopic methods: one subjects matter, for instance, to electromagnetic radiation and observes how it responses. We perform our studies by directing monochromatized synchrotron radiation on isolated molecules or atoms and by detecting angular and energy distributions of any particles that are ejected: electrons, singly or multiply charged ions and photons, sometimes in coincidence with each other. These processes can be understood best in gaseous samples. We carry out research within the Research Group of the Gas Phase Photoemission beamline (Elettra-Sincrotrone Trieste, CNR-IOM and CNR-ISM). The beamline delivers highly monochromatic radiation. in the photon energy range 14-900 eV. Lowest photon energies are suited to studies of valence electron transitions, while the high energy part allows us to induce 1s electron transitions in atoms such as C, N and O. As an example of valence ionization studies, the electronic structure of iron phthalocyanine (FePc) was examined within a joint theoretical–experimental collaboration [J. Chem Phys. **134**, 074312 (2011)]. Particular emphasis was placed on the determination of the energy position of the Fe 3d levels in proximity of the highest occupied molecular orbital. Photoelectron spectroscopy measurements were performed on FePc in gas phase at several photon energies between 21 and 150 eV. In the core region, S 2p photoionization in the SF_6 molecule has attracted much attention because its cross section displays very intense shape resonances. In a combined experimental and theoretical study, Stener et al [J. Chem. Phys. **134**, 174311 (2011)] proved that the effect of the shape resonances extends even up to 80 eV above the S 2p ionization thresholds. In another study of the SF_6 molecule, Auger decays of the S $2p^{-1}$ states and of its first shake-up state, which is characterized by an electron configuration S $2p^{-1}val^{-1}virt^{1}$, could be separated using electron-electron coincidence spectroscopy [J. Chem. Phys. **134**, 094308 (2011)]. We have studied O 1s excitation and ionization processes in the CO_2 molecule using UV-visible fluorescence spectroscopy and VUV photon-photoion coincidence technique [J. Phys. B **44**, 165103 (2011)]. Detected UV and VUV photons are created when the final states of Auger decay dissociate into valence-excited neutral or ionic fragments. Remarkably, the fluorescence yield of a transition in the neutral O atom displays all the single and double excitation features seen in the O 1s absoption spectrum of CO_2. In another study, Kivimäki, Alagia and Richter [Chem. Phys. Lett. **531**, 252 (2012)] exploited x-ray emission-photoion coincidence spectroscopy to study how the CO_2 molecule dissociates when diverse O 1s hole states decay via soft x-ray emission.



Alagia et al [Phys. Chem. Chem. Phys. **13**, 8245 (2011)] used a time-of-flight mass spectrometer to study dissociative double ionization of benzene by VUV synchrotron radiation. The threshold energies of the main dissociative processes were characterized by exploiting the photoelectron-photoion-photoion coincidence technique.

Magnetism and electron correlation at the nanoscale

Written by Silvio Modesti (modesti@ts.infn.it)

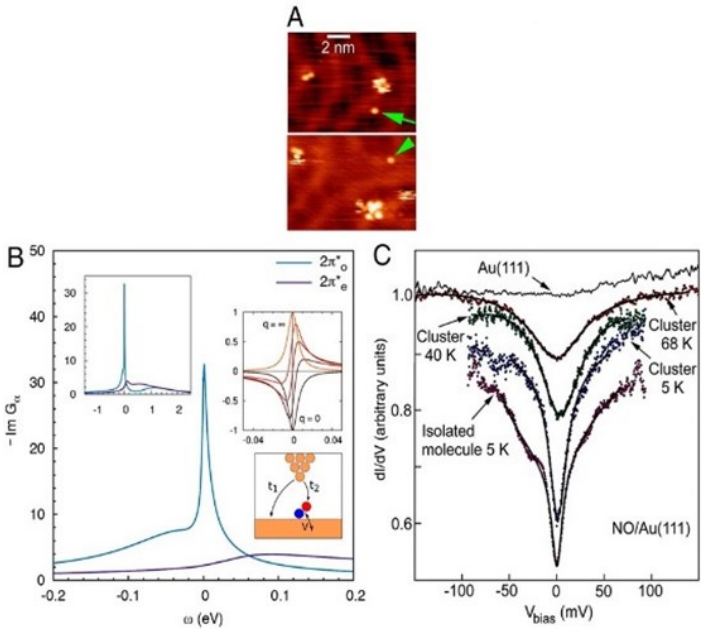
Permanent staff: S. Modesti

Model systems simple enough to be tackled by *ab initio* calculations and containing key ingredients of more complex strongly-correlated systems are useful playgrounds to test the validity of current attempts to describe many-body systems bridging the gap between the approximations based on the Density Functional Theory and on simple model Hamiltonians. The Kondo state is a well-known many body state that arises from the interaction between a localized degree of freedom (e.g. a spin) and a sea of delocalized electrons. The physics of this state is well captured by a model Hamiltonian, but its parameters could not be obtained by *ab initio* methods till now.

In collaboration with a the Tosatti-Fabrizio group at Democritos we have chosen the simplest and exemplary spin ½ molecule – N - physisorbed on the unreactive metallic Au(111) surface to quantitatively compare the spectral function experimentally obtained by scanning tunneling spectroscopy (STS) on single molecules and by photoemission spectroscopy with the predictions of recently-proposed ab-initio methods for Kondo systems.

The prediction of a Kondo state with a Kondo temperature of the order of 15 K is experimentally verified, and the discrepancies between the calculated and the experimental lineshape provide an instructive measure of the approximations used in the modeling.

Other model systems under investigation in the 2010-2012 period by STS and photoemission were simple two-dimensional systems that undergo a metal-insulator transition at high temperature, such us 1/3 of a monolayer of Sn on Si(111) and the clean Si (111)-7x7 surface. In the former case a Mott-Hubbard ground state well describes the experimental STS and photoemission data below 60 K and the metallization at higher temperature, in the latter case a simple Mott-Hubbard mechanism in not enough to explain the transition observed at 20 K and magnetic effects seems important.



A) Isolated NO molecules on Au(111) at 5 K (arrows).
B) Calculated spectral density for the Kondo state.
C) Tunneling spectra showing the Kondo zero bias anomaly from 5 to 70 K

R. Requist et al., PNAS 111, 69 (2014)

Istituto Officina dei Materiali

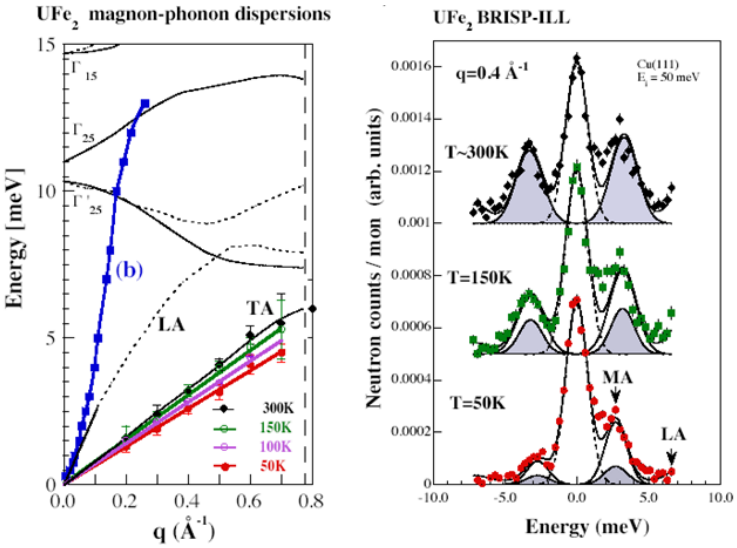
Neutrons and Magnetism

Written by Francesco Sacchetti (sacchetti@iom.cnr.it)

Permanent staff: F.Formisano, C. Petrillo, F. Sacchetti

The neutron scattering has been introduced from the beginning in 1946 as a major tool to study the magnetism at the microscopic level. The characteristics of the BRISP spectrometer at ILL (i.e. the rather high incident neutron energy and the proper coverage of the low scattering angle region) make it a perfect tool to investigate the magnetic dynamics in the energy range up to several tens of meV. Although the most part of research activity on BRISP is devoted to investigate the collective atomic dynamics in disordered systems. In the last years the BRISP spectrometer has been employed to study the magnetic dynamics of different systems. BRISP has been proved to be an efficient tool to study the magnetic dynamics in systems where a single crystal of adequate volume is not available as the instrument allows for studying all systems in the first Brillouin zone while the usual three axis instruments are normally adequate to perform experiments in the second Brillouin zone. This possibility was applied in the study of SrRuO3, a system having a relationship to SrRuO4 which shows a mixed behavior with superconductivity.

The ruthenate $SrRuO_3$ is a weak ferromagnet which shows a dynamics well described by the Moriya model on increasing the temperature. Further experiments are being performed in order to have a complete description of this system (A. Orecchini, C. Petrillo, J. Park and co-workers).The performance of the spectrometer has been shown to be excellent also in the study of the UFe_2 allowing for the description of the anomalous magnetoelastic behavior in this compound [L. Paolasini, F. Formisano, R. Caciuffo, G. H. Lander, G. Lapertot, Journal of Physics: Conference Series **340**, 012063 (2012)].



These experiments were performed using a magnetic field useful to increase the inelastic magnetic signal along the field direction. The successful results are indicating that a proper magnetic field must be provided to improve the performance of BRISP in magnetic studies.

A) UFe_2 phonon dispersion curves. The vertical dashed line indicates the Brillouin zone boundary.
B) Temperature dependence of the neutron scattering intensitieson BRISP at 0.4 $Å^{-1}$.

Magnetization dynamics in ferromagnetic nanostructures

Written by Gianluca Gubbiotti (gubbiotti@fisica.unipg.it)

Permanent staff: G. Gubbiotti, S. Tacchi

The IOM researchers working at the Perugia unit conduct their activity for investigating both the static properties and the magnetization dynamics of low dimensional magnetic systems such as, thin film, multilayers and patterned structures by means of magneto-optic Kerr effect (MOKE), magnetic force microscopy (MFM) and both conventional and micro-focused Brillouin light scattering (BLS) technique. This latter technique, based on the inelastic scattering of light from both thermal and microwave excited spin waves, has proven to be a powerful tool for investigating the magnetization dynamics in the GHz frequency range with high frequency and spatial resolution. BLS experiments are performed either in-situ, by using the ultra-high vacuum chamber available in our laboratory, or ex-situ on samples prepared by other research groups.
The research activity on thin ferromagnetic films and multilayers has be primarely focused, respectively, on the spin excitation properties of Fe film epitaxially grown onto MnAs/GaAs(001) substrate,[1] which exhibits stripe magnetization domain, and out-of-plane magnetized systems such as Co/Ni multilayers [2] which find application as polarizing layers in spin-torque oscillators.
Concerning patterned elements, our attention has been focused either on array of isolated (not-interacting) dots, dipolarly coupled dots and continuous films with regular array of etched holes (see Fig. 1).
New properties of spin excitations have been observed, such as the existence of quantized non-dispersive resonant modes and localized excitations, due to the lateral confinement and to the inhomogeneity of the internal magnetic field, respectively.
When the inter-element separation is sufficiently small (typically below 100 nm) dynamic dipolar coupling leads to the formation of collective modes propagating through the array, with the appearance of Brillouin zones determined by the artificial periodicity. [3]
Finally, the propagation properties of spin wave launched into a continuous permalloy film either from a spin torque oscillator[4] or from a coplanar wave guide [5] have been investigated by means of micro-focused BLS having lateral resolution of about 250 nm.

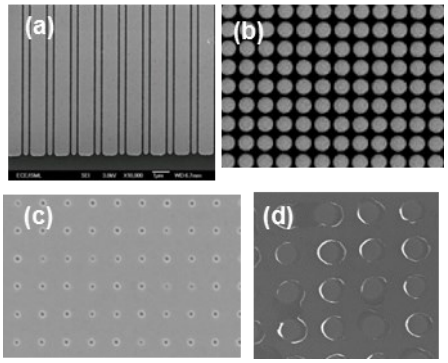


Fig. 1 SEM images of some representative 1D and 2D patterned structure: (a) array of stripes with alternating width, (b) array of circular disks, (c) an permalloy antidot array regular circular holes and (d) an antidot array with holes filled by Co dots.

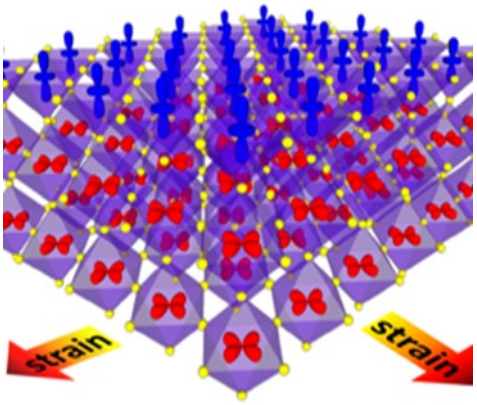
References:

1. C. Helman, J. Milano, S. Tacchi, M. Madami, G. Carlotti, G. Gubbiotti, G. Alejandro, M. Marangolo, D. Demaille, V. H. Etgens and M. G. Pini, Phys. Rev. B 82, 094423 (2010)
2. G. Gubbiotti, G. Carlotti, S. Tacchi, M. Madami, T. Ono, T. Koyama, D. Chiba, F. Casoli, and M. G. Pini, Phys. Rev. B 86, 014401 (2012)
3. Gubbiotti, S. Tacchi, M. Madami, G. Carlotti, A. O. Adeyeye and M. Kostylev , J. Phys. D: Appl. Phys. 43 264003 (2010).
4. M. Madami, S. Bonetti, S. Tacchi, G. Carlotti, G. Gubbiotti, G. Consolo, F. Mancoff, M.A. Yar, and J. Åkerman, Nature Nanotech. 6, 635 (2011)
5. G. Duerr, M. Madami, S. Neusser, S. Tacchi, G. Gubbiotti, G. Carlotti, and D. Grundler, App. Phys. Lett., 99, 202502 (2011)

Strongly correlated magnetic systems

Written by Claudia Mondelli (mondelli@ill.fr)

Permanent staff: F. Bondino, L. Capogna, E. Magnano, C. Mondelli, P. Torelli



The effects of symmetry breaking at free surfaces of ABO_3 perovskite epitaxial films can be combined with substrate-induced epitaxial strain to tailor at will the electron occupancy of in-plane and out-of-plane surface electronic orbitals. *D. Pesquera et al. Nature Communications, Vol. 3, pp. 1189 (2012)*..

Strongly correlated systems, are subject of intense research nowadays because of their uncommon properties due to complex interactions arising from coupling of lattice, spin and charge degrees of freedom.
This research concerns several classes of materials, topics and techniques.
Multiferroic, manganites, perovskite oxides, iron based superconductors, ruthenates, pinictides, vanadates are between the studied materials.
The goal is to study the influence of electronic, chemical, structural properties on magnetism, spin dynamic and conductivity from the fundamental aspect to industrial application and devices.
The number of subjects touched in this research, is quite wide: influence of inhomogeneities and clusterization on the spin dynamic in half doped manganites; topologically protected conducting surface states of so-called topological insulators; metal insulator transition and anomalous electronic properties in highly correlated 3d and 4d oxides magnetic transition and anisotropies in interfaces (AFM/FM, FM/FM.); proximity magnetic effect dilute magnetic semiconductors and their epitaxial interfaces (GaMnAs, Fe/GaMnAs); topological insulators and their interface/doping with magnetic elements; orbital hybridization effects on the magnetic and superconducting properties of iron-based superconductors and in multiferroic systems; orbital occupancy of the Mn 3d-related electron levels in LSMO and LCMO epitaxial thin films; itinerant ferromagnetism, metamagnetic quantum criticality, superconductivity in ruthenates.
We use mainly synchrotron x-ray spectroscopies, neutron diffraction and neutron scattering, with and without polarization analysis.
In particular the determination of magnetic structures are obtained by high resolution neutron diffraction and the study of spin dynamic, spin density, frustration and short range dynamic correlations in manganites and ruthenates, has been done by neutron scattering with and without polarization analysis.
Interfaces properties and orbital hybridizations as well as electronic properties has been studied by mean x-ray absorption spectroscopy and soft x-ray spectroscopy.
The analysis of neutron data are supported by calculations using ab-initio, density functional theory-based methods and classical, force field-based methods to perform structure - including electronic and spin aspects, lattice dynamics and molecular dynamics simulations.

Optical nanomanipulation for biological systems

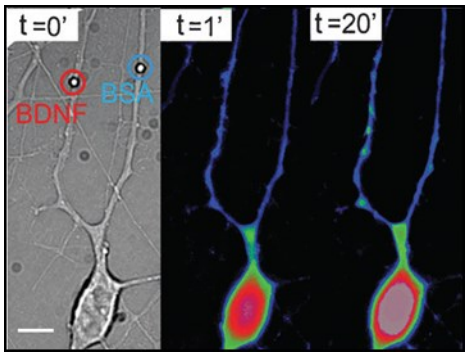
Written by Dan Cojoc (cojoc@iom.cnr.it)

Permanent staff: D. Cojoc, G. Pinato

The aim of the Optical Manipulation Laboratory (OM-Lab) is to develop new optical microscopy instrumentation and techniques for nanotechnology, biophysics and biomedicine.

Optical Manipulation includes the following techniques: optical trapping and manipulation of micro and nano particles, pN force spectroscopy by optical tweezers microscopy, laser microsurgery, digital holographic and speckle microscopy, micro-Raman spectroscopy, TIRF and FRET fluorescence.

Local probing the mechanical properties of living cells and local stimulation of specific compartments of neuronal cells with small amount of neuronal activation molecules represent two main directions of our research activity. Local probing of the mechanical properties employs optical tweezers (OT) force spectroscopy to measure forces exerted by membrane tether membranes on a pulling bead and derive local viscoelastic proeprties of the cell. OT are used also to locally measure cell elasticity by identation method similarly to AFM but with different loading characteristics. These methods are applied at OM-Lab to study the mechanical properties of cancer cells characterized by different levels of disease aggressiveness. On the other hand, digital holohraphic and speckle microscopies are employed to measure the thermal vibration of suspended cells, like red blood cells, and establish protocols to detect cell infection, e.g. malaria.



Brightfield (left) and Ca^{++} fluorescence images (right) of a hippocampal neuron stimulated by two micrometric beads coated with Brain Derived Neurotrophic Factor (BDNF) and repectively Bovine Serum Albumin (BSA). The beads are precisely positioned on two different dentrites. BDNF coated bead induces an increase of the Ca^{++} level in the corresponding dendrite and in the cell body after 20'..

Local stimulation of the neuronal cells has as goal to mimic biomechanical and biochemical interactions between hippocampal neurons, in order to understand synaptic and development mechanisms. These activities are developed in collaboration with SISSA and University of Trieste. Biomechanical interactions are mimicked using optically manipulated beads positioned in front of processes and measuring interaction forces developed there. Micro- and nano-vectors coated or filled with active molecules are instead used to stimulate specific compartments of the neurons. Examples of vectors are: microbeads, quantum dots, PLGA biodegradable beads, liposomes, micro-vesicles released by cells. The vectors are trapped and positioned on cells by optical tweezers microscopy. Stimulation is reached by cell-vector contact (coated beads or QDs), photolysis (liposomes) or by biodegradation (PLGA beasds). The effects induced are observed by optical microcopy, following the cell morphology or/and activation of specific process indicators in the cell. An example of neuronal stimulation with Brain Derived Neurothrophic Factor (BDNF) is shown in the figure above. This work (E. D'Este *et* al, Integrative Biology 2011) was very important since we clearly showed that BDNF not necessarily need to be internalized to trigger the receptor pathway.

We also studied the effect induced by small number of molecules for two molecules of interest (Netrin and Semaphorin 3A) in neuronal signalling (G. Pinato *et a*l, Scientific Reports 2012).

Istituto Officina dei Materiali

Structure and dynamics of molecules of biological interest

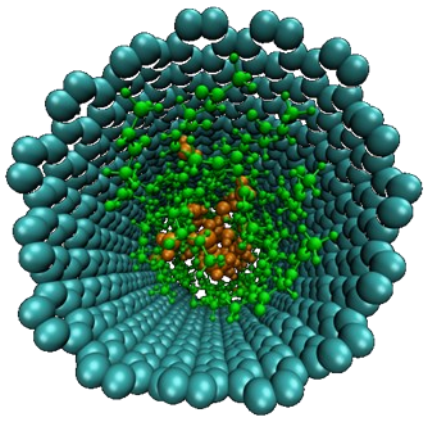
Written by Daniela Russo (daniela.russo@cnr.it)

Permanent staff: A. De Francesco, F. Natali, L. Comez, S. Caponi, D. Russo

The research focuses on several aspects concerning systems of biological interest such as characterization of structure and dynamics of bio-molecules from powders to solution to nano-confined environments. The importance of hydration water on the structure and dynamics of bio-molecules, the understanding of the role of water, at a molecular level, in mechanisms responsible for biocompatibility of biopolymer, together with the interest of adaptation of biomolecules to extreme conditions and solvent free environment are also investigated.

The general research area includes biocompatible polymers, organic hybrid materials, nano-confinement, high pressure effects, protein model interfaces, biological tissues, lipids composites, photosynthesis and biotechnological applications.

The research profile connects the fundamentals of specific biological field with that of applied science through biophysical and biochemical background and expertise with cutting edge experimental techniques such as neutron scattering and depolarized light scattering. Understanding movements on the *ps-ns* time-scale is of great importance, since it means understanding the forces which maintain the bio-molecule structures. Investigations of a variety of bio-relevant systems of different nature, size and complexity, from small hydrophobic and hydrophilic peptides to proteins and whole cells enabled to delineate a landscape as a function of the complexity of the bio-solute. In this context the effect of the environment, with special attention to biomolecules embedded in a variety of organic co-solvents, and bio-compatible/biodegradable bio -polymers, is also investigated for their potential application in bio-technology and nano-medicine. The study emphasized the importance of hydration in biological activity, cell regulation and signal transmission and the strong effect of the solvent in conditioning the dynamical behaviour of the biomolecules. Furthermore the close correlation between dynamics (flexibility/ rigidity), structure and biological functionality are extensively tackled. Focusing on water dynamics an important effort is also devoted to outline the role of hydration water dynamics and structure from cells to protein model interfaces. The nature of the molecular rearrangement connected to the continuous breaking and forming of H-bonds on a ps time scale, translational diffusion coefficient and rotational time associated to time of life of the H-bond network and the relevance of its extent, are investigated under various and well defined conditions, in order to shed light on crucial molecular mechanisms of bio-compatibly and functionality. Investigation on water collective dynamics might provide important insight on the transmission of information possibly correlated to biological functionality. Finally the importance of nano-confinement, in the polypeptide chain of native protein and small molecules, in order to prevent, unfolding, degradation, improve storage, drug preservation and delivery, is also a developing field of investigation.



Confined bio-molecules (green) and water (orange) in carbon nanotubes.

Plasmonic and DNA based Biosensors

Written by Marco Lazzarino (lazzarino@iom.cnr.it)

Permanent staff: M. Lazzarino, N. Marquestaut

The peculiar properties of gold nanostructures have been exploited for many applications with large attention on spectroscopy and biological sensing. The localized surface plasmon resonance and the easiness of gold surface functionalization are the main features that make them an optimal multi-purpose tool.

Tip enhanced Raman scattering

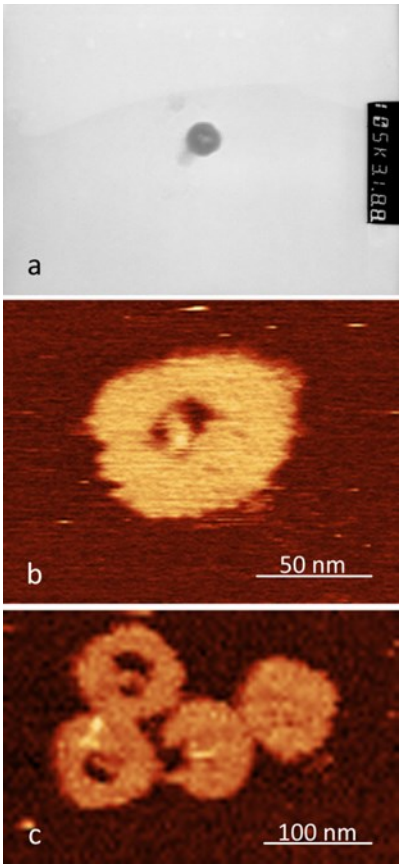
Tip enhance Raman scattering is a microscopic approach to get chemical information at the nanoscale, and combines AFM and plasmonic enhancement. In the past years we investigated two main approaches: (a) surface plasmon polaritons tips, which enabled us to reach the world record of chemical mapping at 7nm. (b) self assembled semiconductor nanowires, that carry a AuNP at their tip which is a natural candidate for low cost and high reproducibleTERS tips.

DNA driven AuNP assembly.

DNA unique recognition properties are particularly useful to create complex hybrid structures. We exploited this combination to create AuNP dimers that behave like plasmon field hot spots in order to build up a plasmonic ruler that can be used to sense in a precise way the distance between two AuNPs. In particular we developed an innovative protocols that allowed us to reach the highest efficiency ever reported in literature to synthesize regular clusters made of few AuNP.

DNA origami

DNA recognition mechanism and it flexibility makes of it an amazing nano-brick to build functional, reliable and inexpensive nano-objects. DNA origami in particular are made of a long bacterial DNA strand which is folded in desired shape by a number of suitable short DNA strands. We used DNA origami approach to create a nanovalve and a nanocontainer for biosensing and drug delivery, respectively. Next step will be the merge of DNA origami and AuNP to form a dynamic plasmonic ruler.



DNA origami nanovalve. (a) TEM image; (b) AFM image showing the the honeycomb structure originated by the alternate coiling of the short staples; (c) AFM image showing open and closed DNA origami valves.

Istituto Officina dei Materiali

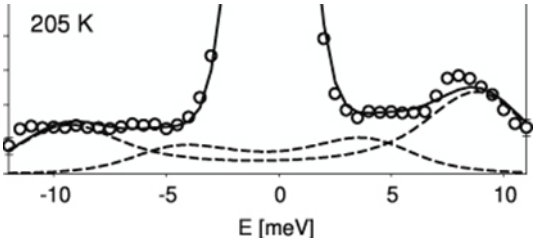
Structure and dynamics in disordered systems

Written by Ferdinando Formisano (formisano@ill.eu)

Permanent staff: F. Formisano, A. De Francesco, E. Guarini, C. Mondelli, C. Petrillo, F. Sacchetti, A. Trapananti.

This research activity is focused on the structural and dynamical properties in disordered systems, i.e. an extremely wide class of disordered materials ranging from the broad family of liquids (simple, metallic, molecular, quantum, ionic), to glasses, including solutions, molten salts, soft (e.g. polymers) and biological matter, and aqueous systems.

Our objective is to obtain a refined characterization of processes ruling the aggregation of atoms and molecules at a microscopic (anisotropic) level, because these processes are those that ultimately determine the macroscopic (isotropic) bulk and chemical-physical properties in matter.



A continuous effort is made since long time to extrapolate the properties of water in the 150-235 K range (no man's land region), where pure water unavoidably crystallizes. Here the effect of temperature on the collective modes in slightly salty water is shown.

This research addresses to both fundamental (e.g. the interaction law, polyamorphism) and technological (e.g. hydrogen storage, fuel cells, confined hydrogen in radioactive waste disposal) aspects, which may require to measure the systems properties in an extended thermodynamic range (P up to few GPa, 1 K<T 1500 K) or, other than in the bulk state, under nanometric confinement.

To reach our objective we mostly use neutron and synchrotron x-ray spectroscopy, which are scattering techniques capable to cover an extended momentum-energy range (0.1- 100 nm^{-1}, 0.1-100 meV), thus allowing encompassing extended time- and length-scales. In particular, we have gained a longstanding experience in the experimental determination of:

- structural properties (atomic and molecular correlations) by means of small- and wide-angle neutron/x-ray diffraction,, and of x-ray absorption spectroscopy;
- dynamical properties such as single-particle (e.g. diffusion) and collective (e.g. sound modes) by means of quasielastic and inelastic neutron scattering techniques (three-axis and time-of-fight spectroscopy) .

We regularly accompany our experimental approach with intense numerical activities::

- molecular simulations (classical, ab-initio) having the twofold goal of experimentally validating a model or potential, and numerically accessing a momentum-energy range even more extended than the experimental one;
- the development of a Bayesian approach in the analysis of neutron scattering data, based on the exploitation of a Reversible Jump Markov Chain Montecarlo algorithm. We are especially interested in this approach as, in the case of intrinsically weak scattering data, it turns out to be extremely powerful in finding the model that better maximizes the statistical information contained in experimental data.

Glass transition – structural arrest: molecular liquids, polymers, glues

Written by Lucia Comez, Silvia Capone (lucia.comez@fisica.unipg.it, silvia.caponi@cnr.it)

Permanent staff: L. Comez, S. Caponi

The research concerns the multiple aspects of the glass transition phenomenon. The formation of a glass can be produced both by physical and chemical paths. The first is the usual way to generate a glass: a liquid in a metastable state is cooled or compressed so as to avoid crystallization; the second represents an alternative practice, i.e. the chemical vitrification: a process involving progressive polymerization of the constituent molecules via the formation of irreversible chemical bonds. The formation of most of the materials used in engineering plastics and the hardening of natural and synthetic resins are based on chemical vitrification.

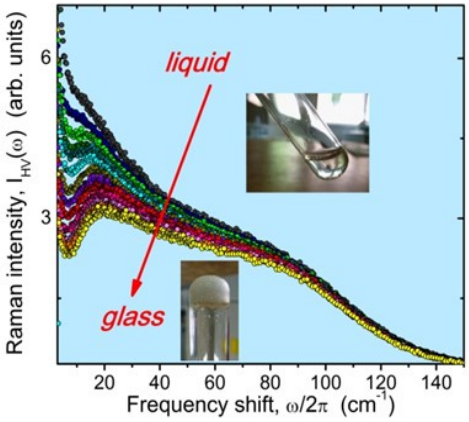


Fig. 1 Representative Raman spectra during a chemical vitrification.

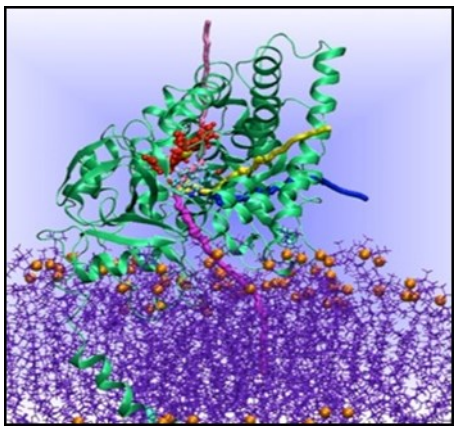
Despite the differences in the molecular processes involved in chemical and physical vitrification, the detection of common ingredients is extremely challenging for the scientific community. However, enormous efforts are necessary to explore the whole progression of the phase transformation. From an experimental point of view, the study of the glass transition requires experiments over a wide frequency band since the dynamical range of processes involved, when the system passes from the liquid to the amorphous state, is very huge (timescales from picoseconds to hundred of seconds). In addition, for achieving results that may have a universal character, several systems belonging to different categories, from conventional glass-formers to polymers capable of undergoing a chemical vitrification, should be considered. On this ground, thanks to the combined use of multiple techniques and the comparison among different systems (glycerol, vitreous silica and germania, epoxy resins), we have observed unexpected similarities in the slowing down of the dynamics and in the thermodynamical properties of the resulting glasses. Our research has been focused to explain such similarities that would improve general understanding of the glass transition and may unveil its universal nature. In particular, we have found that the obtained chemical and physical glasses share numerous features concerning the cooperative, the kinetic and the vibrational dynamics. In detail: (i) The slow dynamics (relaxation time >μs) has been investigated by photon correlation spectroscopy and explained in terms of bond–controlled configurational entropy reduction, identifying a common paradigm to physical and chemical variables; (ii) The fast dynamics (relaxation time ~ps), analyzed by means of Brillouin spectroscopy in different frequency domains, has shown intriguing features addressed by the mode–coupling theory for simple liquids, revealing that chemical bonding surprisingly, yet efficiently, realizes the mechanism of dynamical arrest described by the theory; (iii) The modifications of the vibrational density of states throughout the polymerization, studied by Brillouin and Raman spectroscopies, has been fully explained by the corresponding changes of the Debye level, in a similar manner as in densified glasses. In this last context, we have contributed to also demonstrate the validity of a strong connection, of a general nature, between some acoustic properties, as attenuation and longitudinal compliance, and the density of states of a system when it vitrifies.

Istituto Officina dei Materiali

Molecular Modeling of Biological Systems

Written by Alessandra Magistrato (alessandra.magistrato@sissa.it)

Permanent staff: A. Magistrato



Human Aromatase enzyme embedded on a membrane bilayer. The entrance/exit channels of the androgen substrate are shown.

The Molecular Modeling of Biological systems research line mainly focuses in understanding the molecular principle at the basis of the onset of major human diseases diseases and to the rational design of drugs that can interfere with these mechanism.

These studies rely on the use and development of protocols based on state-of-the-art computational methods such as hybrid quantum-classical (QM/MM) molecular dynamics (MD) simulations; classical all-atom explicit solvent MD simulations, in combination with advanced sampling techniques to simulate rare events. The integrated use of these computational techniques allows focusing deeply in the fundamental aspects of the mechanism of complex biological phenomena, which cannot be fully addressed by experimental techniques. These studies allow interpreting experimental data, providing an explanation of complex biological phenomena at microscopic level. The employment of bioinformatics tools allows to identify mechanisms and facets common across biological families.

Current research lines focus on enzymatic catalysis in proteinaceous and RNA enzymes, recognition of DNA damages by repair enzymes and by specifically tailored tailored inorganic, molecular determinants of allosteric inhibition mechanism of enzymes, role of metal ions in neurodegeneration, transport of nutrients trough biological membranes, or computational design of nanodevices that allows the selective detection and removal of cancer cells. In particular the molecular mechanism of metal containing enzymes or ribozymes is addressed by the integrated use of force filed based and hybrid quantum-classical molecular dynamics simulations in enzyme at the basis of hormone biosynthesis, in charge of silencing specific genes or in self-cleaving ribozymes.[1,2] Enhanced sampling techniques are a key tool to understand how the detection of DNA damages occurs in cells; how it can be modulated by inorganic molecules or to study the the transport of nutrients across biological membranes is associated. The use of these sophisticated techniques allows to dissect the complex free energy landscape[3,4] on which this key cellular processes occur, paving the way for the design of selective drugs.

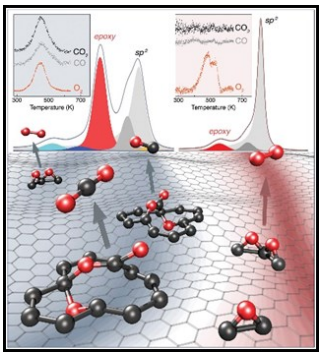
Metal ions are often associated to the onset of neurodegenerative diseases (Parkinsons', Alzheimer's, Prion's Disease), which share the same metal mediated aggregation mechanism. Since the proteins responsible of the onset of these diseases intrinsically unfolded, it is a challenge from both the experimental and the computational side takes singularly to understand how metal ions triggers aggregation at molecular level.[5] In this scenario the integrated use of experimental and computational spectroscopy plays a key role in elucidating structural facets of metal-protein adducts.

1. Sgrignani J.; Magistrato A. 2012, *J. Chem. Inf. Mod.* 2012; 2. Sgrignani J. and Magistrato A. *J Phys Chem B* 2012. 3. Franco, D.; Sgrignani, J.; Bussi, G.; Magistrato A *J. Chem. Info. Mod.* 2013; 3. Bisha, I.; Laio, A.; Magistrato, A.; Giorgetti, A.; Sgrignani J. *J. Chem. Theor. Comput.* (2013); 5. Binolfi A., et al. *Inorg. Chem.* (2010)

Glass transition – structural arrest: molecular liquids, polymers, glues

Written by Simone Piccinin (piccinin@iom.cnr.it))

Permanent staff: S. Fabris, S. Piccinin, P. Umari, F. Ancilotto, S. Baroni, N. Binggeli, A. Dal Corso, P. Decleva, S. de Gironcoli, A. De Vita, G. Fronzoni, R. Gebauer, P. Giannozzi, G. Pastore, M. Peressi, R. Resta, S. Scandolo, P. Silvestrelli, M. Stener, F. Toigo, E. Tosatti



Combined theory-experiment work on the thermal reduction of graphene oxide

We use computer modeling to provide fundamental atomic-scale insights into the physical and chemical processes that govern the functional properties of nano structured materials. Our simulations aim to characterize, engineer and discover materials for innovative applications in nano technologies, renewable energies, electronics, optics, and catalysis. We develop and apply theories and simulation techniques centered on Density Functional Theory, and ranging from empirical modeling to many-body theories and quantum chemistry. Collaborations with the local experimental partners are coordinated by the theory@Elettra group located in the AREA science park. The research projects undertook in the 2010-2012 period can be divided in the following areas

Heterogeneous catalysis. The main systems/processes studied where: i) Ag/Cu alloy catalysts to convert ethylene into ethylene epoxide and the related reaction mechanism; ii) Diffusion and segregation in alloy catalysts such as Ni/Cu; iii) Metal atoms, clusters and interfaces supported by oxide surfaces in the context of fuel cells and H2 production/purification; iii) reliability of DFT-based cluster expansion in modeling phase transitions in oxygen layers on Pd(111); iv) CO2 interaction and activation on metal catalyst surfaces; and v) first-principles NMR characterization of materials for catalytic and biomedical applications.

Solar energy conversion and storage. We focused on materials for artificial photosynthesis and on the electrochemical processes for the direct conversion of sunlight into chemical fuels (H2). We studied the structure, properties and reaction mechanisms promoted by homogeneous and heterogeneous catalysts (metal-organic and inorganic molecules, and amorphous Co-phosphate nano particles) for water oxidation.

Physics and chemistry of graphene. The main research in this area focused on i) the structural and electronic characterization of the main defects and surface functional groups of graphene and graphene oxide; ii) the oxidation of graphene and reduction of graphene oxide; and iii) the properties and reactivity of metal nano cluster supported by graphitic surfaces.

Organic and metal-organic systems. We have characterized novel metal-organic frameworks self-assembled on metal surfaces (benzoic acids coordinating Cu and Fe), porphyrin monolayers on Ag(110), and metal phthalocyanines on Au(110). This research line was strongly linked to experiment.

Computational spectroscopy. The optical, emission and absorption properties of systems like C60, nanoclusters of CdSe as well as molecules like pyrimidine and pyrazine, were studied developing and using a variety of theoretical methods including DFT, TD-DFT and many-body perturbation theory (GW).

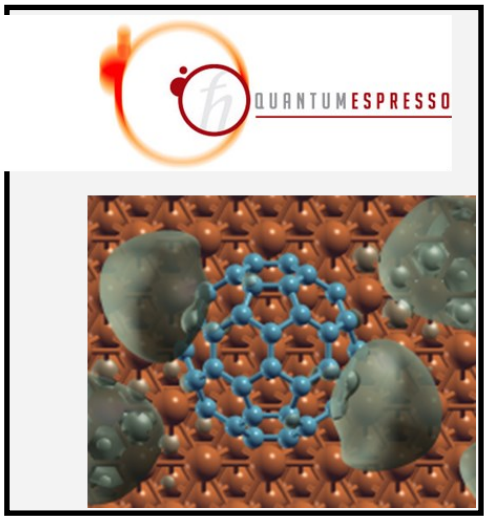
Functional materials. i) Novel theories for topological insulators, for magnetic and electronic polarization in solids; ii) Electronic transport in nano contacts and metal nanowires; iii) Si-based nano structures for (opto-/spin-)electronics, materials at ultra-high pressure and temperature; iv) Chemomechanics in nano structures.

Istituto Officina dei Materiali

Quantum ESPRESSO: an Open Source software distribution for modeling materials properties from first principles

Written by Stefano Fabris (fabris@iom.cnr.it)

Permanent staff: S. Fabris L. Martin-Samos, P. Giannozzi, S. Baroni, S. De Gironcoli, A. dal Corso.



Super Atomic Molecular Orbital of a C60 molecule on top of a Cu surface.

Quantum ESPRESSO (QE) is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials. Quantum ESPRESSO stands for opEn Source Package for Research in Electronic Structure, Simulation, and Optimization. QE is evolving towards a distribution of independent and inter-operable codes in the spirit of an open-source project. Researchers active in the field of electronic-structure calculations are encouraged to participate in the project by contributing their own codes or by implementing their own ideas into existing codes.

This research line is devoted to the coordination of the QE software development, the maintenance of the distribution coherence and the management of developers and users tools and services.

New developments in terms of implementation of new modeling capabilities are included in other specific research lines. The state of the art in 2009 was a distribution of interdependent modules all coming from Quantum ESPRESSO developers (for a review on the capabilities and on the philosophy see: P. Giannozzi et al, J. Phys. Cond. Matter 21, 395502 (2009).

In the period from 2010 to 2012 the main achievement were the adoption of a coherent directory structure for the modules, a new distribution model based on the subdivision of QE into packages and plugins, and a new installation model, enabling automated installation of the required packages and plugins. For instance, the original metadynamics implementation in QE was replaced by the more complete PLUMED plugin; the modeling of electronic and optical properties was enhanced through the automatic installation of YAMBO plugin and of the GWW package; the modeling of transport properties in nanojunctions is now available to users through automatic download, installation and compilation of the WANT package. During this period three main releases: QE-4.2, QE-4.3 and QE-5.0, have been made available to the community. In 2010, the cooperative development environment has been substantially improved with the installation of web portal qe-forge (www.qe-forge.org) and with the migration of the QE repository to a more flexible version manager. In 2012 an undergraduate computer scientist has been hired to design and implement a web interface for using and maintaining the pseudopotential table in an extendable and user-friendly way. The researches involved in this line actively contribute to education and dissemination activities all around the world with particular emphasis on emerging countries.

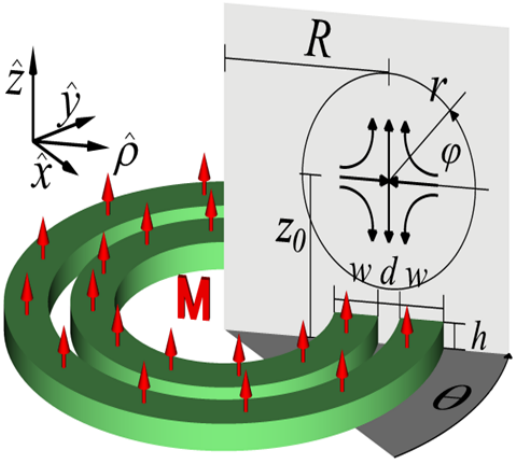
A complete list of workshop, tutorials, schools and contributors is available at :
http://www.quantum-espresso.org/complete-qe-schools-workshops-and-tutorials/
http://www.qe-forge.org/gf/project/q-e/
and in the documentation of the Quantum ESPRESSO distribution.

Quantum Simulations and Quantum Devices with Ultracold Atoms

Written by Andrea Trombettoni (andreatr@sissa.it)

Permanent staff: A. Trombettoni

The research activity on ultracold atoms @ DEMOCRITOS focused on the study of equilibrium and dynamical properties of ultracold atoms trapped in engineerable confined potentials, and in particular in optical lattices. These systems are characterized by the high controllability of their experimental parameters, making them ideal (i) for the implementation of quantum simulations and (ii) for the realization of quantum devices.
In the direction (i), the use of one-dimensional waveguides was used to propose and study the physical implementation of integrable models such as the Lieb-Liniger model [see M. Kormos, G. Mussardo, and A. Trombettoni, Phys. Rev. A 83, 013617 (2011)] and the XXZ chain [studied in D. Giuliano, D. Rossini, P. Sodano, and A. Trombettoni, Phys. Rev. B 87, 035104 (2013)]. In higher dimensions one can use the possibility of using optical lattices to induce topological phase transitions as those studied in M. Burrello, I. C. Fulga, E. Alba, L. Lepori, and A. Trombettoni, Phys. Rev. A 88, 053619 (2013).



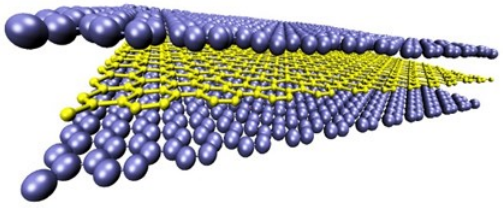
Planar ring structures for the generation of an axially symmetric 2D quadrupole field acting on a cold gas trapped in a ring geometry.

In the direction (ii) recent works @ DEMOCRITOS focused on the tunneling properties of ultracold atoms in presence of multiwell potentials and on the role of interatomic interactions: in particular effective models for interacting fermions at the unitary limit were studied in M. Iazzi, S. Fantoni, and A. Trombettoni, Europhys. Lett. 100, 36007 (2012), showing that the tunneling properties in the unitary limit are well described by a Lawrence-Doniach model. Work in progress concerns the study of the quantum dynamics in presence of tunable impurities, which is relevant for the realization of quantum devices such as gravimeters and gyroscopes. Along this line there is the collaboration with the theoretical and experimental groups of the European STREP project MatterWave: Andrea Trombettoni and Federico Becca are part of the MatterWave consortium, and Giacomo Gori has been hired in July 2013 as a CNR Post-Doc. MatterWave brings together an international team with groups from United Kingdom, Greece , Israel and Italy (CNR-IOM) aiming at making ultrasensitive matterwave-interferometry in a compact and portable device. The current work is focusing on the implementation of a ring confining geometry created using atom chips (see the figure – more material is in www.matterwave.eu). The proposed device is based on the Sagnac interferometric scheme: the rotation is measured by letting interfer two cold gases moving along the ring in opposite directions. Since the sensitivity of the gyroscope depends on the interaction and on the properties of the confining potential, work @DEMOCRITOS is in progress to determine the optimal point for precision measurements of acceleration and rotations.

Theory and simulation of interface dynamics, friction and dissipation at the nano and mesoscale

Written by Andrea Vanossi (vanossi@sissa.it)

Permanent staff: A. Vanossi, E. Tosatti, G.E. Santoro, N. Manini



Atomistic simulation of a confined solid lubricant under shear.

Understanding the complex microscopic processes occurring at the interface of sliding materials is a formidable task, central to pure and applied sciences and relevant to technological areas, including friction, adhesion, lubrication, wear, plastic deformations, fracture, and so on. With increasing device miniaturization in nanotechnology, the large surface-to-volume ratio makes interfacial forces dominant, seriously constraining the performance and lifetime of microdevices. Durable low-friction surfaces, wear-resistant materials, and suitable liquid and solid lubricants are increasingly in demand for hi-tech applications. Despite the practical and fundamental importance and the growing efforts in the field, many key aspects of the dynamics of friction are still open.

We seek to model, simulate, and understand theoretically the physics of sliding friction and of dissipative dynamics at the nano and mesoscale, aiming also at designing efficient methods and algorithms to tune and control the microscopic dissipation strength. We address the multiplicity of phenomena observed in experimental nanotribology, with a variety of tip-based, wear-free atomic scale sliding setups, involving physisorbed and boundary lubrication layers, and including mechanical, electronic, magnetic, and electromagnetic mechanisms. The potential of new experimental techniques such as ultra-sensitive pendulum

AFM are connected with the theoretically expected dissipation changes due to structural, metal-insulator, and magnetic phenomena including phase transitions. Besides these "real" systems, we model theoretically the sliding phenomena which occur in the new artificial setups based on sliding trapped cold ion chains and, especially, on two dimensional colloidal layers, toy systems which hold considerable potential to mimick friction on crystals from the nanoscale upwards. At the fundamental level, we plan to develop and extend the theory of

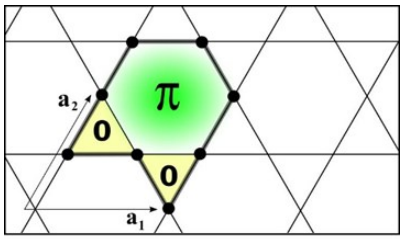
sliding friction beyond linear response, using stick slip nanofriction as a test case, and modeling, simulation and non equilibrium statistical mechanics as our tools. We explore how to build bridging approaches between brute force atomistic simulation and "minimalistic" classic frictional models. The nanoscale results can also be put to use, when appropriate, as building blocks to model mesoscale friction, extending the research activity in practically relevant multi-contact systems, where the tribological behavior is ruled by both the dynamics of single asperities as well as the interplay of collective mechanisms. Finally we intend to move starting steps away from purely classical systems by studying quantum corrections, and also frictional effects in quantum systems submitted to external time-dependent perturbations.

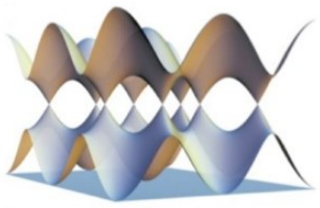
Quantum phases beyond the Landau paradigm

Written by Federico Becca (becca@sissa.it)

Permanent staff: F. Becca, S. Sorella

The research activity on unconventional phases of matter focused on systems having competing (i.e., frustrating) interactions. The search for such exotic phases, which cannot be described by the standard Landau's symmetry breaking theory, represents an important branch in condensed matter physics. In this regard, topological insulators, integer and fractional quantum Hall states, and quantum spin liquids are not characterized by broken symmetries or any kind of local order parameter. Instead, they show global aspects such as unconventional quasiparticles with fractional quantum numbers, edge modes, and, in some cases, emergent gauge degrees of freedom.





The unit cell of the Kagome lattice is shown as shaded region. The variational wave function is described by gauge fields with zero and pi magnetic fluxes piercing triangles and hexagons, respectively. This implies a spinon band with Dirac cones.

We investigated models of interacting spins or bosons on frustrated lattices (e.g., square, triangular, honeycomb, and Kagome lattices) by using improved variational wave functions and Monte Carlo techniques. In particular, we showed that gapless spin liquids can be obtained in frustrated Heisenberg models on the square and Kagome lattices, the latter one being particularly relevant for a family of recently synthetized materials (e.g., Herbertsmithite and Volborthite). Our approach corroborate the scenario in which the low-energy properties of these spin systems is described by asymptotically free spin-1/2 objects (spinons) interacting through emergent gauge fluctuations (visons). [see Y. Iqbal, F. Becca, and D. Poilblanc, Phys. Rev. B 84, 020407 (2011), Y. Iqbal, F. Becca, S. Sorella, and D. Poilblanc, Phys. Rev. B 87, 060405 (2013), and W.-J. Hu, F. Becca, A. Parola, and S. Sorella, Phys. Rev. B 88, 060402 (2013)].

Spin liquids can be also found in frustrated electronic systems, such as the Hubbard model on the anisotropic triangular lattice, with different hopping parameters in different spatial directions. This is especially relevant for a family of organic salts, where strongly dimerized organic molecules are arranged in stacked two-dimensional triangular lattices. We provide solid evidence that a spin-liquid phase is stabilized in the strongly-correlated regime and close to the isotropic limit, while, for a weak degree of frustration, magnetically ordered phases are obtained. [see L.F. Tocchio, H. Feldner, F. Becca, R. Valenti, and C. Gros, Phys. Rev. B 87, 035143 (2013) and L.F. Tocchio, C. Gros, R. Valenti, and F. Becca, arXiv:1403.4497].

Finally, frustrated bosons on the honeycomb lattice have been considered to investigate the existence of the so-called Bose metal, a phase where bosons do not condense or form a crystal down to zero temperature. This kind of research is relevant for ongoing experiments with cold atomic gases trapped in optical lattices. We found that, besides superfluid phases that are stable in a wide region of parameters, a Bose metal can be obtained in a narrow regime with high frustration. Here, bosons should have a fully gapped spectrum but no order whatsoever.

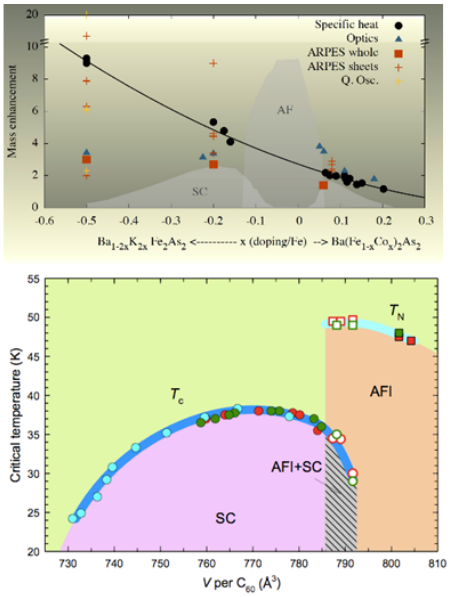
[see J. Carrasquilla, A. Di Ciolo, F. Becca, V. Galitski, and M. Rigol, Phys. Rev. B 88, 241109 (2013)].

Istituto Officina dei Materiali

Superconductivity and electron-electron correlations

Written by Massimo Capone (massimo.capone@sissa.it)

Permanent staff: G. Giovannetti, M. Capone, M. Fabrizio, E. Tosatti



Effective mass of iron-based superconductors as a function of doping (top) and phase diagram of Cs_3C_{60} under pressure (bottom). The proximity to the Mott state influences sueprconductivity in both systems

The research on strongly correlated electrons became one of the most active field in condensed matter theory when high-temperature superconductivity has been discovered in doped Mott insulators based on copper-oxygen planes, the so-called cuprates. After a few decades, despite the lack of consensus on the microscopic origin of superconductivity in the cuprates, the link between electronic correlations and superconductivity is still strong, also thanks to new materials and new experimental evidences. CNR-IOM is active in these directions, exploring the role of strong correlations in cuprates and in iron-based superconductors, as well as in doped fullerides. Our activity is also focused on general properties of strongly correlated systems, including metal-insulator transitions and the non-equilibrium dynamics. The research in this direction at IOM has been primarily financed by European Research Council (ERC) through the standard independent research grant SUPERBAD.

Within this project, we have studied the role of strong correlations in a variety of superconductors and other materials, and we developed theoretical methods able to properly treat the strong competing interactions of these materials. A common thread connects many superconductors, and identifies in the strong correlations the key mechanism to achieve high-temperature superconductivity irrespective of the pairing mechanism. The critical temperature is in fact enhanced by the Mott physics also in alkali-doped fullerides, where the electron-phonon coupling is responsible for Cooper pair formation. In the iron-based superconductors, the undoped compounds are magnetic, but they are not Mott insulators. We have however shown that the physics of these materials is controlled by a Mott state that woud be realized for one hole doped in each iron atom.

A new perspective on the physics of the cuprates is given by the development of pump-and-probe spectroscopies investigating the real-rime dynamics following an impulsive excitation. These advances allow to disentangle different physical processes and even induce dynamical phase transitions. Our research in this direction has focused on both general properties of non-equilibrium correlated systems and superconductors and on the interpretation of experiments in the high-temperature superconductors or other correlated oxides.

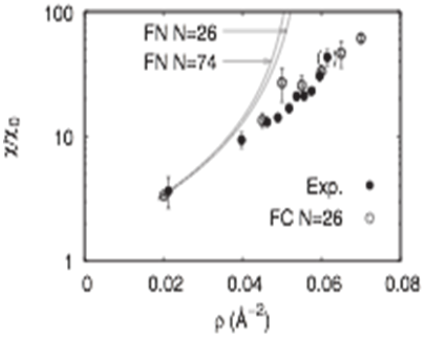
As notable examples, we studied the dynamical phase transition after an interaction quench in the Hubbard model, the properties of two-band models for V_2O_3 and the role of dissipation in the approach to non-equilibrium stationary states in the presence of an electric field .

Quantum Monte Carlo simulations

Written by Stefania De Palo (stefania.depalo@sissa.it)

Permanent staff: S. Moroni, F. Becca, S. De Palo; G. Senatore, S. Sorella

The Quantum Monte Carlo (QMC) method has provided high quality results for a variety of systems in physics, as well as in quantum chemistry, where strong correlations cannot be adequately treated by methods as density-functional theory or within perturbative approaches. It provides exact results for bosonic systems and very accurate information for the fermionic systems for which the sign problem, due to the antisymmetry of the wave function, in general requires approximations. Here we highlight selected applications to challenging physical and chemical systems, as well important methodological advances developed to increase the computational efficiency and/or extend the scope of QMC techniques. Further applications are described in 4) and 6). The engineered confinement of electrons in low dimensions, as in semiconductor heterostructures or in He-3 adsorbed on graphite substrate, enhances their many-body correlations. In solid state devices where the electronic gas is confined in two dimensions (2DEG) spin/valley degrees of freedom are important ingredients in the description of the metallic phase. Fixed-node Diffusion Monte Carlo (FN-DMC) study of 2DEG in AlAs quantum wells, for which is possible to reach very low density (strong correlations) and vary the valley degeneracy, has clarified the role of valley degeneracy in magnetic properties and the importance of including the mass anisotropy present in these devices to obtain very good agreement with experimental findings for spin-susceptibility within a Fermi-Liquid framework. An agreement not-recoverable using perturbative approaches. The liquid phase of the adsorbed He-3 has a Fermi-Liquid behaviour with an effective mass that increases at high densities where the strong correlation regime is achieved and diverges near the freezing density. The computation of the equation of state for He-3 in two dimensions requires to go beyond FN-QMC, since this approximation including with back- flow correlations predicts a polarisation transition experimentally not observed in the fluid phase. The spin susceptibility obtained from the polarisation energy, estimated using the formally exact QMC method we have introduced (fermionic-correlation method), is in excellent agreement with the experimental values (see Figure). This technique, relying on bosonic imaginary–time correlation functions of operators suitably chosen in order to extract fermionic energies, has been used to investigate the itinerant ferromagnetic phase of the Hubbard model. QMC simulations of 2D Bose soft disks have shown a supersolid cluster phase. This indicates that this soft-core interaction, engineerable for ultracold atoms, is a minimal model where to investigate this highly debated phase. Another direction of research in which sizeable progress has been made is the computation of electronic structure using QMC. The calculation of forces with QMC is plagued by stochastic noise that prevent an efficient and reliable computation. We proposed an efficient scheme to compute forces with QMC using the so-called adjoint algorithmic differentiation, through which full structural optimization of systems of few atoms can be performed with the addition of a small computational expense.



Enhancement of the spin susceptibility as a function of the density: (filled circles) as measured in the second layer of 3He on graphite, (open circles) are obtained from the QMC simulations going beyond FN. The corresponding FN-QMC results (solid lines) would diverge at ρ≃0.050 Å-2.

Istituto Officina dei Materiali

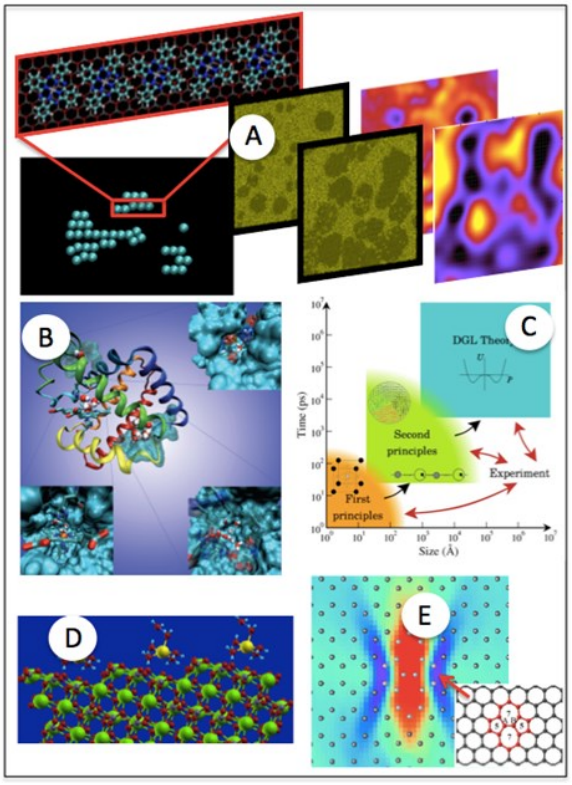
Multi-scale modeling of materials and processes for nanoscience

Written by Alessandro Mattoni (mattoni@iom.cnr.it)

Permanent staff: F. Bernardini, G. Cappellini, M. Ceccarelli, L. Colombo, P. Delugas, A. Filippetti, V. Fiorentini, G.M. Lopez, A. Mattoni, P. Ruggerone, A. Satta

Material modelling is a key issue in the route towards development of nanomaterials for technological applications of industrial relevance. However, it is necessary to fill the the gap between fundamentally accurate theoretical predictions and the practical exploitation of these models for problems of technological relevance.

In this perspective, the modeling activity on materials and processes for nanoscience at the CNR-IOM Cagliari (Sardinian Laboratory for Computational Materials Science) is characterized by a multiscale/multiphysics approach coupling the different modeling levels: quantum mechanical, molecular, up to mesoscopic and continuum models. The theoretical techniques cover the entire hierarchy of state-of-the-art simulation techniques, from classical molecular dynamics to the many-body perturbation theory. Innovative techniques (self-interaction-corrected DFT, QMMM, Divide-&-Conquer methods) are applied to a broad class of nanosystems and materials with applications in optoelectronics, photovoltaics and energy harvesting microelectronics, systems of biological interest, biominerals.



Examples of application of multi-scale modeling strategy; (a) nanostructures and interfaces for photovoltaic optoelectronics [1,2]; (b) systems of biological interest[3,4]; (c) functional oxides for microelectronics and thermolectric applications[5]; (d) biominerals; (e) nanomechanics of graphene[6];

[1] A. Mattoni, L. Ferraro, and L. Colombo, Phys. Rev. B 79, 245302 (2009).
[2] C. Melis, P. Raiteri, L. Colombo, and A. Mattoni, ACS Nano 5, 9639 (2011).
[3] A.V. Vargiu et al., J AM CHEM SOC 133: 10704-7 (2011).
[4] M.A. Scorciapino, A. Robertazzi, M. Casu, P. Ruggerone, M. Ceccarelli, J AM CHEM SOC, 132, 5156–5163 (2010)

[5] A. Filippetti, C.D. Pemmaraju, S. Sanvito, P. Delugas, D. Puggioni, and V. Fiorentini, Phys. Rev. B 84, 195127 (2011).
[6] R. Dettori, E. Cadelano, and L. Colombo, J. Phys. Condens. Matter 24, 104020 (2012).

Nanoarchitectures for solar energy harvesting

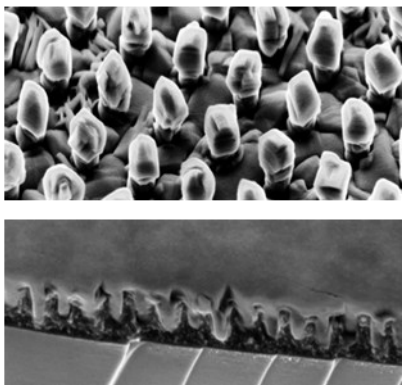
Written by Massimo Tormen (tormen@iom.cnr.it)

Permanent staff: M. Tormen

Efficient and economic technologies to convert the energy from renewable sources to electrical or chemical energy are urged for relieving environmental and geopolitical problems associated with the today's massive use of fossil fuels. Organic photovoltaic (OPV) technologies are among the ones that may concretely contribute solving these problems. Advances in design, synthesis and processing of materials and a better knowledge of device physics, have taken organic cells to ~10% efficiency, which seems not sufficient yet for commercial exploitation.

In the context of OPV, bulk heterojunction organic solar cells represent now the best performing nanoarchitecture for the intermixed donor/acceptor (D/A) in the active layer. However, theoretical predictions show disordered blends of D/A lead to losses, reducing the charge collection efficiency, due intricate percolation paths and high charge recombination probability.

On the contrary, ordered columnar (comb-like) interpenetrated D/A nanostructures with lateral dimension in the order of exciton diffusion length (~10 nm) and height comparable to the light attenuation length should in principle give the best performance for the cells.



a) Nanopillars of PEDOT:PSS coated with an evaporated layer of pentacene
b) PEDOT:PSS lines coated with a conformal layer of pentacene and filled with the acceptor (PCBM)

At IOM-CNR, we are exploring such a possibility, by nanostructuring either the conductive electrodes (such as PEDOT:PSS) or the active layer itself with nanolithography, in particular with the Nanoimprint Lithography, a technology which enables the patterning of large surfaces at low cost and at extreme resolution (<10 nm).

The range of activities in which we are involved include:

Nanofabrication of organic solar cells;
Study of the effects of nanolithography on the electronic properties of the active materials;
Design and fabrication of light harvesting/trapping structures and nanostructures;
Inclusion of novel hybrid materials (e.g. lead halide perovskites) as active layers in nanostructured cells;
Characterization of materials (in collaboration with groups with expertise in XPS, SAXS, XRD @ Elettra synchrotron);
Characterization of cells (power conversion and external quantum efficiency).

Istituto Officina dei Materiali

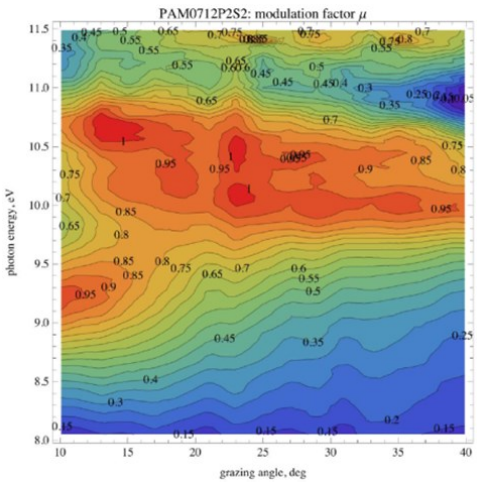
Optical characterization of materials and instrumentation for space optics

Written by Angelo Giglia (giglia@iom.cnr.it)

Permanent staff: A. Giglia, L. Pasquali, M. Malvezzi, S. Nannarone

The research activity is focused on the quantitative analysis and spectroscopy of UV-X-ray optical devices, determination of optical constants of materials, calibration and optimization of devices for FUV polarimetry, nanoparticle systems and organic thin films at surfaces. The study is assisted by modeling and simulation, in particular using the code OPAL (Optical Properties of Anisotropic Layers) that we developed to simulate the wave propagation and then the reflectivity and transmission response of a stratified system made by heterostructures as anisotropic, magnetized or ultrathin materials. These are the main topics:

- Performances and spectroscopic study of UV X-ray optics systems including interferential multilayer mirrors, thin films, UV pass band filters, calibration of spectrometers and detectors, in particular related to space instrumentation or to Free Electron laser transport optics;
- Determination of soft X-ray optical constants of several of the rare-earth materials: thin films with various thicknesses were deposited by evaporation in UHV, and their transmittance was measured in situ. Multi-angle reflectance was used to calculate the precise thickness of the sample through the angular positions of the minima and maxima. Sc, Er, Ce, Eu, Pr, Tm, Lu, Ho and Sr have been measured in several experimental campaigns;
- FUV polarimetry is a powerful technique to interpret the role of the coronal plasma in the energy-transfer processes from the inner parts of the Sun to the outer space, and in particular the Lyman a (121.6 nm) and b (102.6 nm) H spectral lines are for crucial for the study of the solar corona. A part of the activity concerns the design and development of a piezobirefrangence wave retarder, based on an anvil applying an axial stress to a LiF crystal (that can be cooled down to 100 °K to extend transmission above the Lyman b line). The activity consists also in the characterization of polarizers consisting in (Al/MgF2)xn multilayer coatings, tuned at 121.6 nm with high performance in transmission or reflection for one polarization plane and with large polarizing power;



Modulation factor of a (Al/MgF_2)x3 multilayer coating polarizer optimized for Lyman a H line.

-Study of metallic nanoparticle (NP) arrays on nanopatterned LiF(110) in the DUV range. Polarized light absorption measurements in the 3-12 eV range revealed the presence of the characteristic absorption dips correlated with the L-SPR in the 3.9-5.8 eV energy range depending on the NP mean size and the relative orientation of the exciting electric field and the NP ellipsoid. The diffraction properties of Ag NP in the EUV range were also studied with particular attention to the morphology and electronic properties of the NP coating.

- Characterization of ultrathin organic layers at surfaces (principally on metals), appealing systems for molecular electronics and sensors. Attention was given to the molecular bonding, molecular orientation and overall order. Systems were studied with a collection of techniques including XPS, XAS and X-ray reflectivity. The interpretation of the spectral signals was supported by theoretical calculations of the molecular properties through DFT.

Physical techniques for cultural heritage and environment

Written by F. d'Acapito (dacapito@esrf.fr)
Permanent staff: F. d'Acapito, A. Trapananti, C. Mondelli

X-ray Absorption Spectroscopy (XAS) is an ideal technique when dealing with trace elements or systems lacking long range structural order. It allows the determination of the local structure/simmetry of a chosen element as well as its valence state and several details of its electronic structure. These peculiarities are of particular interest in the field of cultural heritage and environmental science where XAS makes possible the investigation of trace (polluting) elements in soils or aerosols, chromophores in artistic manufacts and their chemical evolution upon ageing and exposure to external agents. Neutron scattering (NS) is also of great interest in this field for the possibility of investigating both the structure and the dynamics of materials.

The baptism of Jesus, banner by L. Signorelli (end XV Cen.). Samples from altered Smaltino pigment taken from this artwork were used for an investigation on the deterioration of this pigment (I. Cianchetta et al. J. Anal. At. Spectrom., 2012, **27**, 1941)

Cultural Heritage

Transition metals were frequently used as chromophores in the realization of manufacts. Most of the pigments used in paintings or ceramic decorations are based on metals and their valence state or local simmetry are determinant for the final coloration. A noticeable example is Co^{2+} that gives a deep blue hue when present in a tetrahedral coordination or a pale pink color when in an octahedral site. Since XAS provides information on both oxidation state and local coordination within the same spectrum it allows an effective characterization of the materials under study. Advanced data analysis methods like Full Multiple Scattering calculations of the XANES spectra, multishell structural models to fit the EXAFS spectra or ab-initio structural/dynamical simulation of the materials (DFT, MD-DFT) are used by our group for a detailed description of the specimens. Neutron techniques (diffraction, small angle scattering, inelastic scattering) can also be used in cultural heritage science, namely for the study of structure and dynamics of new nano materials (hydroxides and cements) optimised for the application in conservation science (stones, frescos and paper).

Environment

Soils or air particulate can contain metals of concern for the human health. The speciation of these elements is of paramount importance as a same element can be present in chemical forms of different toxicity. Cr is a typical example as hexavalent Cr^{6+} is considerably more toxic than the trivalent Cr^{3+} form. It is thus important not only to detect the presence of an element but also to determine its chemical state and this is the main task of XAS as a complement of the standard laboratory characterizations. The availability of the high flux beamline GILDA makes possible to carry out experiments directly on samples like soil specimens (contamination at tens of mg per Kg) or single filters of air particulate. Advanced data analysis methods permit a complete description of the samples.

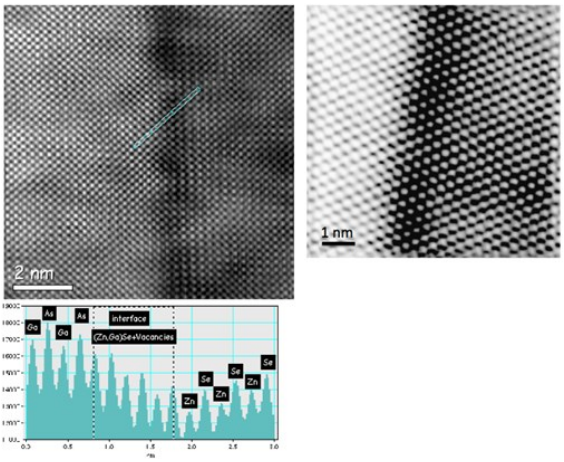
Istituto Officina dei Materiali

Development of electron microscopy methods

Written by Elvio Carlino (carlino@iom.cnr.it)

Permanent staff: E. Carlino, R. Ciancio

EMCD (electron energy loss magnetic chiral dichroism):The aim is to measure the circular dichroism by means of a TEM. Dichroism is the property of certain materials whose photon absorption spectrum depends on the polarisation of the incident radiation. Within the project it has been demonstrated the first direct experimental proof of magnetic circular dichroism in the TEM by comparing Electron Energy Loss Magnetic Chiral Dichroism (EMCD) with XMCD spectra from the same specimen together with theoretical calculations [P. Schattschneider et al._*Nature 441, 486-488 (2006)*]. The experiment shows that chiral atomic transitions in a specimen are accessible with inelastic electron scattering under particular scattering conditions. This result bears dramatic consequences for the study of magnetism on the nm and sub-nm scale, as EMCD offers spatial resolutions down to the sub-nanometre scale and provides depth information.

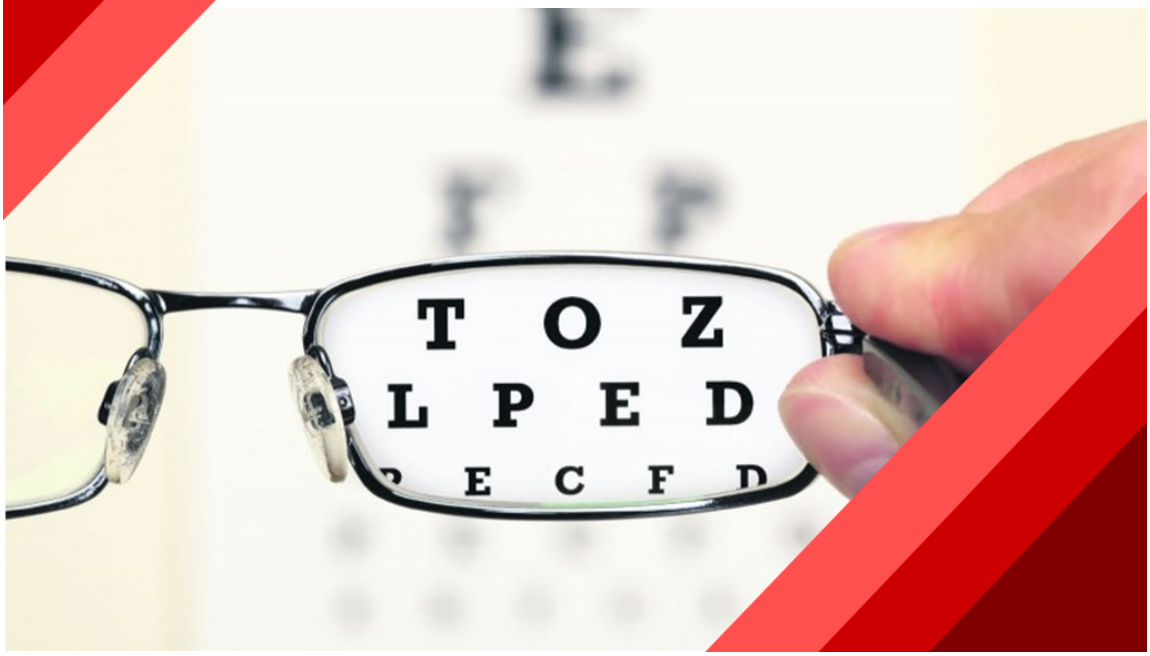


HAADF image of ZnSe/GaAs [100] (left) and [110] (right) interface.
The intensity profile allows to distinguish cations and anions atomic columns.

HAADF (high angle annular dark field imaging): The method (see figure) enables to image structure and chemistry of a specimen at 0.126 nm resolution. [E. Carlino et al. Phys. Rev. B 71 235303 (2005)] as contrast in the HAADF image is proportional to the atomic number of the specimen chemical species (Z-contrast imaging). The approach is based on the experiments in HAADF coupled with relevant simulation of HAADF images, by multislice calculation in the frozen-phonon framework, to derive quantitatively the correlation between experimental image contrast and the relevant chemical composition.

CEDI (coherent electron diffractive imaging): relies on combining information from the high-resolution transmission electron microscopy image of an isolated nano-particle with the relevant nano-electron diffraction pattern. Phase-retrieval algorithms allow one to derive the phase, lost in the acquisition of the diffraction pattern, to visualize the actual atomic projected potential within the specimen at sub-angstroem resolution, overcoming limitations due to the electron lens aberrations. Very recently the approach has been generalized by our group to study extended crystalline specimens. The new technique has been called keyhole electron diffractive imaging (KEDI) because it aims to investigate nano-regions of extended specimens at sub-angstroem resolution by properly confining the illuminated area. In fact, by using the generalized Shannon sampling theorem it is shown that whenever suitable oversampling conditions are satisfied, EDI/KEDI diffraction patterns can contain enough information to lead to reliable phase retrieval of the unknown specimen electrostatic potential. Hence, the KEDI method has been demonstrated by simulations and experiments performed on a Si crystal cross section in the [112] zone-axis orientation, achieving a resolution of 71 pm.

Highlights



Istituto Officina dei Materiali

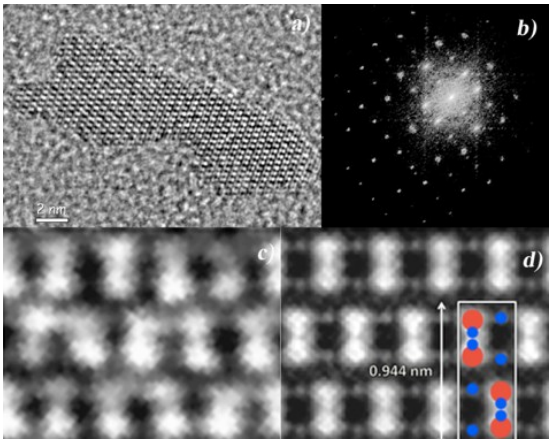
Sub-ångström resolution by TEM coherent electron diffractive imaging

L. De Caro[1], E. Carlino[2], G. Caputo[3,4], P. D. Cozzoli[3,4], C. Giannini[1]

[1]Istituto di Cristallografia (IC-CNR) via Amendola 122/O, 70126 Bari, Italy,
[2]IOM CNR Laboratorio TASC, Area Science Park Basovizza, Building MM SS 14, Km 163.5, 34149 Trieste, Italy,
[3]Scuola Superiore ISUFI, Universita` del Salento, Distretto Tecnologico, Via per Arnesano Km 5, 73100 Lecce, Italy,
[4]National Nanotechnology Laboratory (NNL) of CNR-INFM, Unita` di Ricerca IIT, Via Arnesano, 73100 Lecce, Italy.

High-Resolution Transmission Electron Microscopy (HRTEM) has revolutionized our understanding of nanoscale materials by identifying structure-properties correlations at the atomic level. However, despite the progress of the last years, the ultimate resolution has not yet achieved due to the residual electron lens aberrations. Our research group has developed an approach, based on a Sayre's idea1, that can be implemented also in a conventional transmission electron microscope and enables to achieve a resolution in principle only limited by the electron wavelength. The method uses the phase contrast HRTEM image of an isolated nanometer sized object together with its coherent nano-electron diffraction pattern (n-EDp) to image its structure at sub-ångström resolution and at low dose. The phase information lost in the n-EDp is recovered by using a recursive phasing algorithm starting with the phase information contained in the HRTEM image (figure) achieving a final resolution much higher than the starting HRTEM image, limited by the lens aberration, and enables the reconstruction of the positions of the atomic column also in the case of light elements2. In the example in the figure a spatial resolution of 70pm was achieved in the imaging of a nanorod of TiO2 detecting the small distortion in the lattice related to the properties of TiO2 at the nano-scale2. This is so far the highest resolution achieved in the world by coherent diffraction imaging.

The method has been named coherent Electron Diffraction Imaging (EDI). The work has been developed within the research activity of the Center for Electron Microscopy of the IOM-TASC (MD.P04.006.006) aimed to develop and apply new TEM methods for the study of the crystal, magnetic, electronic and chemical structure of the matter at the highest spatial resolution. The EDI method has very recently been generalised to extended specimen by self confining the TEM illumination to achieve the requirement of the Shannon-Nyquist theorem and allowing to image a nanometric area of any specimen[3]. The method has been named Keyhole EDI (KEDI). In the case study our experiments demonstrated a resolution of 60pm in the imaging of a cross section of Si [112], paving the way for ultimate accuracy and spatial resolution in the study of soft and hard matter..



a) HRTEM image of a nanorod;
b) n-Edp coupled with Fast Fourier Transform of a);
c) Magnified view of area of a);
d) reconstructed image at 70 pm of resolution with superimposed the crystal cell of TiO2 in [100] projection.

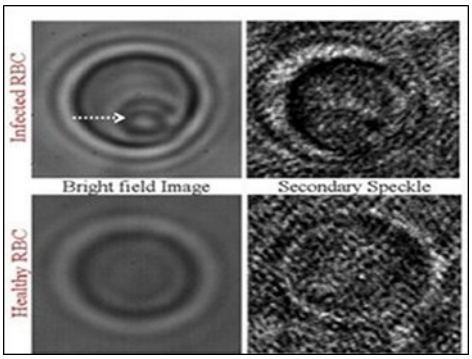
References:
1-Sayre, D. (1952). Acta Cryst. 5, 843.
2-L. De Caro et al. (2010). Nature Nano. 5, 360.
3-L. De Caro et al. (2012). Acta Cryst. A 68, 687.

Speckle sensing microscopy for fast detection of malaria

D. Cojoc [1], S. Finaurini [1], P. Livshits [2], E. Gur [3], A Shapira2, V. Mico[4], Z. Zalevsky [2]

[1] CNR-IOM Institute of Materials, Area Science Park – Basovizza, Trieste, Italy
[2] Bar-Ilan University, Raman-Gat, Israel
[3] Jerusalem College of Engineering, Jerusalem, Israel
[4] University of Valencia, Burjassot, Spain

We propose a new technique called speckle sensing microscopy (SSM), based upon extraction of correlation based statistics of speckle patterns generated while illuminating red blood cells (RBCs) with a tilted laser beam and inspecting them under a microscope. The microscope, by properly adjusting its focus, captures time varied speckle patterns generated due to the thermal vibrations of the RBCs. This movement is characterized using a correlation based algorithm that extracts the changes in position and value of the correlation peak. The statistics is then analyzed using two automated approaches: fuzzy logic based ruling and principle component analysis. Compared to other phase microscopy methods, SSM requires a much simpler setup and experimental implementation. The SSM approach allows to directly measure the movements of the cells rather than the phase changes due to these movements. It is also simpler, in SSM, to convert the parameters of the cell movement (e.g. value, direction, speed) from the dynamics of the speckle pattern. SSM allows also to tune the detection sensitivity by changing the defocusing of the objective lens. Defocusing also changes the size of the speckle patterns which affects the measurement sensitivity.



The image and corresponding speckle for an infected (first row) and unifected RBC (second row). The white arrow indicates the parasite at the trophozoite stage.

A correct diagnosis of malaria allows a life-saving treatment. In endemic areas, laboratories cannot support many technologies, because of their poor setting conditions. For this reason, blood smear microscopy still remains the gold standard. Several efforts have been made to improve the quality of diagnosis, but the ideal tool for infectious diseases in poor countries requires to be rapid, correct, simple to use, portable and low cost, as suggested by World Health Organization.

We have proposed a project to build an opto-microfluidic device for an accurate and fast malaria diagnosis. Combining the SSM with microfluidics the sample analysis is cross-checked by microfluidic test and optical probing, the diagnosis accuracy is largely improved and the results are easily interpretable and unmistakable. This device would allow the parasite identification in a drop of blood (20 uL) in only 30 minutes, without sample treatment and minimizing contact between sample and operator. This will allow screening efficiently many persons per day, with low cost, without the need to go personally to a specialized lab of a hospital. This is a fundamental problem in many regions in Africa, the most affected continent by Malaria.

References:

D. Cojoc, S. Finaurini, P. Livshits, E. Gur, A. Shapira, V. Mico, Z. Zalevsky, "Toward fast malaria detection by secondary speckle sensing microscopy", *Biomed. Opt. Express* 3, 991-1005 (2012).

O. Graydon, "Detecting malaria", *Nat. Photon*. **6**, 343 (2012) – research highlights.

Studies in the cultural heritage field

F. d'Acapito, A. Trapananti

CNR-IOM-OGG c/o ESRF, Grenoble France

Studies in the field of Cultural Heritage have been conducted at IOM-OGG aiming to the chemical/physical characterization of chromophores and pigments and to study their degradation.
The origin of the discoloration of the smaltino pigment has been addressed in [Cianchetta-12]. Smaltino is a potassium based glass additioned with Cobalt to obtain a deep blue color. This pigment is known to turn into a greyish hue under the effect of external agents.
An X-ray Absorption Spectroscopy analysis at the Co-K edge carried out on fresh, artificially aged and original degraded specimens from a Luca Signorelli's banner revealed that the degradation is associated with a coordination change in the coloring ion Co^{2+} from tetrahedral into octahedral. Ab initio simulations of the optical response of the system (via time dependent density functional theory) showed that intermediate distorted "octahedral-like" structures are the best candidates to explain the color change.
Another study, presented in [Cartechini-11], was devoded to understand if the "Naples Yellow" pigment found in renaissance maiolicas (mainly made up of lead antimonate) could have been enriched on purpose with Zn or Fe to alter the chromatic effect. A XAS study, carried out at the Zn-K and Fe-K edges, evidenced that the metals actually can enter the crystal structure of the lead antimonate substituting for Sb. This study was carried out by using advanced XAS analysis methods coupled to Molecular Dynamics for the simulation of the XAS spectra.
A series of studies have been dedicated to the link between color and valence state of transition metals (Cu, Fe, Mn) in glassy mosaic and sectilia panels tesserae of roman [Gliozzo-10] and medieval [Silvestri-12] production. Metallic copper was found to produce the deep red color via the Surface Plasmon Resonance of nanometer sized copper particles embedded in the glassy matrix.
Cuprite particles were found to produce the orange hue whereas blue and green tesserae contain copper in the 2+ valence state. A marked correlation was found between the Cu^{2+} content and the deep coloration of the tesserae. Concerning Fe and Mn the latter was supposed to be added as decoloring agent by promoting the oxidation of Fe to the 3+ state. The ratio between Fe^{3+} and Fe^{2+} determined the color of the manufact. For Fe^{2+} between 30 and 50% an aqua blue color is obtained whereas for lower amounts a light green is obtained. Mn was found in the 2+ state: since it was added as a Mn^{4+} mineral (pyrolusite) this suggests its role as oxidating agent for Fe.

A Sectilia Panel from the roman rural settlement located at the Faragola site. The tesserae were used for the study described in Gliozzo-10.

References:
I. Cianchetta et al. *Discoloration of the smalt pigment: experimental studies and ab initio Calculations* J. Anal. At. Spectrom 2012, 27, 1941.
A. Silvestri et al. *The role of copper on colour of palaeo-Christian glass mosaic tesserae: an XAS study* J. Cult. Herit. 13 (2012) 137
L. Cartechini et al.*Modified Naples yellow in Renaissance majolica: study of Pb–Sb–Zn and Pb–Sb–Fe ternary pyroantimonates by X-ray absorption spectroscopy* J. Anal. At. Spectrom., 2011, 26, 2500
E. Gliozzo et al. *The sectilia panels of faragola (Ascoli Satriano, Southern Italy) a multi analytical study of the green, marbled (green and yellow) blue and blackish glass slabs*. Achaeometry 52, (2010) 38.

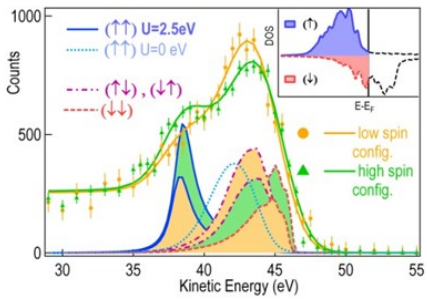
AR-APECS: coincidence spectroscopy as a "two-particle" probe of the electronic structure in magnetic systems

R. Gotter[1], G. Fratesi[2], R. A. Bartynski[3], F. Da Pieve[4], F. Offi[5], A. Ruocco[5], S. Ugenti[5], M. I. Trioni[6], G. P. Brivio[2], and G. Stefani[5]

[1] IOM-CNR Istituto Officina dei Materiali, Area Science Park, I-34149 Basovizza, Trieste, Italy
[2] ETSF, CNISM, and Dipartimento Scienza dei Materiali, Università Milano Bicocca, I-20125 Milano, Italy
[3] Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA
[4] EMAT, University of Antwerp, B-2020 Antwerp, Belgium
[5] CNISM and Dipartimento di Fisica, Università Roma Tre, I-00146 Roma, Italy
[6] ISTM-CNR Istituto di Scienze e Tecnologie Molecolari, I-20133 Milano, Italy

In core-valence-valence (CVV) Auger decays, two holes are created in the valence band (VB). While in conventional Auger spectroscopy, only one of the two electrons leaving the VB is measured (the Auger electron), in AR-APECS (Angle Resolved - Auger PhotoElectron Coincidence Spectroscopy), the coincident detection of the Auger electron and its parent photoelectron, allows one to put constraints on the electron which leaves the valence band and fills the core hole, thereby getting information on the total spin value of the two-hole finale state [1] and providing new insights in the study of magnetic systems [2,3]. In addition, the CVV Auger line shape is sensitive to electron-electron correlation and can be understood within the established Cini-Sawatzky (CS) approach.

The combination of spin selectivity and sensitivity to electron correlation become relevant in the study of itinerant ferromagnets, where majority (↑) and minority (↓) spin split into significantly different sub-bands. In this case one has the possibility to pick two electrons out of the valence band, so that the two-holes in the Auger final state can have different spin pairings, (↑↑), (↑↓), (↓↑) and (↓↓), depending on which sub-band each hole originated in, and thereby probe electron correlations in each sub-band [4]. Due to an interplay among photoemission selection rules, Auger matrix elements and angular distributions of the emitted electrons, one obtains experimental configurations favoring low spin or high spin states. In figure the dashed curves show the SCDOS (Self Convolution of Density of States) for the four possible spin combinations of final state holes, starting from *ab-initio* calculation of the spin-resolved DOS (inset). It is evident that the ~ 38 eV feature, enhanced in the high-spin configuration, is reproduced by applying the CS method only to the (↑↑) contribution, with a correlation energy U=2.5 eV. The CS model gives rise to sharper features located at lower kinetic (higher binding) energy with respect to the (↑↑) SCDOS (U=0 eV dotted line). Finally, a different degree of localization of differently spin oriented holes has been found, by an amount which depends on the thickness of the magnetic film. This may have a relevant impact in spintronics and in the development of magnetic nano-devices.



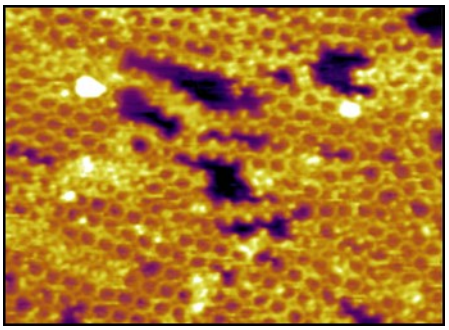
Fe $M_{23}VV$ Auger spectra obtained in the low-spin (orange symbols) and high spin (green symbols) AR-APECS geometries, for a 4 ML Fe/Cu(001) film

References:
[1] R. Gotter, F. Da Pieve, A. Ruocco, F. Offi, G. Stefani, R. Bartynski, *Phys. Rev. B* 72, 235409 (2005)
[2] R. Gotter, F. Offi, A. Ruocco, F. Da Pieve, R. Bartynski, M. Cini and G. Stefani, *Eur. Phys. Lett.* , 94 (2011) 37008
[3] M. Cini, E. Perfetto, R. Gotter, F. Offi, A. Ruocco, and G. Stefani, *Phys. Rev. Lett.* 107, 217602 (2011)
[4] R. Gotter, G. Fratesi, R. A. Bartynski, F. Da Pieve, F. Offi, A. Ruocco, S. Ugenti, M. I. Trioni, G. P. Brivio, and G. Stefani, *Phys. Rev. Lett.* 109, 126401 (2012)

Controlling on-surface polymerization by hierarchical and substrate-directed growth

L. Lafferentz[1,3], V. Eberhardt[2], C. Dri[3], C. Africh,[3] G. Comelli[3,4], F. Esch[3], S. Hecht[2], L. Grill [1]

[1] Department of Physical Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, 14195 Berlin, Germany
[2] Department of Chemistry, Humboldt- Universität zu Berlin, 12489 Berlin, Germany
[3] IOM-CNR Laboratorio TASC, Area Science Park, 34149 Basovizza-Trieste, Italy
[4] Physics Department and CENMAT, University of Trieste, 34127 Trieste, Italy



2D network of trans-Br_2I_2TPP molecules deposited at 80 K on Au(111) after annealing to 250°C

The bottom-up construction of covalently-bound molecular architectures in a well-defined arrangement is a key step in molecular electronics and in the design of novel materials. In particular, step-by-step connection of molecules is required for the formation of rather sophisticated structures . We were able covalently connect molecules in a hierarchical manner by the temperature-controlled selective and sequential activation of specific sites. To this end, we equipped a central molecular porphyrin building block with different halogen–phenyl side groups. These 5,15-bis(4'-bromophenyl)-10,20-bis(4'- iodophenyl)porphyrin (trans-Br_2I_2TPP) molecules have two bromine and two iodine substituents, each in a linear trans configuration, to encode for the two directions of growth. The crucial point is that bromine and iodine substituents, chracterized by different bond dissociation energies, can be selectively removed by heating at different temperatures. We deposited the trans-Br_2I_2TPP molecules on a Au(111) surface kept at 80K and investigated their structure and assembling upon annealing by means of Scanning Tunneling Microscopy (STM). After deposition at low temperature, mainly intact monomers were found, with each molecule containing both kinds of halogen substituents. Upon heating to 120°C, selective activation of the terminal iodine substituents is induced, and linear chains of porphyrin molecules are created, which typically arrange in a parallel manner on the surface and form close-packed islands.

Upon further heating to 250°C, also the remaining bromine substituents are removed, and the chains interconnect in a 2D regular architecture, much less defective and more extended than what achievable by a one-step growth process. The hierarchical growth introduces the possibility of realizing two-component networks for the construction of more complex, heterogeneous architectures, as demonstrated by depositing trans-Br_2I_2TPP in combination with dibromoterfluorene (DBTF). Furthermore, substrate-directed growth and a preferred orientation of the molecular nanostructures can be achieved by deposition on an anisotropic surface as Au(100), for both homo- and hetero-molecular architectures.

References:

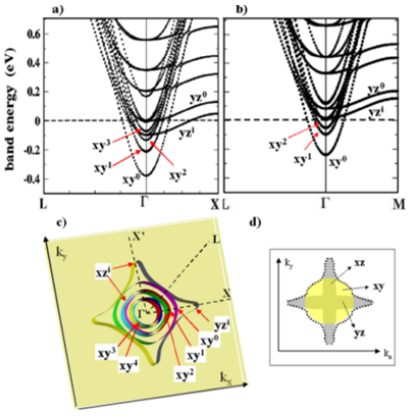
L. Lafferentz, V. Eberhardt, C. Dri, C. Africh, G. Comelli, F. Esch, S. Hecht and L. Grill *Controlling on-surface polymerization by hierarchical and substrate-directed growth* Nature Chem. 4 (2012) 215-220

Electronic and magnetic phenomena in Ti based perovskites

A. Filippetti[1], P. Delugas[1], M. Scarrozza[1], G. Lopez[1], G. Colizzi[1], V.Fiorentini[1,2]

[1] CNR-IOM, UoS Cagliari, c/o Dipartimento di Fisica, S.P. Monserrato-Sestu km 0.700, 09042 Monserrato
[2] Dipartimento di Fisica, Università di Cagliari, S.P. Monserrato-Sestu km 0.700, 09042 Monserrato

The physics of oxides, and of Ti based perovskites in particular, form a variegate field that involves many topics like electronic correlations, dielectric properties, magnetism and many more. In this highlight we point out two papers that deal with 2 different aspects, both treated with theoretical methods based on advanced ab-initio computations. The first paper [1] deals with the SrTiO3-LaAlO3 conductive interface, a popular topic in oxide physics, while the second [2] studies an unconventional class of potential multiferroic materials. The apparently weird formation of a 2 Dimensional Electron Gas (2DEG) at the interface of two strong insulators is generally explained as consequence of a Zener breakdown occuring in the LaAlO3 layer. The 2DEG is present only when aluminate layer exceeds a critical 3 layer thickness and its density increases as the $LaAlO_3$ grows deeper, in principle up to a saturation value of 0.5 per unit cell but observed values are at most 1 magnitude order lower. Paper [1], studying a non-stoichiometric super-lattice configuration with two n-type fully charged interfaces, actually demonstrates that the nature of the confinement is intrinsic and completely independent of the Zener breakdown or other charge transfers scenarios. The confinement is always caused by the discontinuity of the SrTiO3 conduction band that induces a splitting between Ti d_{xy} levels and the other t_{2g} orbitals, the d_{xy} levels form thus a planar band with high mobility along the interface plan and strongly confined in the normal direction. It is also demontrated that this interface splitting grows proportionally with the charge density at the interface. The paper also shows that for charge densities exceeding 0.15 e/u.c. the 2DEG can accommodate only part of the charge. Above this density, the bulk t_{2g} bands are progressively occupied. This part of the charge has a net lower mobility and its confinement is of electrostatic nature and therefore depends on the particular interface.



Bands (a) and 2D Fermi surface (c,d) for full density n_s=0.5 e/u.c. STO/LAO interface. In (b) bands for n_s=0.15 e/u.c.

Paper [2] explores the possibility of engineering a multiferroic material via magnetic doping in $La_2Ti_2O_7$. This is a layered ferroelectric perovskite where at variance with most of ferroelectric titanates, the spontaneous polarization is not caused by the centro-simmetry breaking of octahedra and can be thus compatible with Jahn-Teller distortions. Magnetism is introduced via doping with V ions, which cluster preferentially in linear chains; their d orbitals give rise to a specific orbital ordering and ferromagnetic coupling, preserving the insulating character even for large dopant concentrations.

References:
[1] Spontaneous 2-Dimensional Carrier Confinement at the n-Type SrTiO3/LaAlO3 Interface.
P. Delugas, A. Filippetti, V. Fiorentini, D. Bilc,D. Fontaine,P. Ghosez, Phys.Rev.Lett. 106,166807 (2011)
[2] Ferromagnetism and Orbital Order in a Topological Ferroelectric.
Marco Scarrozza, Alessio Filippetti and Vincenzo Fiorentini – Phys Rev Lett.
109, 217202 (2012)

Computational materials science for solar-energy conversion and storage

S. Piccinin,[1] H. L. Hu,[1,2] C. Ma,[1,2] A. Laio,[1,2] and S. Fabris[1,] C. Melis[3,4], L. Bagolini[3,4], G. Malloci[3], C. Caddeo[3,4], M.I. Saba[3], L. Colombo[3,4], and A. Mattoni[3]

[1] CNR-IOM DEMOCRITOS, Istituto Officina dei Materiali, c/o SISSA Via Bonomea 265, Trieste, Italy
[2] SISSA – Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, Trieste, Italy
[3] CNR-IOM Unità di Cagliari, Istituto Officina dei Materiali, Monserrato (Ca), Italy
[4]Dipartimento di Fisica, Università di Cagliari, Monserrato (CA), Italy

Novel Catalysts for Artificial Photosynthesis. Artificial leaf technologies aim at the direct conversion and storage of solar energy into high-energy chemical fuels. One of the main limiting processes is the light-promoted electrochemical splitting of water molecules into H_2 and O_2. The present challenge of finding stable and efficient catalyst materials for this reaction is undertaken with combined experimental and theoretical approaches, in which numerical materials modeling plays a key role.

In this work (1), we have focused on a class of materials - cobalt-phosphate (Co-Pi), cobalt-borate, nickel-borate, and others – that have been recently discovered and successfully applied to artificial leaf technologies. Their activity relies on ordered and oxidation-resistant active centers embedded in amorphous grains. The structure of these active cores is debated and experimentally elusive because of the complex amorphous structure and composition of the grains. Our computational study provided the first realistic structural model of the Co-Pi catalyst (Fig. 1a), and opened the way for understanding the functionality of these catalysts.

Another work (2) addressed the reaction mechanism of an all-inorganic homogeneous catalyst (Fig. 1b) capable to promote water oxidation with low overpotential and high turnover frequency (3). The reaction thermodynamics predicted by Density Functional Theory calculations for the intermediate reaction steps is in good agreement with the available measurements. Our work shows that the catalytic efficiency stems from the optimal distribution of the free energy cost to form reaction intermediates, in analogy with metal-oxide catalysts, thus providing a unifying picture for the two realms of water oxidation catalysis.

While the oxidation of water to molecular oxygen and the reduction of protons to molecular hydrogen are typically promoted by different catalysts, the Ru(II)-pincer complex recently synthesized (4) has been shown to promote both the thermal driven formation of H_2 and the UV–vis driven evolution of O_2. In our work (5), we adopt an explicit description of the solvent and employ metadynamics coupled with the Car–Parrinello method to study the reaction mechanism and determine the activation free energies (Fig. 1c). Our simulations predict a novel catalytic cycle, which has considerably lower activation energies than earlier proposals, and demonstrate the importance of an explicit description of the solvent

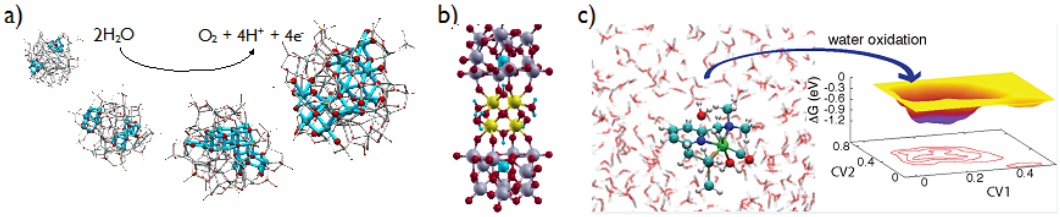


Figure 1. Structural models of a) Co-phosphate nanoparticles (Ref. 1); b) tetraruthenium-polyoxometalate (Ref. 2); c) Ru(II)-pincer complex in solution (Ref. 5).

Modeling nanomaterials for photovoltaics The large scale production of electricity from sunlight by photovoltaic (PV) effect requires the development of efficient solar cells based on low cost and clean synthesis. Nanostructured materials offer great opportunities for PV.
It is possible to cheaply process many nanomaterials from solution by blending organic and inorganic components and to control their optoelectronic properties by tuning the microstructure at the nanoscale.
An atomic-scale control of the interfaces and a better fundamental understanding of the photo-physical processes are important to further improve the performances of nanostructured solar cells.
In these works (6,7,8), we have applied multi-scale modeling by combining model potential and first-principles atomistic simulations, to understand and to improve the properties of several classes of hybrid (6,7) and inorganic (8) nanostructured interfaces for PV.
As for hybrid solar cells, we have enabled an improvement in the performance of the polymer poly(3-hexylthiophene) P3HT/TiO_2 solar cells by engineering the hybrid interface with molecular pyridines interlayer (7). Atomistic simulations coupled to experiments have clarified that a suitable chemical structure of the molecule induces selective intermolecular interactions, a preferential morphological order at the interface and higher power conversion efficiency (6) (Figure 2, left panel).
In the field of low cost inorganic films, we have investigated nanocrystalline silicon (Figure 2, right panel). We have shown theoretically and experimentally the occurrence of quantum confinement in hydrogenated nanocrystalline silicon. Photo-generated positive charges can be confined within the nano-grains due to the embedding within the amorphous matrix. The emission associated to confined states is verified by photoluminescence experiments on nanocrystalline samples. According to this study nanocrystalline silicon is a promising material suitable for oxygen-free optoelectronics, silicon-based memories and photovoltaics (8).

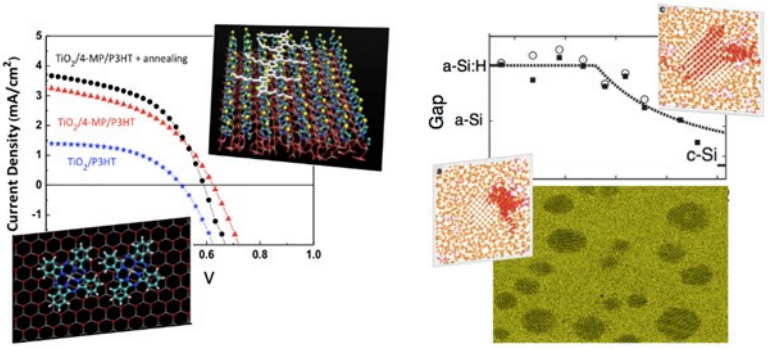


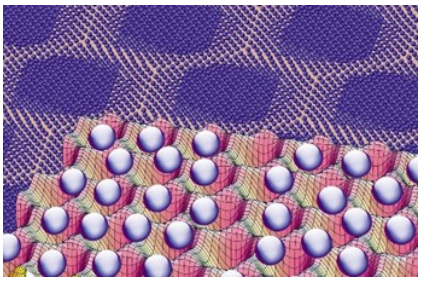
Figure 2 (Left Panel): Polymer/ metal oxide PV cells functionalized by pyridine [6] (top) and ZnPc [7] (bottom) interlayers; (Right Panel): Dependence on crystal size of the electronic gap of nano- crystalline silicon due to quantum confinement and to holes localization [8] effects.

References:
(1) H. L. Hu, S. Piccinin, A. Laio, and S. Fabris, ACS Nano vol. 6, pp. 10497, 2012.
(2) S. Piccinin and S. Fabris, Phys. Chem. Chem. Phys. vol. 13, pp. 7666, 2011.
(3) A. Sartorel et al., J. Am. Chem. Soc., vol. 130, pp 5006, 2008.
(4) Kohl et al. , Science vol. 324, pp. 74, 2008.
(5) C. Ma, S. Piccinin, and S. Fabris, ACS Catalysis vol. 2, pp. 1500, 2012.
(6) C. Melis, P. Raiteri, L. Colombo, and A. Mattoni, ACS NANO, vol. 5, no. 12, pp. 9639–9647, 2011.
(7) E. V. Canesi et al., Energy and Enviromental Science, vol. 5, no. 10, pp. 9068–9076, 2012.
(8) L. Bagolini et al., Physical Review Letters, vol. 104, no. 17, 2010.

Simulating novel laser-controlled frictional systems

A. Vanossi[1], A. Benassi[1], N. Manini[2], E. Tosatti[3,4]

[1] CNR-IOM Democritos & SISSA, Via Bonomea 265, 34136 Trieste, Italy.
[2] Dipartimento di Fisica, Università di Milano, Via Celoria 16, 20133 Milano, Italy.
[3] SISSA & CNR-IOM Democritos, Via Bonomea 265, 34136 Trieste, Italy.
[4] ICTP, Strada Costiera 11, 34104 Trieste, Italy.



MD simulations of a crystalline layer of colloids interacting with a laser-generated periodic potential. Lattice mismatch results in solitonic structures ruling the frictional behavior.

The intimate understanding of sliding friction, a central player in the physics and technology of an enormous variety of systems, from nano up to macroscale, is historically hampered by a number of difficulties. One of them is the practical inaccessibility of the buried interface between the contacting surfaces. Another is the general impossibility to fully control the detailed nature, morphology, and geometric parameters of the tribological system. Addressing both issues, a brand new and exciting alley in microscopic frictional sliding has been recently opened by artificial systems realized with the help of optically trapped charged particles, either cold Ca(+) ions in empty space, or colloidal particles in a fluid solvent, forced to slide over a laser-generated periodic potentials.
Before any data, we recently predicted [1] that in the very near future trapped atomic ions will verify experimentally the mathematically proven one-dimensional Aubry's theory for incommensurate systems, cornerstone of the celebrated transition between superlubric sliding and pinning with static friction. In two dimensions, the sliding of a crystalline layer of charged colloidal particles has already shown the superlubric dynamics of the incommensurate case and the new phenomenon of kinks in flight controlling the colloid mobility, and unexpectedly appearing in a system statically commensurate and kink-free. Our molecular dynamics simulations [2] reveal how these moving solitonic structures that permit the depinning are spawned at the system edges, where the density drops, and commensurability necessarily changes – a physics related to that of real island and cluster depinning. The explored phase diagram versus colloid density and sliding force highlights large asymmetry between solitons and antisolitons in overdense and underdense monolayers, respectively. We then extract and predict the frictional work as a function of mean velocity and corrugation amplitude, loosely mimicking the “load” variable of macroscopic friction laws. Trapped ions and especially colloids possess many controllable elements and added bonuses, including the promise to bridge between nanoscale and mesoscale sizes and phenomena. As recently pointed out [3], it is definitely urgent that theory should set to work to anticipate and accompany the ongoing experimental efforts.

References:

[1] A. Benassi, A. Vanossi, E. Tosatti, “Nanofriction in Cold Ion Traps”, Nature Communications 2:236 (2011).
[2] A. Vanossi, N. Manini, E. Tosatti, “Static and dynamic friction in sliding colloidal monolayers”, PNAS 109, 16429 (2012).
[3] A. Vanossi and E. Tosatti, “Colloidal friction: kinks in motion”, Nature Materials 11, 97 (2012).

Graphene: growth, structural and electronic properties

Prepared by I. Vobornik, S. Fabris and A. Baraldi

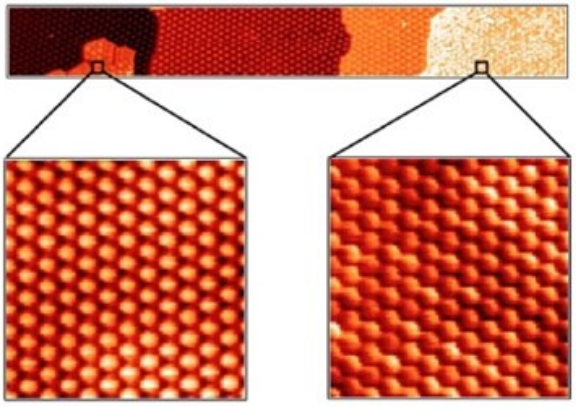
CNR-IOM, Trieste, Italy

Graphene is the lightest and strongest material with extraordinary heat and electrical conductivity. Among a number of envisioned applications, it also represents a top candidate for substituting silicon in future electronic devices. Our Institute is strongly involved in the research on this material, with the aim of developing new synthesis strategies, of improving its structural and transport properties and exploring its unique chemical and physical properties.

The so far exploited synthesis approaches result in graphene sheets whose electronic properties are often altered by interactions with the substrate. We identified different approaches in producing non-interacting graphene layers. **Graphene on cubic 3C-SiC (β-SiC):** Due to its cubic lattice, β-SiC would not appear suitable for graphene growth. Contrary to common belief, we found that high quality graphene can be successfully grown on cubic β-SiC and the interaction with the substrate is almost negligible when compared to α-SiC exactly due to strong lattice mismatch with the substrate[1]. **Bilayer graphene on Ru(0001):** In special growth conditions (high level ethylene exposure) a condition may be realized where the first graphene layer acts as a buffer and the second layer behaves basically as an isolated graphene sheet[2]. Alternative strategies were found, based on the **funtionalization/intercalation with light elements**,[3] or by the **growth of a silica layer between graphene and Ru(0001)** using transfer-free processes[4].

The thermal properties of graphene were also studied using different approaches[5]. The stability and break-up of epitaxial graphene was investigated by combining DFT calculations and high-energy resolution photoemission. The latter experimental technique resulted to be extremely successful also in providing information on the graphene thermal expansion.

Thermal reduction of graphene oxide: X-ray photoelectron spectroscopy, temperature programmed desorption, and DFT calculations were used to identify a dual path mechanism for the reduction of oxidized graphene governed by the coverage of oxygen atoms (6). The numerical modeling allowed to identify the surface functional groups that are the precursors for CO/CO2 evolution (7). Our DFT calculations demonstrate that O diffusion on graphene governs the **unzipping and cracking of the oxidized C network** (8). This forced a revision and extension of the current models of graphene oxidative unzipping and cutting.



Bilayer graphene on Ru(0001) (from reference 2)

Istituto Officina dei Materiali

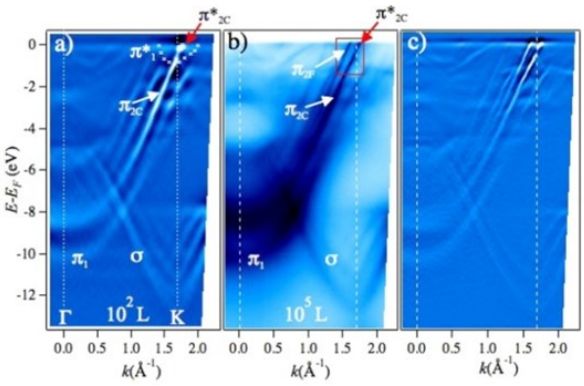
(2) New bilayer graphene phase on Ru(0001)

M. Papagno[1,2], D. Pacilé[1,2], D. Topwal[3], P. Moras[1], P.M. Sheverdyaeva[1], F.D. Natterer[4], A. Lehnert[4], S. Rusponi[4], Q. Dubout[4], F. Calleja[4], E. Frantzeskakis[4], S. Pons[4], J. Fujii[5], I. Vobornik[5], M. Grioni[4], C. Carbone[1] and H. Brune[4]

[1] CNR-ISM, Trieste, Italy
[2] Physics Department, University of Calabria, Rende (Cs), Italy
[3] Elettra – Sincrotrone Trieste S.C.p.A. Trieste, Italy
[4] IPMC, EPFL, Lausanne, Switzerland
[5] CNR-IOM, Laboratorio TASC, Trieste, Italy

The electronic properties of graphene strongly depend on the interaction with the supporting substrate. When graphene is placed on top of another graphene layer in a Bernal (AB) stacking, the weak interlayer coupling is sufficient to modify the dispersion of the charge carriers from linear (massless fermions) to hyperbolic (massive chiral fermions). A suitable way to reduce this interaction and restore a nearly free-standing band behavior is to introduce a relative displacement of the two layers. We were able to synthesize a bilayer graphene phase with these structural and electronic properties on the Ru(0001) surface by performing a large ethylene exposure. This novel phase displays an AA stacking sequence and a relatively weak structural modulation, that result in a p-doped linearly dispersing Dirac state.

At an exposure level of 10^2 L of ethylene the Ru(0001) surface (held at a temperature of 1600 K) allows the formation of a full graphene layer in contact with the metallic substrate, plus patches of a second graphene layer. In angle-resolved photoemission spectroscopy map along the ΓK direction of the graphene Brillouin zone (Fig. 1a) the respective band features are identified as the paraboliclike π_1 and π_1^* states, ascribed to the first graphene layer, and the sharp and n-doped π_{2c} Dirac cone and σ band, accompanied by several replicas, which are associated to the patches of the graphene bilayer.



Electronic band structure of bilayer grapheme on Ru(0001)

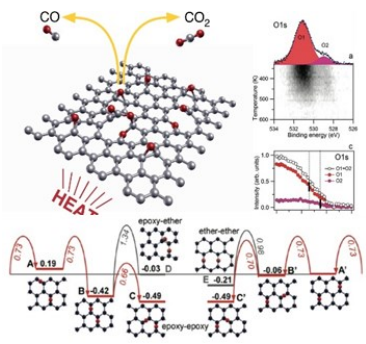
Figs. 1b-c display the changes occurring in the electronic structure of the system upon further exposure to 10^5 L of ethylene with the Ru surface at 1600 K. In addition to the previously observed bands, we find a new π state (π_{2F}) that displays a linear dispersion, characteristic of a free-standing graphene layer, with a Dirac point above the Fermi level (p-type doping). Scanning tunneling microscopy measurements show that this new phase consists of weakly interacting graphene layers arranged in an AA stacking sequence. These features sizably differ from those of bilayer graphene synthesized on Ru(0001) at much smaller ethylene exposures. Our results prove that the first graphene layer grown on Ru(0001) can be used as a template to grow almost free-standing graphene on top.

(6)(7)(8) Structure and chemistry of graphene oxide

T. Sun[1,2] R. Larciprete[3] S. Baroni[1,2], P. Lacovig[5] A. Baraldi,[6] S. Lizzit[5], S. Fabris[1,2]

[1] CNR-IOM DEMOCRITOS, Istituto Officina dei Materiali, c/o SISSA Via Bonomea 265, Trieste, Italy
[2] SISSA – Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, Trieste, Italy
[3] CNR-Institute for Complex Systems, via Fosso del Cavaliere 100, I-00133 Roma, Italy
[5] Sincrotrone Trieste S.C.p.A., Strada Statale 14 Km 163.5, I-34149 Trieste, Italy
[6] Physics Department and CENMAT, University of Trieste, Via Valerio 2, I-34127 Trieste, Italy

The efficient reduction of graphene oxide while preserving optimal transport properties would greatly widen the versatility of graphene in electronics and optoelectronics. The actual structure of graphene oxide, which mostly comprises surface O, and OH groups and C vacancies, is presently debated. Graphene can be easily produced by thermally reducing graphene oxide. However, defect formation in the C network during deoxygenation compromises the charge carrier mobility in the reduced material. Thermal reduction of graphene oxide occurs around 450 K with the release of H_2O, CO, and CO_2 in the gas phase, which implies surface mobility of adsorbates and defects. In this group of papers we have identified i) the mechanisms of the thermal reaction of graphene oxide and shown their dependency on the O coverage (1); ii) the relevant surface precursors for the thermal reduction and the role of O mobility (2); and iii) the nucleation and growth of extended defects on oxidized graphene leading to oxidative unzipping and cutting of graphene (3). In this work (1) we combined spectroscopic tools and ab initio calculations to probe the species residing on the surface and to identify a dual path mechanism in the thermal reduction of graphene oxide driven by the oxygen coverage. At low surface density, the O atoms adsorbed as epoxy groups evolve as O_2 leaving the C network unmodified. At higher coverage, the formation of other O-containing species opens competing reaction channels, which consume the C backbone. The reduction of graphene oxide surfaces yielding molecular CO/CO_2 was further studied using density functional theory calculations (2). This reaction can proceed exothermically only from surface precursors containing more oxygen atoms than strictly needed to produce CO/CO_2 in the gas phase. The main reaction precursors were shown to be lactone groups either in lactone-ether or in ether-lactone-ether forms. Our calculations also show that the formation of surface structures capable to initiate the unzipping and cracking of the oxidized C network is strongly influenced by the constraint of the graphitic lattice on the surface functional groups. We find that these processes are rate limited by O diffusion and driven by the local strain induced by the O adspecies. O mobility is ultimately recognized as a key factor to control and to prevent the C-network breakdown during thermal processing of oxidized graphene.



a) Precursors for the thermal reduction of graphene oxide. b) O1s core level spectra measured during thermal reduction. c) Calculated activation energies for epoxy group diffusion.

References:
(1) V. Aristov et al., Nano Letters, Vol. 10 - 3 (2010)
(2) M. Papagno et al., ACS Nano, Vol. 6 - 10, pp. 9299-9304 (2012)
(3) R. Balog et al., Nat. Mater. 9, 315 (2010); R. Larciprete et al., ACS Nano 6, 9551 (2012)
(4) S. Lizzit et al., Nano Letters 12, 4503 (2012)
(5) E. Miniussi et al., Phys. Rev. Lett. 106, 216101 (2011); M. Pozzo et al., Phys. Rev. Lett. 106, 135501 (2011)
(6) R. Larciprete et al., JACS, Vol. 133, pp. 17315-17321 (2011)
(7) T. Sun, S. Fabris, and S. Baroni, J. Phys. Chem. C, Vol. 115, pp. 4730-4737 (2011)
(8) T. Sun and S. Fabris, Nano Letters, Vol. 12, pp. 17-21 (2011)

Istituto Officina dei Materiali

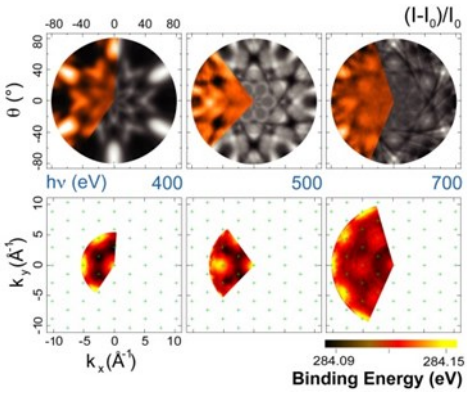
Band dispersion in the deep 1s core level of graphene

S. Lizzit[1], G. Zampieri[2], L. Petaccia[1], R. Larciprete[3], P. Lacovig[1,4],
E.D.L. Rienks[5], G. Bihlmayer[6], A. Baraldi[4,7], Ph. Hofmann[5]

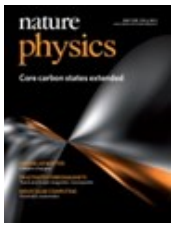
[1] Elettra – Sincrotrone Trieste S.C.p.A., Trieste, Italy
[2] Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica, Bariloche, Argentina;
[3] CNR-Institute for Complex Systems, Roma, Italy
[4] Physics Department and CENMAT, University of Trieste, Italy
[5] Institute for Storage Ring Facilities and Interdisciplinary Nanoscience Center (iNANO), University of Aarhus, Denmark
[6] Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany
[7] CNR-IOM, Laboratorio TASC, Trieste, Italy

Chemical bonding in molecules and solids arises from the overlap of valence electron wave functions, forming extended molecular orbitals and dispersing Bloch states, respectively. Core electrons with high binding energies, on the other hand, do not participate in the bonding being localized on their respective atoms. This implies well defined core level binding energies and the absence of splitting and band like dispersion, a fact that is exploited in several powerful experimental techniques, such as X-ray Photoelectron Spectroscopy. Here it is reported the observation of band formation and considerable dispersion (up to 60 meV) in the 1s core level of the carbon atoms forming graphene, despite the high C 1s binding energy of ~284 eV. The dispersion shows up as an emission-angle dependent C1s binding energy modulation.

High resolution C1s core level photoemission spectra were measured at the SuperESCA beamline of Elettra on graphene grown on Ir(111). The fitting of all the C1s spectra of the extensive data set measured is obtained with a single component with the same line-shape parameters. Strong intensity modulations are observed which are due to photoelectron diffraction effects. The intensity modulation function is perfectly reproduced by multiple scattering simulations for a flat, free-standing graphene layer. The resulting binding energy modulation shows also a periodicity with the point symmetry of the graphene lattice. However, when displayed as a function of $k_{||}$, the wavevector component parallel to the surface, which is the only relevant wavevector for a two-dimensional system such as graphene, the modulation is periodic in the reciprocal space of graphene but the pattern does not coincide with the reciprocal lattice mesh. Among the different mechanisms that could led to the observed binding energy variations, the one that explains all the experimental findings is the formation of bonding and anti-bonding bands between the 1s states of the two atoms in the unit cell of graphene. The apparently wrong periodicity of the binding energy modulation is due to a Young's double slit-like interference effect, caused by the presence of two atoms in the unit cell of graphene, which modulates the intensity of the two bands: for some reciprocal lattice points only the bonding band is observed, for others only the anti-bonding band. A very similar dispersion is also found by *ab initio* calculations.



Intensity (top) and binding energy (bottom) modulation in C1s core level of graphene on Ir(111)



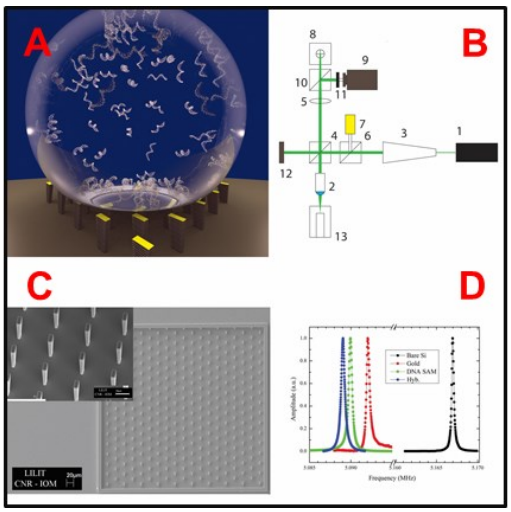
References:
S. Lizzit et al., Nature Physics, Vol. 6, pp. 345-349 (2010)
Selected as Cover Article of Nature Physics, Issue May 2010.

Fast detection of biomolecules in diffusion limited regime using micromechanical pillars

Mauro Melli[1], Giacinto Scoles[2,3] and Marco Lazzarino[1]

[1] CNR-IOM – Area Science Park Basovizza – ss 14 km 163.5 34149 Trieste, Italy
[2] Elettra Sincrotrone Trieste S.C.p.A, Area Science Park Basovizza – ss 14 km 163.5 34149 Trieste, Italy
[3] University of Udine, Dept. of Biological and Medical Science, Ospedale della Misericordia 33100 Udine, Italy

We have developed a micromechanical sensor based on vertically oriented oscillating beams, in which, contrary to what is normally done (for example with oscillating cantilevers) the sensitive area is located at the free end of the oscillator. This confines the adsorption on a small area surrounded by a much larger area with no adsorption of the analyte of interest. As a consequence the kinetics of adsorption on the tip of our micro-pillars is more than three orders of magnitude faster than on a typically 200x20 micron large cantilever.
This is because, at the high dilutions typical in equilibrium recognition bio-sensing, the volume from which the analyte molecules have to diffuse to saturate the surface is, in our case, a sphere of radius more than two orders of magnitude smaller than the corresponding linear distance valid for adsorption on a macroscopic surface. Pillar oscillations are detected by means of an optical lever method, but the geometry is suitable for multiplexing with compact integrated detection. We demonstrate our technology investigating the formation kinetics of a DNA self assembled monolayer consisting of less than 10^6 DNA molecules and measuring their hybridization efficiency. We show that the adsorption kinetics is 1000 times faster than on a "macroscopic" surface. We also show that the hybridization of a SAM of maximum density DNA is 40% or 4 times the value reported in the literature concluding that this discrepancy is very likely due to incomplete saturation of the surface in the published studies due to the slower adsorption kinetics on the "macroscopic" surfaces used in these studies.



(A) Schematics of superhydrophobic conditions.
(B) Experimental configuration
(C) SEM images of the sample
(D) typical resonance curves acquired during DNA-SAM formation and its hybridization.

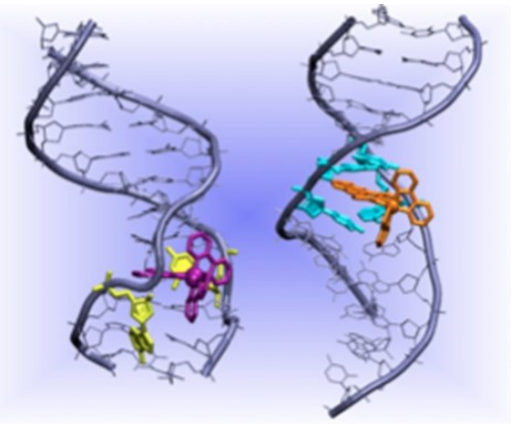
References:
M. Melli, A. Pozzato, M. Lazzarino, Inverted tapered pillars for mass sensing, **Microelectron. Eng**., 87 (2010) 730 –733. Doi:10.1016/j.mee.2009.12.021
M. Melli, G. Scoles, M. Lazzarino, Fast detection of biomolecules in diffusion-limited regime using micromechanical pillars, **ACS nano**, 5 (2011) 7928–7935. Doi:10.1021/nn202224g

Detecting DNA mismatches with inorganic molecules. Insights from computational studies

Attilio V. Vargiu[1], Duvan Franco[2] and Alessandra Magistrato[3]

[1]CNR-IOM, SLACS, c/o Dipartimento di Fisica, Università di Cagliari, s.p. Monserrato-Sestu, 09042 Monserrato, Italy
[2] International School for Advanced Studies (SISSA/ISAS), via Bonomea 265, 34136, Trieste, Italy
[3]CNR-IOM, Democritos National Simulation Center , International School for Advanced Studies\, via Bonomea 265, 34136, Trieste, Italy

Molecules that selectively recognize DNA mismatches (MMs) play a key role as nucleic acids probes and as chemotherapeutic agents. Metallo-insertors bind to the minor groove (mG) of double strand (ds) DNA, expelling the mismatched base pair and acting as its π-stacking replacement. In contrast, metallo-intercalators bind to the major grove of ds DNA and π-stack to adjacent base pairs. In this study we initially focused on structural and electronic properties of Δ–$[Rh(bpy)_2(chrysi)]^{3+}$ (**1**), Δ–$[Ru(bpy)_2(ddpz)]^{2+}$ (**2**) and Δ-$[Ru(bpy)_2(eilatin)]^{2+}$ (**3**) as prototypical examples of metallo-insertors and intercalators. For all molecules we characterized both insertion and intercalation into a DNA dodecamer via force field based molecular dynamics (MD) and hybrid quantum-classical MD simulations. A structural analysis of the **1**-**3**/DNA non-covalent adducts reveals that insertion provokes an untwist of the DNA, an opening of the mG and of the phosphate backbone in proximity of the mismatch, while intercalation induces smaller changes of these structural parameters. This behavior appears to be correlated with the size of the inserting/intercalating ligand in proximity of the metal coordination site. Moreover, by using advanced sampling techniques we studies the de-intercalation path of **1** and **2**, showing that the they have comparable de-intercalation barriers. A striking difference between dppz and chrysi is found in their intercalation modes, being their longest axes, respectively, perpendicular and parallel to the P-P direction between opposite DNA strands. This leads the two ligands to de-intercalate from the DNA through different mechanisms. Compound **2** goes through the formation of a metastable short-lived intermediate, with an overall free energy barrier of ~14.5 kcal/mol, in line with experimental findings. Compound **1** must cross a similar barrier (~15.5 kcal/mol), but does not form intermediates along the de-intercalation path. Thus, the shape of the intercalating moiety significantly affects the dissociation mechanism of these inorganic molecules. Understanding the factors which tune a specific insertion is of crucial importance for designing specific luminescent probes that selectively recognize MMs, as well as for developing more effective anticancer drugs active in MM repair deficient cells lines.



Simplified view of insertion (left) and intercalation (right) binding mode for **1** (violet) and **2** (orange), respectively. Mismatched bases, expelled from ds DNA upon insertion, are yellow colored. Intercalating bases are cyan colored.

References:
A.V. Vargiu, A. Magistrato Detecting DNA mismatches with metallo-insertors. A molecular simulation study. Inorganic chemistry 51 (4), 2046-2057 (2012)

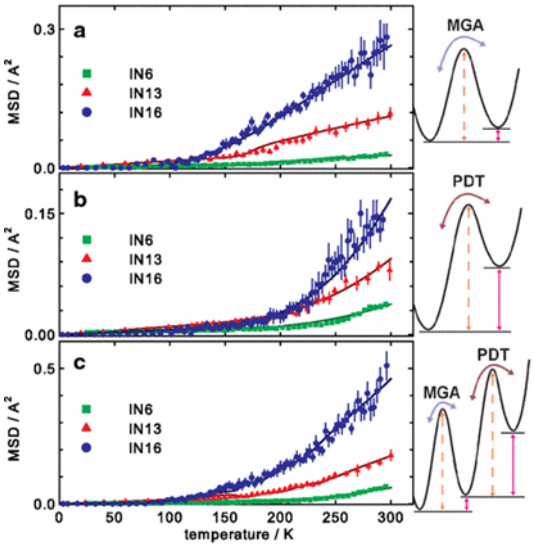
Physical origin of anharmonic dynamics in proteins: new insights from resolution-dependent neutron scattering on homomeric polypeptides

G. Schiro' [1], F. Natali [2], A. Cupane[1]

[1] Dipartimento di Fisica, Universita´ di Palermo, via Archirafi 36, I-90123, Palermo, Italy
[2] CNR-IOM, c/o Institut Laue Langevin, 6 Rue Jules Horowitz, BP 156-38042 Grenoble, France

Neutron scattering reveals a complex dynamics in polypeptide chains, with two main onsets of anharmonicity whose physical origin and biological role are still debated [1-3]. In this study [4] the dynamics of strategically selected homomeric polypeptides is investigated with elastic neutron scattering using different energy resolutions and compared with that of a real protein. Our data spotlight the dependence of anharmonic transition temperatures and fluctuation amplitudes on energy resolution, which we quantitatively explain in terms of a two-site model for the protein-hydration water energy landscape. Experimental data strongly suggest that the protein dynamical transition is not a mere resolution effect but is due to a real physical effect.

Elastic incoherent neutron scattering (EINS) data on D_2O-hydrated protein powders, which probes the mean square displacements (MSDs) of protein nonexchangeable H atoms, reveals two deviations from harmonic dynamics, at 100–150 K and at 220 K [1-3]. The first one is attributed mainly to thermally activated motions of CH_3 methyl groups. The second one is called "protein dynamical transition" (PDT) and its interpretation is still a challenge. Activation barriers and free energy values obtained for the protein dynamical transition allow us to propose that the protein/hydration water landscape structure, responsible for the PDT, is related to the two-wells potential for supercooled water: as proposed by S.-H. Chen and coworkers [5], the low-density à high-density liquid-liquid transition involves changes in the H-bond network dynamics of hydration water, which is coupled to protein internal motions, thus inducing the protein dynamical transition-related backbone and side chains fluctuations revealed by EINS.



MSD measured in dry (a) and hydrated (c) poly-A and hydrated poly-G (b); lines: MSD model calculated according to the potential pictured on the right (magenta and dashed orange arrows indicate ΔG and ΔG*, respectively). Picture taken from [4].

References:
[1] JH Roh, VN Novikov, RB Gregory, JE Curtis, Z. Chowdhuri, and AP Sokolov, Phys.Rev Lett. 95, 038101 (2005).
[2] W. Doster, S. Cusack, and W. Petry, Nature (London) 337, 754 (1989).
[3] G. Schiro´, C. Caronna , F. Natali, and A. Cupane, J. Am. Chem. Soc. 132, 1371 (2010).
[4] G. Schiro´, F. Natali, and A. Cupane, Phys. Rev. Lett. 109, 128102 (2012).
[5] M. Lagi, X. Chu, C. Kim, F. Mallamace, P. Baglioni, and S.-H. Chen, J. Phys. Chem. B 112, 1571 (2008).

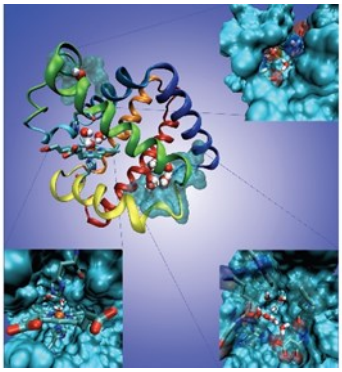
Computational study of biological systems

M. Ceccarelli[1,2], A. V. Vargiu[1,2], M. A. Scorciapino[2,3], P. Ruggerone[1,2]

[1]Dipartimento di Fisica, Università di Cagliari
[2] CNR-IOM Cagliari, Istituto Officina dei Materiali, 09042 Monserrato (CA), Italy
[3] Dipartimento di Scienze Chimiche e Geologiche, Universita' di Cagliari

Multidrug resistance (MDR) mechanisms in bacteria render a large spectrum of chemically unrelated antibiotics ineffective and represent one of the most serious impediments to improved healthcare today. One of the main mechanisms of MDR is the active transport of drugs out of the cell through specific protein complexes called efflux pumps. Thus, a part of the computational works we have performed has been devoted to the study of efflux pumps of the RND family in Gram-negative bacteria, which comprise many human pathogens that are very difficult to treat. To identify possible determinants of the action of these systems we have investigated the effects of the F610A mutation in AcrB, the RND transporter of of *Escherichia coli*. This mutation has been shown to significantly reduce the minimum inhibitory concentration of doxorubicin and many other substrates, although F610 does not appear to interact strongly with them. In our study [1] we shown that the compound slides deeply inside the binding pocket after mutation, increasing the strength of the compound-transporter interaction. To extend our knowledge in this field we have focused our attention on the binding properties of imipenem and meropenem, two potent antibiotics of the carbapenem family, to MexB, the RND transporter of the major efflux system of *Pseudomonas aeruginosa* [2]. Experimental evidence indicates meropenem as a compound strongly affected by MexB contrary to imipenem, which is apparently poorly transported by the same pump. According to our results, this different behavior is mainly due to the hydration properties of the nonpharmacophore part of the two compounds, being that of imipenem less bulky and hydrophobic. Our results indicates how subtle interactions determine the functionality of multidrug transporters. A project on efflux-mediated bacterial resistance has been financed by Basilea Pharmaceutica Ltd as continuation of a previous one on translocation of specific compounds through bacterial porins.

Hydration properties have been computationally studied also in myoglobin [3]. Our study pointed out that water is able to interact with proteins in diverse ways (see figure), leading to different kinds of perturbations in their intrinsic dynamic behavior. In particular, for myoglobin it was found that a water molecule can (i) "block" entry/escape of ligands to/from a particular docking site, (ii) act as a "wedge" modulating the dynamics of internal cavities, or (iii) join a "flow" of waters taking a ligand into (or "washing" a ligand away from) the protein interior. The information gathered in this work allowed us to provide a fingerprint of protein solvation state, the hydration sites map, which may represent a novel tool for comparing different forms/species of globular proteins.



The three ways water can interact with the protein surface, here with myoglobin

References:

[1] A.V. Vargiu et al., *Effect of the F610A mutation on substrate extrusion in the AcrB transporter: explanation and rationale by molecular dynamics simulations*, J AM CHEM SOC 133: 10704-7 (2011)

F. Collu et al., *Recognition of imipenem and meropenem by the RND-transporter MexB studied by computer simulations*, J AM CHEM SOC 134: 19146-58 (2012)

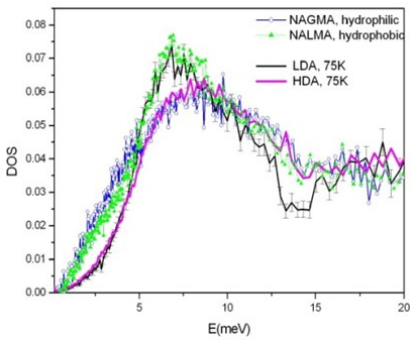
M. A. Scorciapino, A. Robertazzi, M. Casu, P. Ruggerone, and M. Ceccarelli, *Heme proteins: the role of solvent on the dynamics of gates and portals*, J AM CHEM SOC 132: 5156-5163 (2010)

Vibrational density of states of hydration water at biomolecular sites: hydrophobicity promotes low density amorphous ice behaviour

D. Russo[1]*, J. Teixeira[2], L. Kneller[3,4] J. R. D. Copley[3], J. Ollivier[5], S. Perticaroli[6], E. Pellegrini[5], M. A. Gonzalez[5]

[1] CNR-IOM c/o Institut Laue Langevin, 6 rue J. Horowitz BP156, F□38042 Grenoble, France
[2] Laboratoire Léon Brillouin (CEA/CNRS), CEA Saclay, 91191 Gif-sur Yvette Cedex France
[3]National Institute of Standards and Technology, Gaithersburg, MD 20899-6102
[4] Institut Laue Langevin, 6 rue J. Horowitz BP156, F□38042 Grenoble, France
[5]Università degli Studi di Perugia, Dipartimento di Chimica,

Neutron scattering reveals a complex dynamics in polypeptide chains, with two main onsets of anharmonicity whose physical origin and biological role are still debated [1-3]. In this study [4] the dynamics of Inelastic neutron scattering experiments and molecular dynamic simulations have been used to investigate the low frequency modes, in the region between 0 and 100 meV, of hydration water in selected hydrophilic and hydrophobic biomolecules. The results show changes in the *plasticity* of the hydrogen bond network of hydration water molecules depending on the biomolecular site. At 200 K the measured low frequency density of states of hydration water molecules of hydrophilic peptides is remarkably similar to that of high density amorphous ice (HDA), whereas, for hydrophobic biomolecules, it is comparable to that of low density amorphous ice (LDA) behaviour[1,2]. It is tempting to interpret our results within the context of the evaluation of water density at the vicinity of hydrophobic interfaces. It is generally accepted that water density or, more exactly, the molecular volume is modified in the vicinity of hydrophobic surfaces. On the contrary, the volume occupied by water molecules in the first layer above a hydrophilic substrate is smaller than in the bulk[3]. Such an effect may be due to the formation of deformed hydrogen bonds between water molecules and the interface along with disruption of the open tetrahedral water structure. The results that we discussed above show clearly that, for the intermolecular O-O-O bending vibration, the behaviour of hydration water is similar to that of HDA in the case of a hydrophilic substrate and similar to that of LDA for the hydrophobic situation. A way to interpret the apparently higher density is that the formation of hydrogen bonds between water and the organic substrate drastically changes the local tetrahedral structure generating a layer where the bonds are very distorted, thus similar to the situation of HDA. In contrast, close to a sufficiently large hydrophobic interface, particularly at low temperature, water molecules generate a relatively stable and open hydrogen bond network not substantially different from that of LDA and associated with a lower "density". Consequently, with this simple analogy strictly based on the analysis of the vibrational density of states, our results may support the idea that the apparent local density of water is greater in a hydrophilic environment. Our work contributes to assigning the specific contribution of the distinct sites to the polymorphism state of protein hydration water at low temperature.



Low density of states of hydrophilic and hydrophobic hydration water protein model compared to high density (HDA) and low density (LDA) amorphous ice.

References:
1) Russo D, et al. J. Am Chem Soc 133(13) 4882-4888 (2011)
2) Russo D, Chem Phys Letters, 517(1-3) 80-85 (2011)
3) Helmy R, et al, J Am Chem Soc.,127, 12446 (2005)

Extended Frequency Range Depolarized Light Scattering Study applied to Biomolecule - Water Solutions

S. Perticaroli[1], L. Comez[2], M. Paolantoni[3], P. Sassi[4], A. Morresii[2], D.Fioretto[3]

[1] Dipartimento di Chimica, Università di Perugia, via Elce di Sotto, I-06123 Perugia, Italy
[2] IOM-CNR c/o Dipartimento di Fisica, Università di Perugia, Via Pascoli, I-06123, Perugia, Italy
[3] Dipartimento di Fisica, Università degli Studi di Perugia, Via Pascoli, I-06123 Perugia, Italy

Water plays a vital role in determining structural and dynamical properties of biological molecules, but the molecular organization and the dynamical restructuring of the hydration water are in turn strongly influenced by the biomolecular interface. From literature, it is well known that the dynamics of water molecules in contact with the biomolecule surface are to some extent retarded as compared to the bulk, but the level of this retardation, its molecular origin, and the number of water molecules involved in such hydration process are matter of discussion. Since the possible solvated interfaces are numerous and many-sided, much effort has been made to find out model systems capable to reproduce a number of general aspects of the dynamics of water molecules in the hydration layers. We focused our study to the amphiphilic model peptide N-acetyl-leucine-methylamide (NALMA), which is attractive since, despite its small size, it involves both hydrophilic and hydrophobic moieties that may mimic the behaviour of some sub-unities of proteins (see Fig 1).
In detail, we have studied the effect of NALMA on the dynamics of water using extended frequency range depolarized light scattering (EDLS).[1] EDLS, sensitive to molecular polarizability and operating in the GHz-THz range, has proved to be particularly able to disentangle the dynamics of the solute from that of water, and relaxation processes of bulk from those of hydration water. [1,2]
Focusing on water we have measured the characteristic times of bulk and hydration relaxation processes associated to the continuous restructuring of H-bonds at a picosecond time scale.
In particular, for a diluted solution, in the temperature range 5-65 °C, a retardation factor x from 9 to 7 is found for water hydrating NALMA, and a hydration number from 62 to 50 is observed, corresponding to more than two hydration layers. These findings delineate a profound difference with simpler molecules of comparable size, sugars, alcohols, osmolytes, where the retardation factor is lower and the perturbation extends only up to the first hydration shell.[3-6] On the other hand, the value of x falls within the range found for lysozyme aqueous solution,[2] thus suggesting an ability for this small peptide to mimic some properties of more complex molecules.

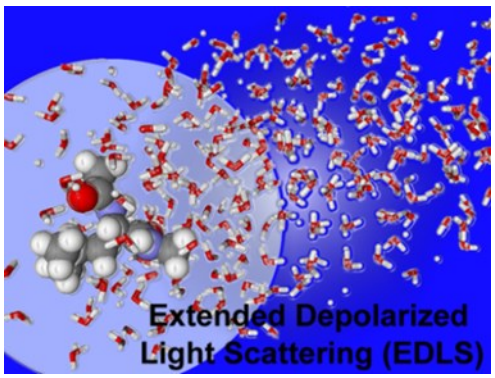


Fig.1 Schematic of NALMA molecule in solution.

References:
1. S. Perticaroli, L. Comez, M. Paolantoni, et al., J. Am. Chem. Soc., , **133**, 4882, 2011.
2. S. Perticaroli, L. Comez, M. Paolantoni, et al., J. Phys. Chem. B, **114**, 8262, 2010.
3. L. Lupi, L. Comez, C. Masciovecchio, et al., J. Chem. Phys., **134**, 055104, 2011.
4. B. Rossi, L. Comez, D. Fioretto, et al., J. Raman Spect., **42**, 1479, 2011.
5. L. Comez, L. Lupi, M. Paolantoni, F. Picchiò, and D. Fioretto, J. Chem. Phys., **137**, 114509, 2012.
6. L. Lupi, L. Comez, M. Paolantoni, D. Fioretto, B.M. Ladanyi, J. Phys. Chem. B., **116**, 7499, 2012.

Electronic structures of dilute magnetic semiconductor

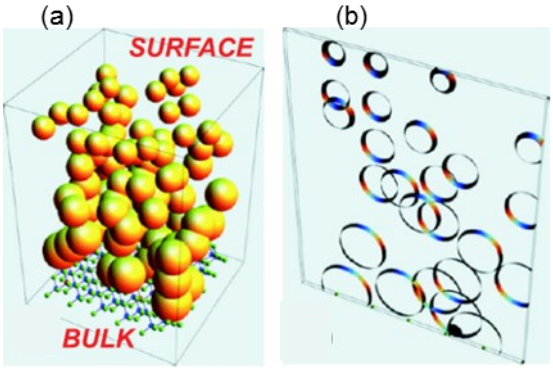
J. Fujii

Laboratorio TASC, IOM-CNR, S.S.14, Km163.5, AREA di Ricerca, Basovizza 34149 Trieste

Although the extensive effort in understanding the mechanisms at the origin of ferromagnetic order in dilute magnetic semiconductors (DMS) [1], which possess great potential as the key material in spintronics applications, controversy still remains as to their electronic structures and the nature of the states producing ferromagnetic coupling. Two extreme limits have been discussed for explaining ferromagnetism of DMS, which are called valence band model and impurity band model [2], where the Mn induced states are either delocalized or localized. Simply speaking the former model has been supported by the measurements with spectroscopic techniques which are often surface sensitive and the latter model has been supported by transport measurements which are bulk sensitive. Here we investigated $Ga_{1-x}Mn_xAs$, which is a prototypical DMS material, by means of conventional photoelectron spectroscopy (PES) and hard x-ray photoelectron spectroscopy (HAXPES), which are surface sensitive and bulk sensitive, respectively [3,4].

The experimental results are compared to theoretical calculation based on local density approximation and dynamical mean field theory, and the model calculation which takes into account configuration interaction using Anderson impurity model.

Doping- and temperature- dependent Mn 2p core level spectra reveal the presence of a distinct electronic screening channel in the bulk. Comparison with model calculations identifies the character of the Mn 3d electronic states and clarifies the role, and the difference between surface and bulk, of hybridization in mediating the ferromagnetic coupling in $Ga_{1-x}Mn_xAs$ (Figure). Only in the bulk the *d* electrons can percolate through the lattice, favoring long-range ferromagnetism. Mn-derived states, which extend well above the top of the host GaAs valence band up to the Fermi energy, are observed in the valence band spectra, suggesting the existence of the localized character (impurity band) as well as the merged states with GaAs bands.



(a) The electronic clouds of partially localized Mn *d* electrons with a radius proportional to the screening length. (b) 2D cross section of panel *a*.

References:
[1] D.D. Awschalom et al., Nature Phys. 3, 153 (2007).
[2] S. Ohya et al., Nature Phys. 7 342 (2011).
[3] J. Fujii et al., Phys. Rev. Lett. 107, 187203 (2011).
[4] A.X. Gray et Al., Nat. Mater. 11, 957 (2012).

Magnetic proximity effect as a pathway to spintronic applications of topological insulators

I.Vobornik[1], U. Manju[2], J. Fujii[1], F. Borgatti[3], P. Torelli[1], D. Krizmancic[1] , Y.S. Hor[4], R.J. Cava[4], and G. Panaccione[1]

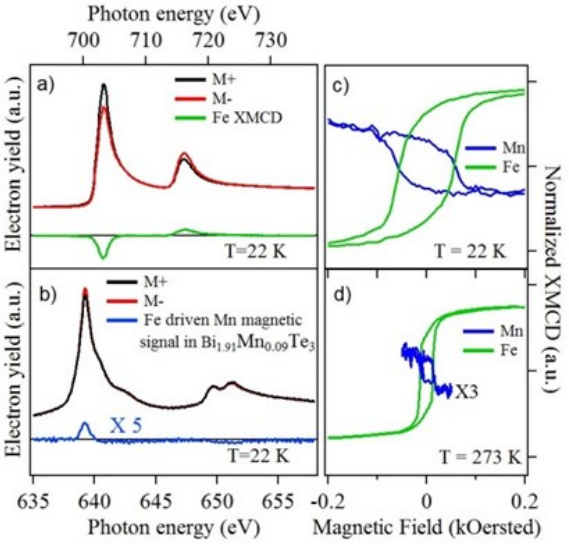
[1] Istituto Officina dei Materiali (IOM)-CNR, Laboratorio TASC, in Area Science Park, S.S.14, Km 163.5, I-34149 Trieste, Italy
[2] International Centre for Theoretical Physics (ICTP), Strada Costiera 11, I-34100 Trieste, Italy
[3] ISMN-CNR, via Gobetti 101, I-40129 Bologna, Italy
[4] Department of Chemistry, Princeton University, Princeton, New Jersey, 08544 USA

Three-dimensional topological insulators are the materials that are insulators in the bulk but do conduct at the surface via special surface electronic states. Unlike the ordinary surface states, the topological surface states cannot be destroyed by impurities or imperfections. Similar to graphene, they are characterized by Dirac dispersion and can be realized uniquely in systems with strong spin-orbit coupling. Some known families of three dimensional topological insulators are Bi_2Se_3, Bi_2Te_3, $TlBiSe_2$, etc.

The topological insulators can be magnetically doped. Mn doped Bi_2Te_3 can be magnetized: the Mn magnetic moments align ferromagnetically below 12 K, with easy magnetization axis perpendicular to the surface. The question is whether magnetism in topological insulators can be controlled and the Curie temperature risen to values that allow practical applications. We addressed this question by applying the magnetic proximity effect.

We evaporated Fe on freshly cleaved $Bi_{1.91}Mn_{0.09}Te_3$ and found that Fe films with thicknesses larger than 0.6 nm may be magnetized within the sample plane. In order to understand the impact of Fe magnetization on Mn within $Bi_{1.91}Mn_{0.09}Te_3$, we used magnetic circular dichroism (XMCD), a technique that measures element selective magnetic properties.

Figure 1a represents the 2p absorption spectra of Fe measured with circular photon polarization, at two different directions of magnetization and T=22 K (higher than the bulk Tc of 12 K). The difference spectrum (green; Fe XMCD) is the dichroic signal and represents a characteristic signature of a magnetic system. In our experimental geometry it reveals the Fe is magnetized within the surface plane. The dichroic signal measured on the Mn 2p edge (Fig.1b) is finitie, although significantly smaller. Its sign is opposite to the one of Fe, indicating antiferromagnetic coupling between the two. Figure 1c-d shows the hysteresis curves obtained by measuring the Fe and Mn dichroic signal as a function of the applied magnetic field. The data indicate that the interfacial magnetization remains even at room temperature..



References:
I. Vobornik et al., Nano Lett., 2011, 11 (10), pp 4079–4082, DOI: 10.1021/nl201275q

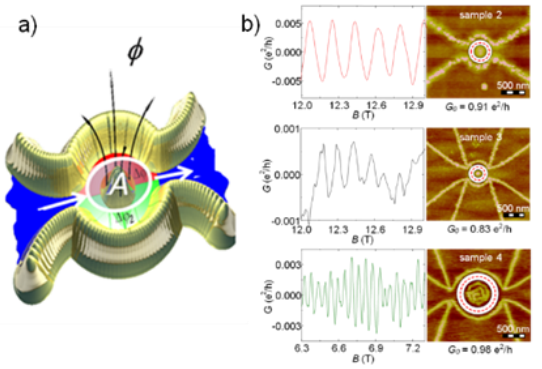
Correlation-induced single-flux-quantum penetration in quantum rings

A. J. M. Giesbers[1], U. Zeitler[1], M. I. Katsnelson[2], D. Reuter[3], A. D.Wieck[3], G. Biasiol[4], L. Sorba[4,5] and J. C. Maan[1]

[1] High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands,
[2] Theory of Condensed Matter, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands
[3] Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany
[4] Laboratorio Nazionale TASC INFM-CNR, Trieste, Italy
[5] NEST INFM-CNR and Scuola Normale Superiore, Pisa, Italy.

Magneto-quantum oscillations in solid-state systems are based on either discrete (Landau) energy levels or the interference of electron waves propagating through a closed loop. The former lead to a 1/B–periodic modulation of e.g. the magneto-conductance (Shubnikov-de Haas effect), the latter cause B-periodic oscillations when electrons propagate phase-coherently through a ring (Aharonov-Bohm effect). We report on a novel type of B-periodic high-field magneto-conductance oscillations in semiconductor quantum rings which are caused by the spatial discreteness of Landau orbits, the quantum mechanical analogue of classical cyclotron orbits.

The electronic eigenstates of a two-dimensional electron system in a high magnetic field consist of Landau orbits with quantized energies. They are situated at discrete spatial positions and occupy a quantised area given by the magnetic flux quantum h/e divided by the applied magnetic field. Combined with the repelling Coulomb interaction, this discreteness of space leads to a discretisation of the electronic size of any mesoscopic structure in a quantizing magnetic field which changes periodically whenever a flux-quantum enters the structure.



a) Schematic representation of a QR with flux through the center and the two different phases accumulated in both arms of the ring. B) AFM images and high-field oscillations of 3 rings.

Our experiments have shown the spatial discreteness of the Landau orbits in high B by means of magnetoconductance oscillations in semiconductor quantum rings (QRs).

The structures were fabricated from high-mobility shallow 2D electron systems in a GaAs/AlGaAs heterojunction using local anodic oxidation with an atomic force microscope. The period of these new high-field oscillations is determined by the number of flux quanta penetrating the conducting area of the structure, i.e. the QR rim. Thus, they are distinctively different from the well-known Aharonov-Bohm oscillations whose period is governed by the number of flux quanta penetrating the entire ring.

Our experiments show explicitly that high magnetic fields do not only quantize the energy but also the size and position of the electronic states, an effect known implicitly since the early times of Landau in the thirties of the last century.

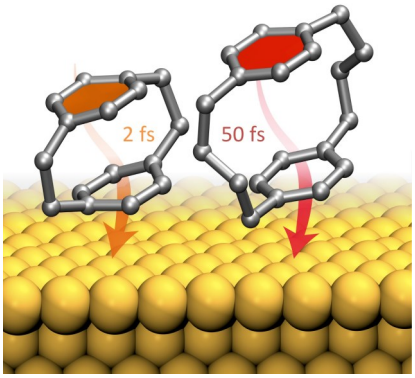
References:

A. J. M. Giesbers, U. Zeitler, M. I. Katsnelson, D. Reuter, A. D. Wieck, G. Biasiol, L. Sorba and J. C. Maan: «Correlation-induced single-flux-quantum penetration in quantum rings», Nature Physics 6, 173 - 177 (2010).

Towards a mulecular circuitry: the charge trasport at a metal-organic hybrid contact

A. Morgante

CNR-IOM, Tirieste, Italy



Investigations of charge transfer processes at interfaces and measurements of charge transport in single molecule junctions are among the most crucial field of research in molecular electronics that promise to produce advances in the understanding of the behaviour of organic material based devices and to give hints for improvement of their performances. We have applied X-ray spectroscopies and theoretical methods to correlate the electronic structure of model interfaces and the charge transfer times measured with core hole clock methods with single molecule conductance measurements.

Using photoemission spectroscopy, we determine the relationship between electronic energy level alignment at a metal–molecule interface and single-molecule junction transport data. We measure the position of the highest occupied molecular orbital (HOMO) relative to the Au metal Fermi level for three 1,4-benzenediamine derivatives on Au(111) and Au(110) with ultraviolet and resonant X-ray photoemission spectroscopy. We find that the energy difference between the HOMO and Fermi level for the three molecules adsorbed on Au(111) correlate well with changes in conductance and agree well with quasiparticle energies computed from first-principles calculations incorporating self-energy corrections. On the Au(110) that presents Au atoms with lower-coordination, critical in break-junction conductance measurements, we see that the HOMO level shifts further from the Fermi level. These results provide the first direct comparison of spectroscopic energy level alignment measurements with single molecule junction transport data.

We have also used the core-hole clock implementation of resonant photoemission spectroscopy to study the femtosecond charge-transfer dynamics in cyclophanes, which consist of two precisely stacked π-systems held together by aliphatic chains. These results can be compared with transport data obtained on the same systems by conductance measurements. We studied two systems, with inter-ring separations of 3.0 and 4.0 Å, respectively. We find that charge transfer across the latter (4.= Å) is 20 times slower than in the first one. In particular, in the case of extended π-conjugated systems, this quantitative understanding of charge dynamics from core-level spectroscopy can directly be translated to valence exciton dynamics that are relevant to organic photovoltaics and organic light-emitting diodes operating in the visible spectrum. These results present the first measure of through-space charge-transfer time as a function of inter-ring distance in a π-stacked system.

References:

A. Batra, G. Kladnik, H. Vazquez, J.S. Meisner, L. Floreano, C. Nuckolls, D. Cvetko, A. Morgante, L. Venkataraman, Nat. Commun. 3, 1086 (2012).

M. Dell'Angela, G. Kladnik, A. Cossaro, A. Verdini, M. Kamenetska, I. Tamblyn, S. Y. Quek, J. B. Neaton, D. Cvetko, A. Morgante, and L. Venkataraman, Nano Lett. 10, 2470 (2010).

Metalation of 2H-tetraphenyl-porphyrins by picking-up a substrate metal atom

A. Goldoni[1], C.A. Pignedoli[2], G. Di Santo[1], C. Castellarin-Cudia[1], F. Bondino[3], E. Magnano[3], A. Verdini[3], D. Passerone[2]

[1]Elettra – Sincrotrone Trieste S.C.p.A., Trieste, Italy
[2] EMPA, Dübendorf, Switzerland
[3] CNR-IOM, Laboratorio TASC, Trieste, Italy

The possibility to obtain systems where the magnetic or catalytic atoms are well separated and arranged in regular arrays is allowed at the nanoscale by using molecular self assembly of π-conjugated molecules containing metal ions. Porphyrins, are a class of π-conjugated molecules with a planar macrocycle that can accept metal ions of different kind at the center, thus forming metallo-porphyrins. Using synchrotron radiation spectroscopy we demonstrate that depositing at room temperature one monolayer of 2H-Tetraphenyl-Porphyrins (2H-TPP) on Fe and Ni substrates, a substrate ad-atom binds directly to the macrocycle and metalates the porphyrins. Fig. 1 shows the N 1s core level photoemission spectra of 2H-TPP monolayers deposited at room temperature on Ni(111), Fe(110) and Ag(111) compared with the 2H-TPP multilayer. While in the multilayer and monolayer on Ag(111) the N 1s spectrum is composed of two peaks, corresponding to non equivalent iminic and pyrrolic nitrogen atoms, both in the case of Ni(111) and Fe(110) substrates the spectra consist of one single peak. This is the clear confirmation that Fe-TPP and Ni-TPP are formed. Energetics obtained by Density Functional Theory calculations confirms that this redox reaction happens on Fe and Ni substrates at room temperature. For Ni(111), the calculations demonstrate that the redox metalation reaction would be exothermic with an energy gain of 0.89 eV upon embedding Ni adatom in the macrocycle. In the monolayer regime upon adsorption at room temperature, TPP exhibits a conformational adaptation with a considerable rotation of the phenyl substituents with respect to the macrocycle plane, mainly due to the steric effect of hydrogen atoms. This causes the macrocycle to be at a distance d between 2.5 Å < d < 5 Å depending on the possible distortion of the macrocycle ring. Our data indicate that, even considering the large macrocycle distance, the metalation may occur. Obviously, this does not happen on all substrates, as demonstrated by the Ag and even Au cases, although both Ag and Au form stable metallo-porphyrin complexes. In conclusion high-resolution x ray spectroscopy and density functional theory calculations show that 2H-tetraphenyl-porphyrins metalate at room temperature by incorporating a surface metal atom when a (sub)monolayer is deposited on Fe(110) and Ni(111). The calculations demonstrate that the redox metalation reaction would be exothermic when occurring on a Ni(111) substrate embedding a Ni adatom in the macrocycle.

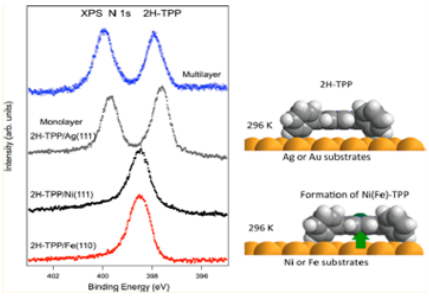


Fig.1 Left: N 1s XPS of a 2H-TPP multilayer and monolayers on Ag(111), Ni(111) and Fe (110). Right: Sketch of the adsorption of 2H-TPP molecule on Ag and Au or on Fe and Ni at RT

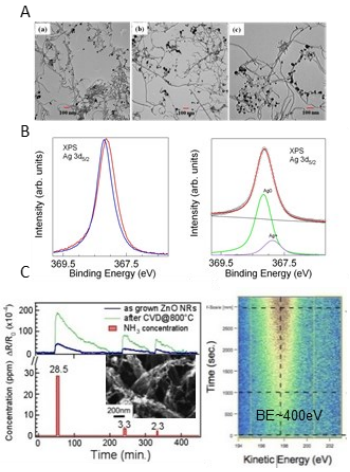
Original work: A. Goldoni C.A. Pignedoli, G. Di Santo, C. Castellarin-Cudia, F. Bondino, E. Magnano, A. Verdini, D. Passerone, *ACS Nano 6, 10800-10807 (2012).*

References:
G. Di Santo, S. Blankenburg, C. Castellarin-Cudia, M. Fanetti, P. Borghetti, L. Sangaletti, L. Floreano, A. Verdini, E. Magnano, F. Bondino, C. A. Pignedoli, M.-T. Nguyen, R. Gaspari, D. Passerone and A. Goldoni, *Chem.; Eur. J 17, 14354–14359 (2011).*
G. Di Santo, C. Castellarin-Cudia, M. Fanetti, B. Taleatu, P. Borghetti, L. Sangaletti, L. Floreano, E. Magnano, F. Bondino, and A. Goldoni, *J. Phys. Chem. C 115, 4155–4162 (2011)*

Advanced X-ray spectroscopy for the characterization of carbon nanotubes as 1-D sensors for gases and chemical processes

P. Singh[1], G. Lamanna[1], C. Mnard-Moyon[1], F. Toma[2], E. Magnano[3], F. Bondino[3], M. Prato[2], S. Verma[4], and A. Bianco[1]
P. Mbuyisa[5], S. P. Bhardwaj[3], F. Rigoni[6], E. Carlino[3], S. Pagliara[6], L. Sangaletti[6], A. Goldoni[7], M. Ndwandwe[5] and C. Cepek[3]

[1] CNRS, Institut de Biologie Molculaire et Cellulaire Laboratoire d'Immunologie et Chimie Thrapeutiques Strasbourg, France
[2] Dipartimento di Scienze Farmaceutiche, Università di Trieste, Trieste, Italy
[3] CNR-IOM, Laboratorio TASC, Trieste, Italy
[4] Department of Chemistry, Indian Institute of Technology-Kanpur, Kanpur, India
[5] Department of Physics and Engineering, University of Zululand, SouthAfrica
[6] Università Cattolica del Sacro Cuore, Brescia, Italy
[7] Sincrotrone Trieste S.C.p.A, Trieste, Italy



A) TEM images of Ad-MWCNT hybrids complexed with Ag NPs. B) left: Ag $3d_{5/2}$ XPS spectra of Ad-MWCNT (red) and metallic Ag (blue); right: fitting procedure results. C) Right: response of pure ZnO (blue) and CNDs (see inset) grown at 800°C (green) upon NH_3 doses. Right: 2D N 1*s* spectra acquired during NH_3 exposure (spectra acquisition time <1sec.).

Because of their nanoscale dimensions, high aspect ratio, huge surface area and lightweight, carbon nanotubes (CNTs) can be exploited in efficient catalytic processes and sensors. Actually pure, non-defective CNTs are weekly reactive, and proper functionalization and/or defects were demonstrated to enhance their sensitivity, improving the efficiency of many catalytic processes and gas absorption. Advanced synchrotron-based spectroscopy allows unravelling many intrinsic structural and electronic properties of materials, which would not be possible using more conventional techniques. Here high-flux, high-resolution XPS performed at BACH beamline was used to reveal the catalytic mechanisms of functionalized multi-wall CNTs (MWCNTs) and the NH_3 adsorption mechanism of defected nanostructured carbon. The oxidation state of silver nanoparticles at the surface of MWCNTs used as a catalyst for the oxidation reaction of methylhydroxyquinone to methylbenzoquinone adsorption mechanism was established by XPS measurements [1]. We demonstrate that by covalent functionalization of oxidized MWCNTs with a modified adenine moiety it is possible to tailor the coordination of Ag-NPs onto MWCNT surface. Indeed, the presence of the adenine functional groups on MWCNTs induces the formation of Ag-NPs via the metal-adenine coordination. MWCNT/Ag nanohybrids resulted in an efficient and re-usable heterogeneous catalyst for hydroquinones oxidation. The absorption and desorption chemistry of NH_3 on ZnO NRs and ZnO-Nanostructured C hybrids grown by CVD were studied by fast XPS. We demostrated that CVD on nanostructured ZnO can synthesize different C nanostructures, spanning from amorphous C cups, covering the ZnO NRs, to nanostructured porous, 1D C nano-dentrites, preferentially aligned along the directions of the pristine NRs (Fig.C, inset) [2]. This latter sample, made of pure C, due to high defect density, show a very high sensitivity to low NH_3 concentration, virtually unexplored in literature in other pure C materials. Our fast XPS data show that ammonia chemisorbs on the hybrid structure while on ZnO NRs and pure CNTs physisorbs (Fig. C, right) [3].

References:
[1] P. Singh , G. Lamanna , C. Ménard-Moyon , F.M. Toma, E. Magnano, F. Bondino, M. Prato, S. Verma, and A. Bianco, *Angewandte Chemie - International Edition, Vol. 50 - 42, pp. 9893-9897 (2011)*
[2] P. Mbuyisa, S. P. Bhardwaj, F. Rigoni, E. Carlino, S. Pagliara, L. Sangaletti, A. Goldoni, M. Ndwandwe and C. Cepek, *Carbon 50, 5472-5480 (2012)*
[3] E. Magnano, F. Bondino and C. Cepek, work in progress

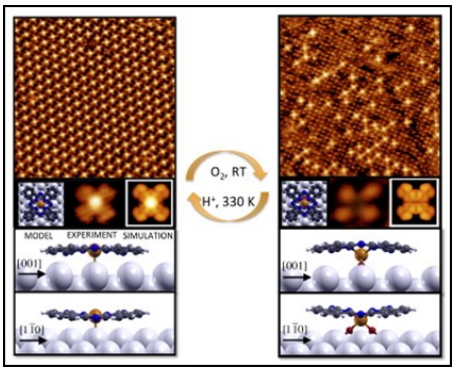
Switching Catalysts at Surfaces

F. Sedona[1], M. Di Marino[1], D. Forrer[1], A. Vittadini[1,2], M. Casarin[1,2], A. Cossaro[3], L. Floreano[3], A. Verdini[3], M. Sambi[1]

[1] Dipartimento di Scienze Chimiche, Università di Padova, Italia
[2] CNR-ISTM, Via Marzolo 1, Padova, Italia
[3] CNR-IOM, Basovizza SS-14 Km 163.5, Trieste, Italia

Chemists and materials scientists are studying simplified synthetic analogues of heme as an alternative to platinum catalysts to promote the Oxygen Reduction Reaction (ORR) in fuel cells: artificial Porphyrins (Pps) or the closely related Phthalocyanines (Pcs). It was recently recognized that a major obstacle to a full understanding of the catalytic mechanisms and to the design of new and more efficient catalysts is the lack of detailed information about the active site structure and how this evolves when oxygen coordination occurs. Recently, we have provided precisely this information for a model system constituted by FePc deposited on a Ag(110) single-crystal substrate. By converging and coherent evidence from a rich set of complementary experimental results and calculations comprising STM, XPS, XAS and DFT, the local chemisorption geometry of the catalyst molecule on the substrate in the catalytically active phase was elucidated and its evolution upon oxygen adsorption was revealed. The catalytically active FePc phase corresponds to slightly less than 1 Monolayer (ML) of FePc, where each molecule sits with its Fe atom on-top a substrate Ag atom (see Fig. 1a). When a full ML is completed, the system undergoes a sharp phase transition to a denser phase, with FePcs shifted to bridge sites, and the catalytic activity sharply disappears. When the sub-ML phase is exposed to oxygen, STM gives a characteristic fingerprint of oxygen binding to FePc in the form of a bright/dim switch of the Fe-centered density of states (compare Fig. 1a and 1b). The switch is reversible: the bright bump reappears even at room temperature and during dosing. This shows that dim adsorbates are not stable. A labile Fe-O bond compatible with the reversible bright/dim switch was found by DFT calculations, where the Fe atom on-top an Ag surface atom is laterally coordinated by two oxygens sitting at nearby Ag bridge sites (Fig. 1b).

Angle-dependent C 1s XAS data are fully compatible with the reversible out-of-plane distortion of the macrocycle upon oxygen dosing and subsequent annealing, as proposed on the basis of STM and DFT results. O 1s XPS spectra show that oxygen reduced by the molecular catalyst in our ultra-high vacuum environment is left in the silver topmost layers, while in solution the oxide produced at the cathode surface is removed by protons provided from the anode. In order to remove this oxygen and fully close the catalytic cycle, low energy ion bombardment by means of ionized hydrogen has been used. The ion treatment almost exactly restores FePc molecules in their state prior to oxygen dosing (Fig. 1a, b), with no overall loss of catalyst. Cycles of oxygen dosing and removal can be repeated several times.



STM images of the catalytically active FePc phase before and after oxygen dosing. Single molecule models, STM images and DFT simulations are shown in the middle stripes.

References:
F.Sedona, M. Di Marino, D. Forrer, A. Vittadini, M. Casarin, A. Cossaro, L. Floreano, A. Verdini, M. Sambi, "Tuning the catalytic activity of Ag(110)-supported Fe phthalocyanine in the oxygen reduction reaction." Nat. Mater. **11,** 970-977 (2012). DOI:10.1038/NMAT3453

Magnetization dynamics in nanostructured magnetic materials

G. Gubbiotti and S. Tacchi

[1]Istituto Officina dei Materiali (CNR-IOM), Sede di Perugia, c/o Dipartimento di Fisica, Via A. Pascoli, I-06123 Perugia, Italy

Micro-focused Brillouin light sattering (μ-BLS) is a powerful technique for resolving the spatial profile of spin waves in magnetic nanostructures, and it has been applied by the IOM researchers to directly observe the propagation of spin waves launched from a spin torque oscillator with a nanoscale electrical contact into an extended Permalloy film through the spin transfer torque effect.[1] The STO is out-of-plane magnetized and the spin waves are unidirectionally emitted from the nanocontact region into the continuous NiFe ferromagnetic thin film up to several micrometres away from the nanocontact. The spin wave intensity has been represented by the intensity $J(r)= ((J_0/r)e^{-r/\lambda})$ with λ=2.1 μm, obtaining a very good agreement with the experimental data. We have verified that the spin wave emission occurs only for the positive polarity of the injected dc current, which corresponds to electrons drifting from the free to the fixed magnetic layer. Both current (250 MHz/mA) and magnetic field (20 MHz/mT) frequency tunability of the emitted spin wave have been observed with a threshold current of about 35-40 mA.

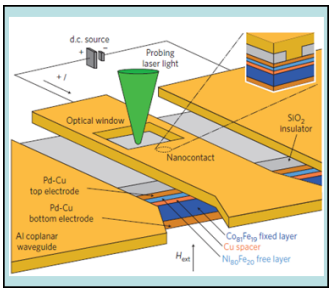


Fig. 1 Cross-section of the nanocontact sample, revealing the layers of the spin valve mesa and the active area of the STO device. An optical window is etched into the central conductor of the waveguide close to the nanocontact where the laser beam is scanned.

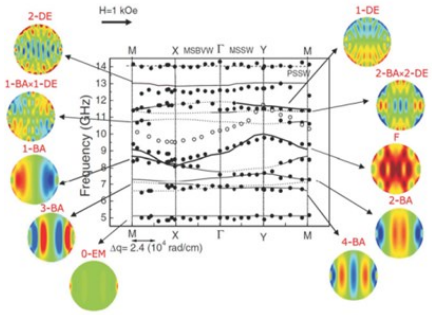


Fig. 2 Measured (dots) and calculated (curves) frequencies along the principal directions of the 1st BZ, for an external magnetic field H=1.0 kOe. The calculated spatial profiles of the different eigenmodes are reported as insets.

Wave-vector resolved Brillouin light scattering technique to achieve a complete mapping of the spin-wave dispersion curves, along the principal symmetry directions of the first Brillouin zone (BZ), for a two-dimensional (2D) MC consisting of a square array of $Ni_{80}Fe_{20}$ disks with in-plane magnetization (see Fig.2). The fourfold symmetry of the geometrical lattice is reduced by the application of the external field and therefore equivalent directions of the first BZ are characterized by different dispersion relations of collective spin waves. The formation of the magnonic band structure, provoked by dynamic dipolar interactions between standing waves in the nanodiscs, has been observed. The physical mechanism underlying the mode frequency dispersion has been explained introducing the concept of a bi-dimensional effective wave vector k_{eff}, which allows to explain the dispersion of any band in any direction in the reciprocal space.

References:
1. M. Madami et al Nature Nanotech **6**, 635 (2011).
2. S. Tacchi et al, Phys. Rev. Lett. **107**, 127204 (2011).

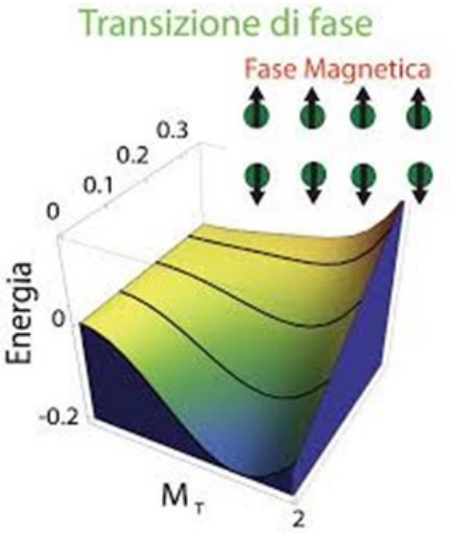
Quantum phase transitions and correlations in iron superconductors

G. Giovannetti[1] C. Ortix[2], M. Marsman[3], M. Capone[1], J. van den Brink[2] and J. Lorenzana[4]

[1] CNR-IOM, UoS SISSA and International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste (Italy)
[2]IFW Dresden, Helmholtzstraße 2001069 Dresden (Germany)
[3] Faculty of Physics and Center for Computational Materials Science, University Vienna, Sensengasse 8/12, Vienna A-1090, Austria.
[4] CNR-ISC, UoS Sapienza and Sapienza University of Rome, Piazzale Aldo Moro 2, 00185, Rome (Italy)

In several materials, unconventional superconductivity appears close to a zero-temperature (or quantum) phase transition where long-range magnetic order vanishes as a function of a control parameter like charge doping, pressure or magnetic field. The nature of the quantum phase transition is of paramount relevance, because continuous second-order transitions are expected to favour superconductivity, due to strong critical fluctuations. Discontinuous transitions, on the other hand, are not expected to have a similar role. Here we determine the nature of the magnetic quantum phase transition, which occurs as a function of doping, in the iron-based superconductor $LaFeAsO_{1-x}F_x$.

We use constrained density functional calculations for the magnetic phases and we extract ab initio coefficients for a Landau order parameter analysis. The outcome is intriguing, as this material turns out to be remarkably close to a quantum tricritical point, where the transition changes from continuous to discontinuous, and several susceptibilities diverge simultaneously. We discuss the consequences for superconductivity and the phase diagram.



Energetic landscape close to the quantum tricritical point in iron-based superconductors

References:
Proximity of iron pnictide superconductors to a quantum tricritical point G. Giovannetti, C. Ortix, M. Marsman, M. Capone, J. van den Brinkand J. Lorenzana Nature Communications 2, Article number: 398 doi:10.1038/ncomms1407 (2011)

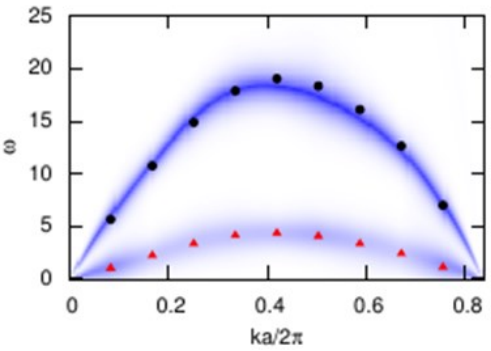
Bose soft disks: a minimal model for supersolidity

S. Saccani [1], S. Moroni [1,2], M. Boninsegni [3]

[1] SISSA, Via Bonomea 265, I-34136, Trieste, Italy
[2] CNR-IOM DEMOCRITOS, Istituto Officina dei Materiali, Trieste, Italy
[3] Department of Physics, University of Alberta,
Edmonton, Alberta, Canada T6G 2G7.

Conclusive experimental evidence of a supersolid phase in any known condensed matter system is presently lacking. On the other hand, a supersolid phase has been recently predicted [1] for a system of spinless bosons in continuous space, interacting via a repulsive soft-core potential with a dipolar tail. Such an interaction can be engineered in assemblies of ultracold atoms, providing a well-defined pathway to the unambiguous observation of this fascinating phase of matter. We have studied by first principles computer simulations a model of Bose soft disks in two dimensions [2]. A supersolid cluster phase exists, within a range of the model parameters, analogous to that predicted for softened dipolar interactions [1]. These findings indicate that a long-range tail of the interaction is unneeded to obtain such a phase, and that the soft-core repulsive interaction is the minimal model for supersolidity. The supersolid phase is a solid with multiply occupied sites and coherent hopping of particles between them. In many respects it is analogous to a self-assembled Bose-Hubbard model. The elementary excitation spectrum [2] features two distinct acoustic modes in the supersolid phase, namely, a solidlike phonon and a softer collective excitation, related to broken translation and gauge symmetry, respectively (see Figure).

Similar features can be introduced in phenomenological mean-field theories with phase and density degrees of freedom independent of the number of sites [3], but first-principles simulations offer conclusive information onto which interactions support this kind of excitations (e.g. soft-core but not Helium-Helium interactions). Further physical insight can be obtained from the calculated spectrum. A third, very low-energy branch with spectral weight proportional to k^4 is currently under investigation. Its tentative assignment to Rayleigh scattering from non-uniform occupation of the lattice sites may challenge the Andreev-Lifshitz scenario for supersolidity [4] and the proposed glass phase [5] in cluster crystals



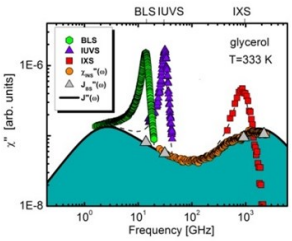
Dynamic structure factor of supersolid soft disks. Colormap: analytic continuation of imaginary-time correlations of density fluctuations; data points: n-pole approximation

References:
[1] F. Cinti, P. Jain, M. Boninsegni, A. Micheli, P. Zoller, G. Pupillo, Phys. Rev. Lett. 105, 135301 (2010).
[2] S. Saccani, S. Moroni, M. Boninsegni, PRB 83, 092506 (2011); Phys. Rev. Lett. 108, 175301 (2011).
[3] Y. Pomeau, S. Rica, Phys. Rev. Lett. 72, 2426 (1994).
[4] F. Cinti, T. Macrì, W. Lechner, G. Pupillo, T. Pohl, Nature Comm. 5, 3235 (2014).
[5] R. Diaz-Mendez, F. Mezzacapo, F. Cinti, W. Lechner, G. Pupillo, arXiv:1402.0852.

On the link between acoustic dissipation and density of states in glass-former systems

L. Comez*

*Istituto Officina dei Materiali (CNR-IOM), Sede di Perugia, c/o Dipartimento di Fisica, Via A. Pascoli, I-06123 Perugia, Italy



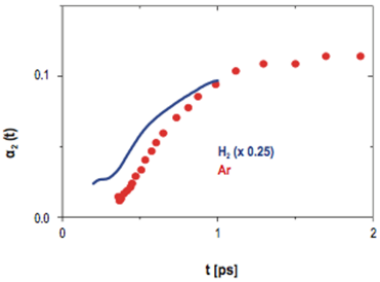
The dynamics of glass-forming systems covers a broad frequency range. Among the many molecular aspects, of particular interest for the scientific community is a fast relaxation dynamics (GHz-THz) that occurs, in light and neutron scattering spectra, as a broad quasielastic contribution (QES). The existing literature proposes a connection between the QES intensity and the damping of the acoustic waves, suggesting that the temperature behavior of these two quantities might be the same. The main limitation, in the past, for putting this concept to the test was the lack of experimental data for the acoustic attenuation in a frequency range wide enough to be directly compared to the QES data. Approaching the case-study glycerol, we have described how the combined use of Brillouin spectra, collected in different frequency -visible, ultra-violet and x-ray- regions, and incoherent neutron spectra (Fig. 1) represents a powerful tool for overcoming the previous experimental limitations.[1] By using a standard field-theory approach we have found a direct link between the density of states, g(w), and the dissipation of acoustic energy, or equivalently the damping, G(w), of acoustic phonons as estimated from the width of Brillouin peaks. Our approach holds in an astonishingly wide frequency range, from the liquid to the supercooled and the glassy regime, thus promising to provide a general link between single particle and collective properties of disordered systems.

Comez, L; Monaco, G; Masciovecchio, C; Paciaroni, A; Gessini, A; Scarponi, F; Ruocco, G; Fioretto, D
Acoustic Dissipation and Density of States in Liquid, Supercooled, and Glassy Glycerol, Phys Rev Lett 106(15) 2011

Non-Gaussian self-dynamics of liquid hydrogen

Ferdinando Formisano – formisano@ill.eu

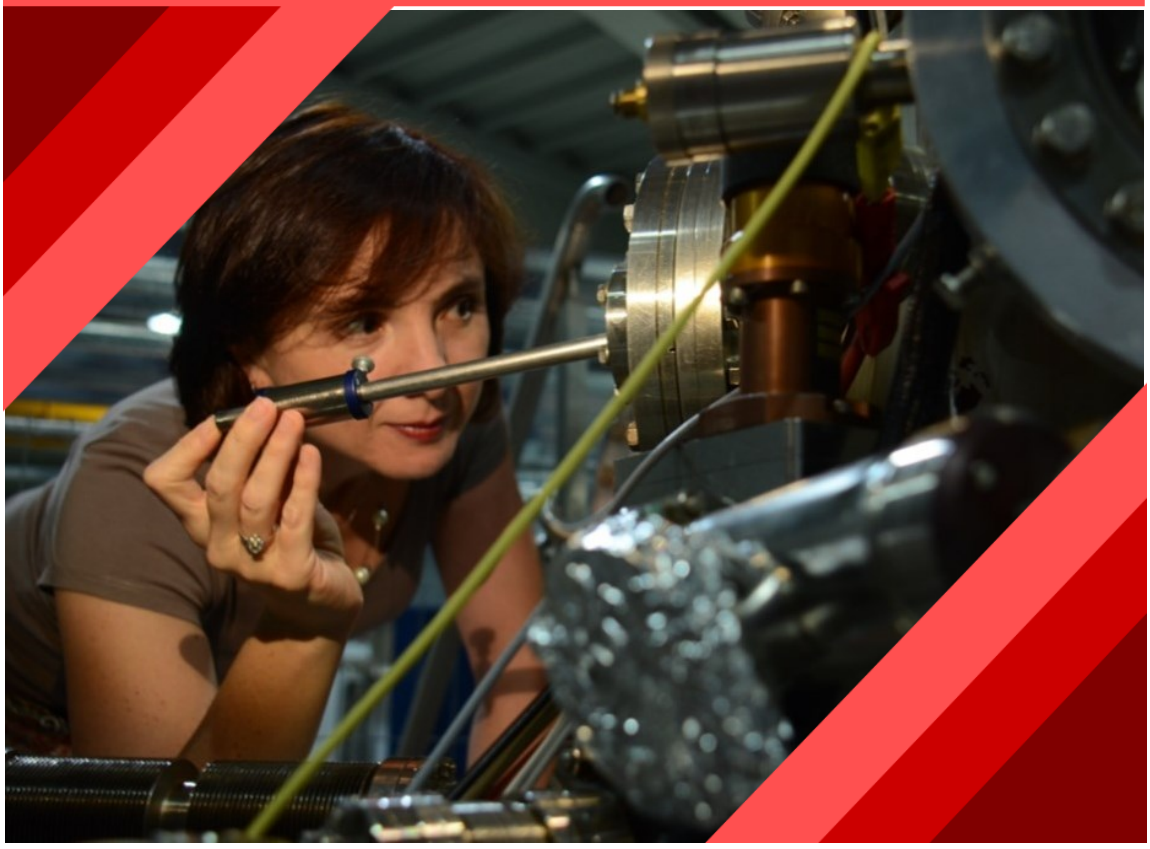
Hydrogen is the most abundant substance in the universe, made of the simplest nuclei bound together in pairs to form the simplest molecules, and its role in the progress of science has been immense. The accurate description of the dynamics remains an open problem for the quantum Boltzmann liquids which feature relevant quantum delocalization effects but can still be thought of as consisting of distinguishable particles obeying Boltzmann statistics. The diffusive motions in the liquid H_2 are traditionally described using the Gaussian approximation (GA), which is known to be valid at small and large wave vector Q. We used two ILL spectrometers (BRISP and IN4) to measure the self part of the dynamic structure factor of liquid H_2 as a function of energy E, in a wide range of Q values. Our work has proven the failure of the GA in the Q interval between 10 and 40 nm-1. This result will help in testing quantum algorithms for the simulation of all dynamical properties of a fundamental system such as H_2, including those relevant for the advance of its present technological applications, particularly as an energy carrier and storing medium.



This work provided the first semi-quantitative determination of the strength of non-Gaussian effects. Interestingly, this appears to be quite larger than in a classical liquid like argon.

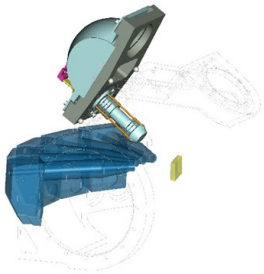
M. Celli, U. Bafile, D. Colognesi, A. De Francesco, F. Formisano, E. Guarini, M. Neumann, M. Zoppi, Phys. Rev. B 84 (2011) 140510(R)

Equipment



ALOISA

Contact: Luca Floreano (floreano@iom.cnr.it)

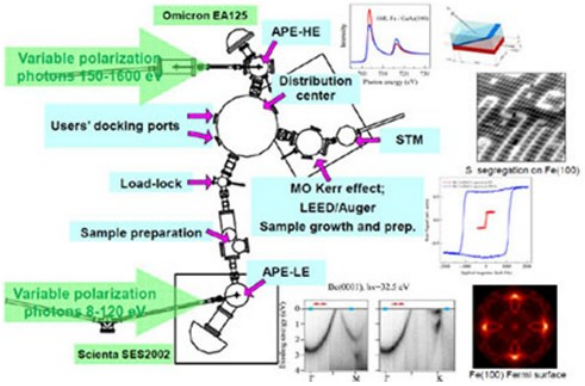


ALOISA is a Synchrotron beamline where it is possible to perform in-situ both medium energy electron spectroscopy and high energy surface x-ray diffraction for the purpose of investigating both the chemistry and the structure of surfaces, adsorbates and ultrathin films. A grating-crystal monochromator is employed to cover a wide photon energy range (130-1500 eV and 3-8 keV). The UHV end-station is equipped with a combination of angle resolved electron spectrometers and energy-resolved photodiodes (see drawing in the figure) to perform in-situ complementary investigations, such as XPS, PED, NEXAFS, RESPES, APECS, SXRD, XRR.ALOISA has an additional branch line that exploits the low energy section of the dispersive system and offers a flexible output for coupling to Users' owned endstations.
At present, the branch line is equipped in alternative:
- with the HASPES experimental chamber made by a Helium Atom Scattering apparatus, equipped with a custom-made 150mm electron analyzer with a 2D delay-line detector, for real time He diffraction and XPS;
-with the ANCHOR experimental chamber (FIRB project, Rif. Albano Cossaro) that has been installed in between the Exit Slits and the HASPES endstation. ANCHOR is equipped with a PSP 150mm electron analyzer (with an 2D delay-line detector) with a monochromatized SPECS X-ray source for in- and off-line XPS and UPS

APE beamlines within NFFA demonstrator

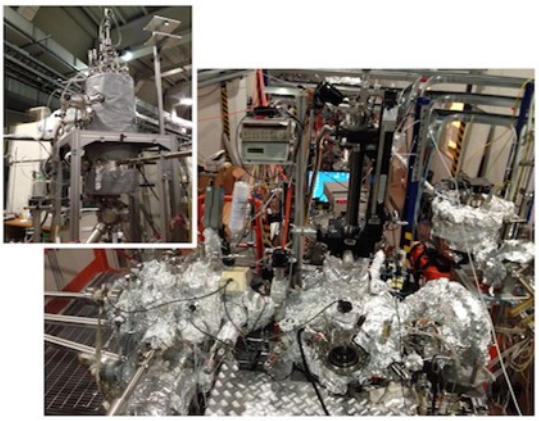
Contact: Ivana Vobornik (vobornik@iom.cnr.it)

APE is a facility for spectroscopic investigation of solid surfaces and nanostructured matter for which the sample preparation and survey represent crucial and integral part of the experiment.
The APE concept is based on a state-of-the-art surface science laboratory as a support facility for advanced spectroscopies at two distinct beamlines using polarized synchrotron radiation in the ultraviolet and soft X-ray range from the Elettra storage ring.
A number of spectroscopic techniques (ARPES, XAS, XMCD/LD, XPS, Mott magnetometry) is therefore coupled with sophisticated off-line preparation/growth and characterization tools (atomically resolved STM, LEED-Auger, magneto-optical Kerr effect; http://www.elettra.trieste.it/elettra-beamlines/ape.html).
From 2013 APE became an integral part of the NFFA project demonstrator (www.nffa.eu) that allowed for the integration of an extra suite of growth and analysis chambers with the APE beamlines. The integral setup will become an open access facility for sample growth, sample characterization and advanced on-line spectroscopic characterization, including spin-resolved ARPES that is also being implemented within NFFA.



BACH beamline

Contacts: Federica Bondino (bondino@iom.cnr.it), Elena Magnano (magnano@iom.cnr.it)



The beamline BACH at Elettra synchrotron storage ring works in the UV-soft x-ray photon energy range (35-1650 eV) with selectable light polarization (linear horizontal and vertical, circular and elliptical), high energy resolution, high intensity and brilliance and time resolution. The beamline offers a multi-technique approach for the investigation of the electronic, chemical, structural, magnetic and dynamical properties of materials. A multi-spectroscopy investigation with photoemission from 35 to 1650 eV including polarization and photon energy-dependent ARPES and RESPES, x-ray emission, x-ray absorption with partial and total electron and photon yield and x-ray magnetic circular dichroism XMCD are possible in the same endstation.
A second endstation is dedicated to XMCD in high variable magnetic fields (± 6.5 Tesla) along the beam and variable temperature from 1.8 K to 340 K. Both stations allow a time synchronization of an external laser source and the synchrotron radiation to study the dynamics of the photo-induced excited states of electronic and magnetic systems with pump-probe time-resolved x-ray absorption spectroscopy. The sample environment is completely in ultra-high-vacuum and in-vacuum connected chambers allow for the preparation of thin films and solid samples in-situ. Measurements in liquid environment are also possible.

BEAR beamline

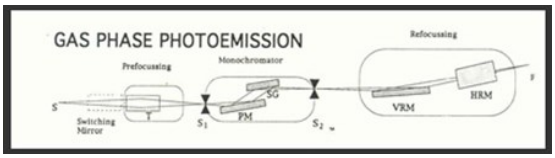
Contact: (Angelo Giglia Angelo.giglia@elettra.eu)

The BEAR (Bending magnet for Emission, Absorption and Reflectivity) beam line is installed at the left exit of the 8.1 bending magnet of Elettra. The beamline can be accessed by submitting a scientific proposal (http://www.elettra.trieste.it/elettra-beamlines/bear.html).

The beamline operates in the 3-1600 eV spectral region, delivering selectable light polarization from linear to circular and offers many spectroscopic tools as specular and diffuse reflectivity, XAS, fluorescence and luminescence yield and XPS-UPS. The beamline is equipped with two coupled UHV endstations, one for the preparation of samples, and the second for the analysis. The analysis station is intended for photon-in-photon out experiments as specular and diffuse reflectivity and for electron emission spectroscopies as photoemission and Auger. The sample manipulator features 6 degrees of freedom, while the detector assembly covers a sphere around the sample. The whole assembly can as a rigid body rotate around the direction of photon beam (continuous scan from s to p incidence). The preparation chamber is dedicated to the in -situ preparation of surfaces, interfaces and multi-layers.

Gas Phase Photoemission (GaPh) beam line and its instrumentation

Contact: Marcello Coreno (marcello.coreno@cnr.it)



The optical scheme of the GAPH beam line [J. Synchrotron Radiation **5**, 565 (1998)]. The monochromator is composed of a spherical grating (SG), a planar premirror (PM), entrance (S_1) and exit slits (S_2). http://www.elettra.eu/elettra-beamlines/gasphase.html

The Gas Phase Photoemission (GaPh) beamline offers a multi-technique approach for investigation of electronic properties of free atoms, molecules and clusters in a wide energy range (13-900 eV) with high flux, high resolving power ($E/\Delta E \geq 10000$) and small spot size (≈250 μm) at the target. A differential pumping section decouples the UHV section of the mirror chambers from the experimental end-station.

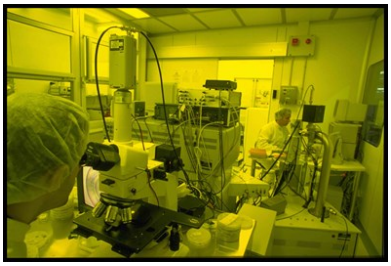
GaPh is operated by a joint Research Team of Elettra Sincrotrone Trieste and Italian National Research Council (CNR-IOM and CNR-ISM). In contrast to other beam lines at the ELETTRA, the end-station is not fixed, but several interchangeable apparatuses are available for users' experiments:

- UV-visible fluorescence spectrometer equipped with a 1200 g/mm grating and a CCD detector
- VG -220i electron analyzer, also usable in PEPICO configuration with a TOF ion mass spectrometer
- SCIENTA SES-200 electron analyzer (in collaboration with Uppsala University)
- window-less double ionization chamber for measurements of absolute photoabsorption cross section
- TOF spectrometer with position sensitive detector, for discrimination of spatial momenta of ionic photofragments
- Velocity Map Imaging detector for electron and ions, also available for PEPICO configurations
- Multi-electron coincidence apparatus, composed of ten small hemispherical electron analyzers

GaPh also hosts a low energy branch line (13-250 eV) equipped with a tunable laser (Tsunami, SpectraPhysics), which can be synchronized to the synchrotron beam at 1/6th of the storage ring frequency (~83 MHz).

LILIT—Laboratory for Interdisciplinary Lithography

Contact: Filippo Romanato (romanato@iom.cnr.it)



L.I.LIT. installed at Elettra Synchrotron is a beam line for X-ray lithography that also gives the name to the lithographic group acitve at TASC laboratory of IOM-CNR at one bending. The design of the beamline allows to select the spectral range of interest continuously, from soft (1.0 keV) to hard (12 keV) X-Rays. The configurations devoted to deliver a soft X-ray spectrum (photon energy between 1 and 2 keV) are optimized to achieves the highest lithographic resolution.

The beam line can provide also spectra in the hard X-ray region (photon energy higher than 10 keV) where sensitive materials of thickness of several tens of microns can be successfully exposed. The X-ray exposure are performed in a class 10 clean room, where also the lithographic processes are developed. Many new applications can be envisaged both at hard and soft X-rays, such as fabrication of hard X-ray optics, micromachinig devices, plasmonic and photonoc band gap crystals. Several industries requires X-ray lithography for the generation of master devoted to hot embossing and imprinting process of heavvy mass production of high resolution micromecanical pieces.

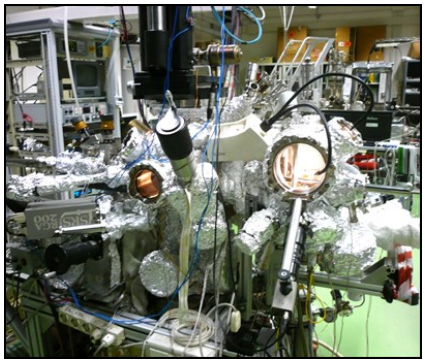
TEM

Contact: Elvio Carlino (carlino@iom.cnr.it)

TEM laboratory, established during 2002, is part of the Centre for Electron Microscopy (CEM) of IOM-CNR whose equipment includes the sample preparation facilities, the laboratory for simulating TEM images and spectra and the SEM facility. CEM has the mission to represent a EM facility for the scientific and industrial community and to explore and to develop new TEM methodologies to be applied to the study of hard and soft matter. The latter strongly take into account the location of the CME: inside TASC laboratory and close to the synchrotron storage ring of ELETTRA and to the FEL FERMI.
A JEOL JEM 2010F UHR TEM/STEM is installed in a dedicated laboratory on a vibration-insulation foundation. The TEM laboratory is kept at constant temperature with a drift rate < 0.1°C/min, with low noise and minimal turbulence. The microscope demonstrated unique performances in the world and it is equipped by a energy-disperse x-ray spectrometer (EDS) with ultra-thin window to enhance detection of light elements (Z > 5). The scanning TEM (STEM) attachment coupled with EDS can be used to obtain chemical profiles with high spatial resolution. STEM is also equipped by high angle annular dark field detector, and a method has been developed at CEM capable to image the structure and chemistry of a specimen at a resolution of 0.123nm.

Variable Temperature and Low Temperature Scanning Tunneling Microscopes

Contact: Cristina Africh (africh@iom.cnr.it)

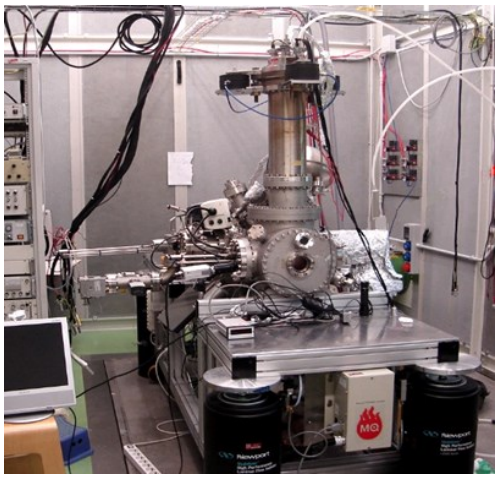


A first UHV chamber hosts a variable temperature Omicron VT-STM that has been modified in-house to allow in-situ and in-operando measurements in the 140 – 900 K temperature range under exposure to reactive gases (O2, H2, CO, NO, etc.) at pressures up to 10-6 mbar. This system is ideal for the investigation of the kinetics of surface processes, such as elementary steps of catalytic reactions or growth and self-assembling, as well as for atomic resolution structural characterization of metal and oxide surfaces.
Recently, the instrument capabilities have been further improved with the development of FAST, an add-on module that allows switching from STM acquisition with conventional speed (few tens of sec/image), to the acquisition of video-rate movies. A second UHV system is equipped with a low temperature Omicron LT-STM, for imaging at 4K, capable of atomic scale resolution on weakly interacting adsorbates such as CO2 and organics of biological interest such as amino- and carboxyl- functionalized molecules.
The LT system has been integrated with a home-built set-up for single molecule vibrational spectroscopy measurements. Maximum sample size: 7mmx7mmx1mm (VT), 8mmx8mmx5mm (LT). Standard UHV surface preparation equipment and LEED are available in both preparation chambers.

Istituto Officina dei Materiali

Scanning tunneling spectroscopy at 5 K

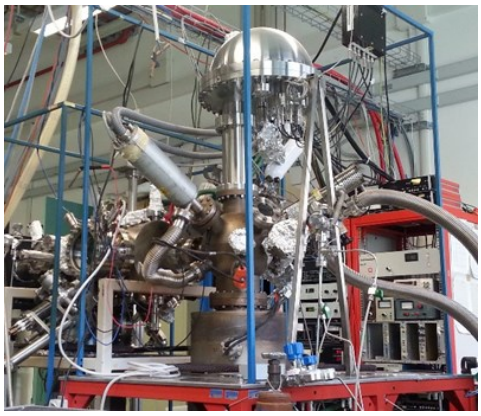
Contact: Silvia Modesti (modesti@ts.infn.it)



Home made UHV scanning tunneling spectroscopy and microscopy system. Temperature range 5-300 K. Facilities for sample preparation and characterization in UHV, ion bombardment, low-energy electron diffraction, Auger spectroscopy,….It is currently used for the measure of the spectral function of low-dimensional correlated electron systems, such as Kondo systems on surfaces and two-dimensional Mott -Hubbard insulators. It has been used for cross-sectional STM-STS of nanostructures in semiconductors and transport measurements of single molecules with the break-junction technique.

Analytical Laboratory

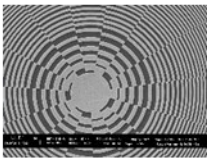
Contact: Cinzia Cepek (cepek@iom.cnr.it)

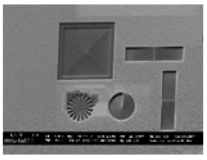


The laboratory consists of an ultra high vacuum (UHV) experimental apparatus (base pressure: ≈ $4x10^{-11}$mbar), equipped with instrumentation devoted to the growth and to the study of the chemical composition, electronic structure and atomic arrangement of surfaces and thin films. The mainly studied systems in the last years are nanostructured carbon-based materials, like fullerenes, CNTs, graphene, porous nanostructured carbon, etc. .
The available experimental analysis techniques are ultra-violet and X-ray photoemission spectroscopy (UPS and XPS), Auger electron spectroscopy, electron energy loss spectroscopy (EELS) and low energy electron diffraction (LEED).
The thin film growth instrumentations include several UHV evaporators for molecular beam epitaxy, many gas lines for chemical vapour deposition (CVD), a plasma enhanced chemical vapour deposition reactor (PECVD) and a supersonic cluster beam source..
All the above systems are directly connected \with the UHV chamber, enabling the in-situ study via electron spectroscopy just after the growth of the samples, avoiding any possible contribution due to atmospheric contamination. A sizeable part of the work of the group is performed via access to international synchrotron radiation facilities.

Cleanroom nanoimprinting

Contact: Massimo Tormen (tormen@iom.cnr.it)



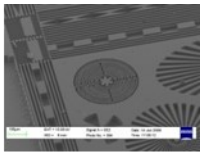


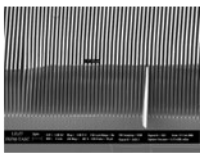
LEO-ZEISS Cross-Beam 1540 XB system, is a high resolution SEM with focused ion beam column (FIB) and gas inlet system (GIS). Its special functions: high resolution imaging even at low energies, nano-etching and –deposition, electron beam, and Ga ion beam lithography system. The writing process is controlled by ELPHY Quantum pattern generator. As Scanning Electron Microscope (SEM) it has an ultimate resolution of 1 nanometer. The operating voltage range of the electron beam is from 0.7-30kV, and the probe current (10pA - 5nA) with high stability (0.2%/h). The ion beam probe voltage is st to 30 keV and the current range is 1pA – 500nA

Key features of this microscope are the in-column secondary electron detector that provides low-noise imaging during FIB material removal as well as imaging at very low voltages.The unique objective lens design uses an electrostatic field below the lens (unlike competing design which utilizes a strong magnetic field, causing limitations in overall performance.

Cleanroom litography

Contact: Massimo Tormen (tormen@iom.cnr.it)





The STS MESC MULTIPLEX ICP is a manual wafer lock, high frequency ICP (Inductively Coupled Plasma) etch system. The plasma is inductively coupled at 13.56 MHz via a matching unit and coil assembly. Independent energy control is provided by a 13.56 MHz biasing of the electrode (platen) via automatic power control and impedance matching. The BOSCH process process consists of alternating cycles of etching and surface passivation to achieve high aspect ratios. The system can be used for deep Si etching of up to 6-inch substrates.

The systems can be used also in continuous mode for nanostructure fabrication, down to the 10-nm scale in lateral resolution and aspect ratios of up to 10. Cooling of the platen is provided by a DI (de-ionized) water chiller. Helium gas is used for aiding backside cooling of the substrate. Other gases configured with this system include SF6 (Sulfur Hexafluoride), C4F8 (Octofluorocyclobutane), O2 (Oxygen), and Ar (Argon). An aluminum load lock allows manual loading of a single wafer to be processed.

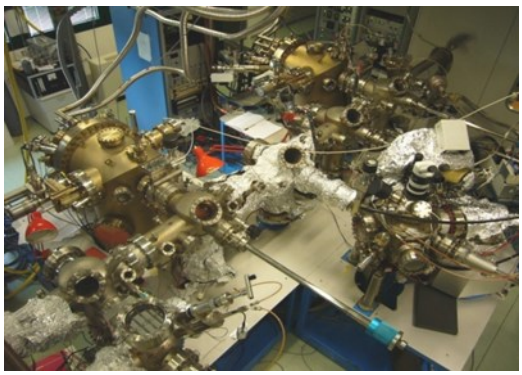
High Mobility Molecular Beam Epitaxy HM-MBE

Contact: Giorgio Biasiol (biasiol@iom.cnr.it)

The High Mobility Molecular Beam Epitaxy is a facility dedicated to the growth of high purity III/V semiconductors in UHV with atomic layer control on compositions and thicknesses . The model is a Veeco Gen II machine with a dedicated design for high mobility, equipped with As (2X), Ga (2X), Al, In effusion cells and Si and C doping sources for growth on 2" GaAs wafers.
Grown structures range from high mobility two-dimensional electron systems in GaAs/AlGaAs (with mobilities up to 8.6 X 106 cm2/Vs) and metamorphic In0.75Ga0.25As/ In0.75Al0.25As heterostructures, to photonic structures and self-assembled nanostructures.
The facility is completed by a variable temperature magneto transport equipment for electrical characterization (T in the 1.5 – 400 K range , magnetic field up to 7 T).
The HM-MBE system accomplishes the double function of facility for synthesis of high purity materials and devices open to external users and collaborators, and of providing nanostructured samples for internal research.
Areas of application of the materials synthesized in the HM-MBE facility include nanophotonics, coherent transport, biosensors, spintronics, plasmonics, detectors for large infrastructures, surface science

Molecular Beam Epitaxy (MBE) laboratory

Contact: Silvia Rubini (rubini@iom.cnr.it)



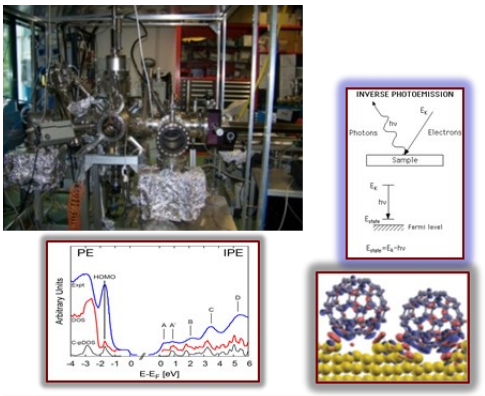
Multichamber UHV system including:
• two twins Riber 32P molecular beam epitaxy growth chambers for III-V (Al, Ga, In)As an II-VI (Zn, Cd)(Se, Te) semiconductor compounds;
• an analysis chamber for x-ray photoemission spectroscopy (XPS) equipped with a monochromatic Al Ka source (1486,7 eV) , overall resolution 0.9 eV.;
• a chamber for the deposition of metals at room temperature.

The system can grow
• Undoped, n-type and p-type epitaxial layers of (Al, Ga, In)As and diluted nitrides on GaAs;
• Undoped and n-tpe (ZnCd)(SeTe) on GaAs;
• III-V and II-VI nanowires on GaAs and on Si.

Spectroscopies and Inverse PhotoEmission laboratory SIPE

Contact: Maddalena Pedio (pedio@iom.cnr.it)

The scientific activity of the SIPE Laboratory is focused on the interconnection between the empty electronic configuration of condensed matter systems and their structure and dimensionality. It is focused on topics related to low dimensional systems, carbon-based materials, molecular thin flms and organic-inorganic interfaces.
IPS technique is complementary to Photoemission (PES) and combined PES-IPS data provide information on the surface electronic transport gap of sample. Figure shows the main SIPE chamber, a schematic of the IPS process and an example of organic-inorganic PES-IPS measurement. The equipment includes two ultra high vacuum (UHV) chambers and a transfer load lock.
The preparation chamber has standard Surface Science tools, with a CMA for AES and Low Energy Electron Diffraction (LEED) and is also used for the growth of the films of the organic molecules and metals. The connected second UHV chamber is devoted to the empty electronic states analysis by means of Inverse Photoemission, with Geiger Mueller detectors and a highly collimated electron gun, overall resolution <0.3 eV. This configuration allows an Angular Resolved IPS acquisition (KR-IPS), i.e. the mapping of unoccupied electronic states *vs* the wave-vector $k_{//}$. The Load lock is a movable UHV chamber which can be connected with other TASC apparatus, including beamlines at nearby ELETTRA facility, to complement the KR-IPS with Direct Photoemission (PES), Core level photoemission and NEXAFS.



Combined PES and IPS of C_{60} forming directional bonds with Au(110)

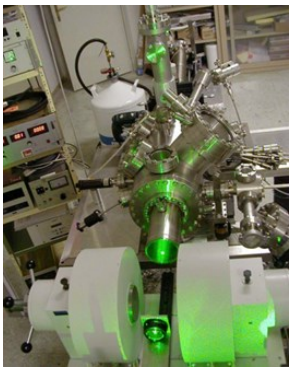
Elcid High Performance Computing HPC

Contact: Stefano Cozzini (cozzini@iom.cnr.it)

Elcid is the High Performance Computing (HPC) platform in use at the CNR-SISSA center Democritos. The system, put into production on June 2013, is composed of a blade system with 8 blades, each with four cpu AMD 6376 by 16 cores. The total number of computational cores is therefore 512 cores. The system is equipped with a Lustre parallel file system that provides 15 TB of disk space. There is also a node equipped with cards GPPGPU for running GPU enabled codes. The system can be further expanded in the case of available funds and increased computational demands.
The system jointly acquired by all the research groups of Democritos is made available to all researchers of the center CNR-IOM Democritos through a policy of resource sharing ("fairshare") according to which the amount of hours of computing time is proportional to the investment of each group. A portion of the funding comes from a commercial contract with eXact Lab rsl, an innovative start-up and spin-off of the institute that is interested in the development of cloud technologies in the field of HPC and is actively working on these issues with the group manager of the platform. The platform can be made available for further computational groups.

UHV evaporation chamber for growth and in-situ characterization of ultrathin magnetic films

Contact: Gianluca Gubbiotti (gubbiotti@fisica.unipg.it)



A UHV chamber, specially designed to be directly interfaced with the optical table for in-situ Brillouin light scattering (BLS) and Magneto-optic Kerr effect (MOKE) measurements, is operative and used by the IOM researchers to growth and study structural and magnetic properties of ultrathin magnetic films deposited either on metallic or semiconductor substrates. As shown in the picture, it is a compact chamber mounted on top of a mobile frame, equipped with standard UHV tools, such as e-beam evaporators, quartz micro -balance, LEED-Auger apparatus, RHEED, load-lock system. A horizontal XYZ manipulator, with primary and secondary rotations, is used to position the evaporated film at the end of the so called *BLS tube* which is a protuberance about 20 cm long and 10 cm in diameter, terminating with a glass viewport for BLS and SMOKE measurements.

The temperature of the specimen can be varied in the range 110-1400 K. The whole frame can be translated just aside the BLS optical table, inserting the BLS tube within the poles of an external four-inches electromagnet. The sample holder allows to measure the spin wave frequency as a function of the both the incidence angle of light and the in-plane angle of the applied magnetic field, with field intensity up to 6 kOe. MOKE hysteresis curves can be measured in the longitudinal configuration to determine the magneto-crystalline anisotropy and its evolution with the film thickness.

Conventional and micro-focused Brillouin light scattering setups

Contact: Gianluca Gubbiotti (gubbiotti@fisica.unipg.it)

Two optical tables are operative and used by the IOM researchers to perform conventional and micro-focused Brillouin light scattering (BLS) measurements. In the conventional BLS apparatus a laser beam from a solid state laser (532-nm line) is focused onto the sample surface using a camera objective of numerical aperture 2 and focal length 50 mm. The backscattered light was analyzed by a Sandercock-type (3+3)-pass tandem Fabry-Pérot interferometer. BLS measurements of the spin-wave frequency, can be performed as a function of the intensity of the applied magnetic field H up to 1T, the incidence angle of light, and the in-plane direction of H, with a spatial resolution of about 30 μm, determined by the diameter of the laser spot.

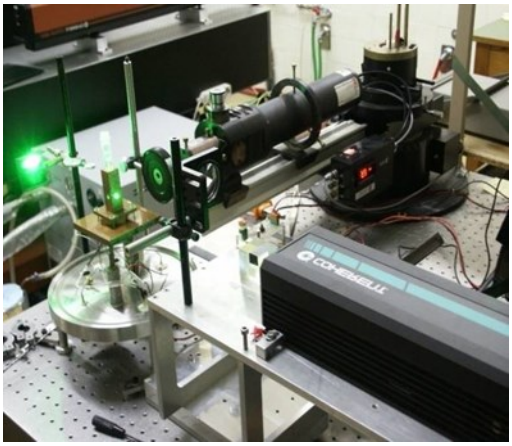
The micro-focused BLS apparatus is characterized by a spatial resolution of about 250 nm. The light source is a single-frequency, Diode-Pumped Solid-State laser (532-nm line). A dark -field objective, with numerical aperture NA=0.75 and long working distance 4.7 mm, focuses light perpendicularly on the sample surface. Using the same objective, a coaxial viewing system based on a collimated LED light source, a beam expander, and a CCD camera is used to visualize the laser spot and the sample region under investigation. The sample holder is controlled by a software which provides an active stabilization of the lateral and vertical position of the sample by compensating for position drifts. Microwave generator (frequency range 250 kHz - 20 GHz) and three-axes positioning stages of picoprobes can also be used for the rf-excited spin-wave experiments.

Istituto Officina dei Materiali

@ Perugia

Photon Correlation Spectroscopy (PCS) Set-up

Contact: Lucia Comez (lucia.comez@fisica.unipg.it)



The photoncorrelation device (Photon correlator Brookhaven BI 9000 AT) consists of a laser source (Coherent: 532nm, 400mW), a goniometer with a special accommodation for samples and a correlator board installed in a computer. The digital correlator works using three sections of channels (low, mid and high speed with different sampling time range) and is able to cover a dynamic range over ten decades (25ns-1310s). The apparatus consents to calculate, in the time domain, the autocorrelation functions of the intensity of the electric field scattered by the selected sample. The spectra can be recorded using either a fixed geometry or varying the scattering angle, thus allowing access to several exchanged vectors ($q=0.01\text{-}0.035 nm^{-1}$).
Photoncorrelation Spectroscopy (PCS) can be successfully applied to study of the slow dynamics of a large variety of disordered systems: aqueous solutions, molecular liquids, polymers and glues. For biosystems in solution, this technique allows to determine the hydrodynamic radius (simple particle sizing calculation) and the diffusion constant of the solute by varying temperature and/or concentration. For molecular liquids, polymers and glues, it represents a unique tool to detect the structural relaxation during the vitrification and/or gelation of the system, under the action of chemical or physical agents.

@ Grenoble

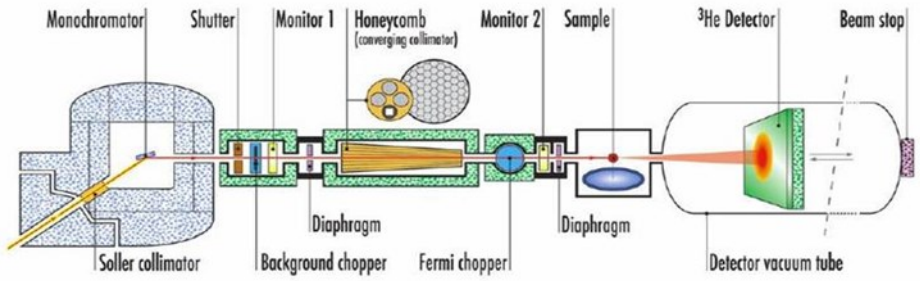
GILDA beamline

Contact: Francesco d'Acapito (dacapito@esrf.fr)

GILDA is a synchrotron radiation beamline operative on a bending magnet source of the European Synchrotron Radiation Facility in Grenoble (F). The beamline is dedicated to X-ray Absorption Spectroscopy experiments and it covers the energy range of hard X rays from 5 to 90 keV allowing investigations of elements from Cromium to the actinides. The main feature of the beamline is the high photon flux (10^{10} ph/s on the sample) obtained by an efficient X-ray focusing optics and a high energy resolution (10^{-5}).
The instrumentation of GILDA includes 2 arrays of High Purity Germanium detectors for the analysis of diluted samples (trace elements, dopants, solutions) and 2 experimental facilities (ReflEXAFS chamber and Grazing Incidence sample manipulator) for the analysis of thin films. Typical limits are 50 ppm for trace elements or 0.3 Monolayers for thin films. Additional apparata (N_2/He cryostat, solid-gas reaction cell) complete the ancillary equipment of the instrument. The scientific activity at GILDA covers a variety of topics like materials science, physics, chemistry, biophysics and medicine, earth science, environment and cultural heritage.

The Neutron Spectrometer BRISP

Contact: Ferdinando Formisano (formisano@ill.fr)



In the framework of an Italian (CNR) - German (Marburg University) collaboration, the BRIllouin SPectrometer BRISP has been constructed at ILL's High Flux Reactor to provide the scientific community with a neutron spectrometer able to perform advanced investigations of the atomic (e.g. collective excitations) and spin (e.g. magnons) dynamics in the low-momentum region (0.1¸1.8 $Å^{-1}$) with relatively high incoming neutron energies (20-80 meV). The use of the time-of-flight technique in combination with a two-dimensional position sensitive small-angle detector, which ensures an efficient data collection, makes this new spectrometer particularly suited for measuring changes in the dynamic structure factor induced by varying external parameters such as pressure, temperature and magnetic field in rather different materials ranging from biological and magnetic systems to disordered systems, like dynamically soft glasses, liquids and compressed gases.
Beam time on BRISP is allocated to external proposers on an international peer review basis: 70 % of the beam time is attributed only to research team including Italian and/or German users, while the remaining 30 % is attributed to users from all over the world

IN13 beamline

Contact: Francesca Natali (natali@ill.fr)

The thermal backscattering spectrometer IN13 at the Institute Laue-Langevin (Grenoble, France), is operated by a French-Italian CRG (Collaborative Research Group).
The relatively high energy of the incident neutrons (16 meV) makes it possible to span a wide range of momentum transfer Q (from 0.3 to 4.9 $Å^{-1}$) with a very good energy resolution (~ 8 μeV, FWHM). Thus, IN13 allows the investigation of a space -time window of about 1 Å and 0.1 ns, providing information on the single particle motions (jump reorientation, rotational and translational diffusion, tunneling). IN13 is mainly devoted to life sciences, in particular to the study of the dynamical features of macromolecular compounds in the μeV energy region, but scientific applications can be also found in areas of materials science, solid-state physics, geophysics and chemistry. IN13 is mainly devoted to life sciences, in particular to the study of the dynamical features of macromolecular compounds in the μeV energy region, but scientific applications can be also found in areas of materials science, solid-state physics, geophysics and chemistry. Beam time is allocated by the Scientific Advisory Committee. Italian and French groups receive on the average a total number of days that reflects their financial participation. Proposals can be submitted by external groups via collaborations with the funding partners. Proposals are selected on the basis of their scientific merit.

Projects & grant

Projects

Type of project	Coordinator	Title	IOM Leader	Location	Grant €
UE	DESY	PRE XFEL - Preparatory activities for the implementation of the European X-Ray free-electron laser facility	G. Rossi	Trieste,-Area Science Park	120.000,00
UE	CNR-IOM	NFFA - Nanoscience Foundries and Fine Analysis	G. Rossi	Trieste-Area Science Park	703.728,00
UE	VTT	NAPANIL - Nanopatterning production and application based on nanoimprinting lithoghraphy	M. Tormen	Trieste-Area Science Park	812.136,00
UE	SISSA	NANOSCALE - Understanding interactions between cells and nanopatterned surfaces	M. Tormen	Trieste-Area Science Park	606.770,96
UE	Integra Renewable Energies S.r.l.	ORION - Optimization of sisolar cells plastic materials and technologies for the development of more efficient concentration photovoltaic system	F. Romanato	Trieste-Area Science Park	750.000,00
UE	INSTITUT LAUE LANGEVIN	NMI3 - Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy	F. Sacchetti	Perugia	85.350,00
UE	INSTITUT LAUE LANGEVIN	NMI3-II - Neutron Scattering and Muon Spectroscopy Integrated Initiative	F. Sacchetti	Perugia	50.126,00
UE	University of Cambridge	TECHNOTUBES - Technology for wafer-scale carbon nanotube applications	C. Cepek	Trieste-Area Science Park	189.143,25
UE	CNR-IOM	H2OSPLIT - Water splitting catalysts for artificial photosynthesis	S. Fabris	Trieste SISSA	100.000,00
UE	Trinity College - Dublin	ATHENA - Advanced theories for functional oxides: new routes to handle the devices of the future	A. Filippetti	Cagliari	242.585,00
UE	CBM S.C.R.L.	SMD - Singlr or few molecules detection by combined enhanced spectroscopies	M. Lazzarino	Trieste-Area Science Park	287.563,14
UE	Stichting Katholieke Universiteit	IFOX- Interfacing oxides	G. Panaccione	Trieste-Area Science Park	239.319,00
UE	CNR-SPIN	OXIDES - Engineering Exotic Phenomena of Oxide interfaces	A. Filippetti	Cagliari	177.398,50
ERC	CNR-IOM	SUPERBAD - Understanding high-temperature superconductivity from the foundations: superconductivity as a cure for bad metallic behaviour	M. Capone	Trieste SISSA	1.000.000,00
ESF	CNR	NOMCIS - Nanomanipulation of metallic cluster on insulting substrates	F. Esch	Trieste-Area Science Park	100.000,00
ESF	CNR	EBIOADL - An Integrated frame work for Engineering bio-mimetic adhesive interface	P. Decuzzi	Trieste SISSA	100.000,00
ESF	CNR	AFRI - Atomic Friction	E. Tosatti	Trieste SISSA	100.000,00

Istituto Officina dei Materiali

Projects

Type of project	Coordinator	Title	IOM Leader	Location	Grant €
MIUR - Progetto strategico	CNR-IOM	NFFA - Nanoscience Foundries and Fine Analysis- nell'ambito della RoadMap ESFR	G. Rossi	Trieste-Area Science Park	2.465.500,00
MIUR - FIRB	Università di Trieste	Approcci nanotecnologici per la teragnostica dei tumori	M. Lazzarino	Trieste-Area Science Park	248.496,00
MIUR - FIRB	CNR-IOM	Ancoraggio di molecole tramite l'interazione Cooh-NH2 su superfici funzionante	A. Cossaro	Trieste-Area Science Park	331.016,00
MIUR - FIRB	CNR-IOM	Beyond graphene: tailored C-layers for novel catalytic materials and green chemistry	F. Bondino	Trieste-Area Science Park	182.400,00
Progetto Bandiera	CNR-NANO	NANOBRAIN - NANOMAX - Nanotechnology-based therapy and diagnostics of brain deseases	F. Romanato	Trieste-Area Science Park	123.576,92
MIUR PRIN	Università Roma La sapienza	Controllo della struttura e delle funzioni di nanostrutture organiche su superfici metalliche	S. Fabris	Trieste SISSA	40.000,00
MIUR PRIN	Università Roma Tor Vergata	Spettroscopia auger di sistemi magnetici a bassa dimensionalita': correlazione elettronica e dicrosmo	R. Gotter	Trieste-Area Science Park	25.720,00
MIUR PRIN	CNR-SPIN	Spettroscopie ottiche, caratterizzazione strutturale e calcoli ab-initio applicati allo stadio dei gas bidimensionali alle interfacce di ossidi funzionali	B.A. Davidson	Trieste-Area Science Park	15.272,00
MIUR PRIN	CNR-ITM	Hierarchical Photosynthetic Nano-Structures for Carbon-Neutral Renewable Energy HI-PHUTURE	C. Cepek	Trieste-Area Science Park	61.582,00
MIUR PRIN	Università di Padova	DESCARTES - "Development of Energy-targeted Self-assembled supramolecular systems: a Convergent Approach through Resonant information Transfer between Experiments and Simulations	L. Floreano	Trieste-Area Science Park	51.300,00
MIUR PRIN	CNR-SPIN	OXIDE - Interfacce di ossidi: nuove proprietà emergenti, multifunzionalità e dispositivi per l'elettronica e l'energia	G. Panaccione	Trieste-Area Science Park-Trieste-Area Science Park	58.023,00
PIK	Elettra	ULTRASPIN - Utrafast spectroscopy with SPIN polarization	G. Panaccione		230.000,00
PIK	Università di Bologna	EX-PRO-REL - EXcitation PROcesses and RELaxation in condensed matter and nanostructures: methodological, instrumental, and scientific challenge	M. Pedio, F. D'Acapito, M. Malvestuto	Trieste-Area Science Park	93.000,00
Region	Università di Trieste	NANO-PV - Sviluppo di un nuovo materiale fotovoltaico nanostrutturato	E. Carlino	Trieste-Area Science Park	15.000,00
Region	SISSA	NANOCAT - Nanocatalisi su fili e fibre di carbonio: una promessa per l'energia e l'ambiente, una sfida per la simulazione numerica	S. Fabris	Trieste SISSA	85.084,01

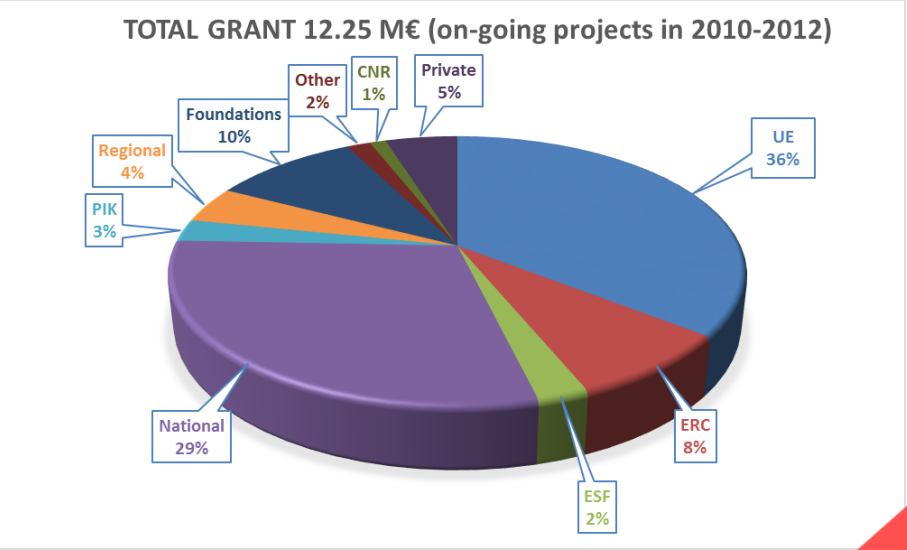
Projects

Type of project	Coordinator	Title	IOM Leader	Location	Grant €
Region	CNR-IOM	MASTER & BACK - Studio delle proprieta' elettroniche dei materiali superconduttori	F. Bernardini	Cagliari	44.982,75
Region	CNR-IOM	MASTER & BACK - Interfacce di ossidi perovskitici di tipo isolante-isolante e metallo-metallo da compiere attraverso simulazioni con metodologie ab-initi	V. Fiorentini	Cagliari	47.580,85
Region	CNR-IOM	M4C - Modellazione multiscala della meccanica dei materiali compositi	L. Colombo	Cagliari	94.000,00
Region	CNR-IOM	MASTER & BACK - Interazione tra superfici biominerali rilevanti nel degrado dei beni architettonici ed ambientali e ambiente: assorbimento di acqua, CO2 e molecole organiche	A. Satta	Cagliari	68.450,73
Region	CNR-IOM	Dispositivi microelettronici per la spintronica basati su ossidi nano strutturati	B.A. Davidson	Trieste-area Science Park	181.408,00
Fond. BDS	CNR-IOM	Silicio nano-cristallino per applicazioni fotovoltaiche ed optoelettroniche	L. Colombo	Cagliari	17.000,00
Fond. BDS	CNR-IOM	Ferroelettricita' e magnetismo in manganiti e titanati di terre rare con drogaggio multiplo	V. Fiorentini	Cagliari	50.000,00
Fond. BDS	CNR-IOM	Assorbimento di metalli pesanti nel terreno: uno studio teorico della biomineralizzazione	A. Satta	Cagliari	10.000,00
Fond. BDS	CNR-IOM	Struttura, proprieta' elttroniche e di trasporto in eterostrutture e basse ossidi	G. Lopez	Cagliari	30.000,00
Fond. BDS	CNR-IOM	Impiego di carbonato di calcio nel problema dell'inquinamento da piombo cadmio e zinco	A. Satta	Cagliari	17.850,00
Fond. BDS	CNR-IOM	Materiali innovativi per applicazioni di microelettronica e spintronica: studio di effetti magnetoelettrici in titanati e manganiti a bassa dimensionalita' con drogaggio di ossigeno	G. Lopez	Cagliari	19.850,00
Fond. BDS	CNR-IOM	Studio di eterostrutture di ossidi con eccezionali proprietà di trasporto e di potere termoelettrico	A. Filippetti	Cagliari	14.850,00
Fond. IIT	Università di Firenze	MYOMAC - Myosin based machines	D. Cojoc	Trieste-area Science Park	126.400,00
Fond. IIT	CNR-IOM	POLYPHEMO - Polymer based Hybrid Nanomaterials for photovoltaic: improving efficency by theoretical modelling	A. Mattoni	Cagliari	390.000,00
Fond. IIT	CNR-ISC	NEWDFESCM - New density functional for the electronic structure of complex materials	A. Filippetti	Cagliari	190.000,00

Istituto Officina dei Materiali

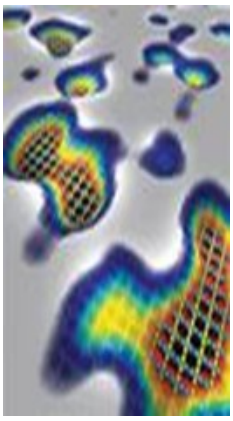
Projects

Type of project	Coordinator	Title	IOM Leader	Location	Grant €
AIRC	CRO Aviano	Application of Advanced Nanotechnology in the Development of Innovative Cancer Diagnostics Tools	M. Lazzarino	Trieste-Area Science Park	338.250,00
//	Elettra	Simulazione numerica della struttura atomica ed elettronica dei materiali e dei relativi fenomeni dinamici ultraveloci	S. Fabris	Trieste SISSA	150.000,00
Consorzio AUSI - UNICA	CNR-IOM	Inquinamento di materiali pesanti: un modello teorico dell'assorbimento di ioni metallici di parte di superfici di biominerali	A. Satta	Cagliari	45.600,00
CNR-DMD FOTONICA 2015	CNR-IOM	Fully integrated optically-pumped organic microlaser	M. Prasciolu	Trieste-Area Science Park	15.000,00
CNR-DMD FOTONICA 2015	CNR-IOM	Enhancing the light absorption in thin films by 2D multiple scattering	M. Tormen	Trieste-Area Science Park	15.000,00
CNR	CNR-IOM	Accordo di cooperazione scientifica CNR/FCT	F. D'Acapito	Grenoble	5.000,00
IOM Start-up Project	CNR-IOM	Cristalli liquidi di nDNA: modellizzazione di strutture G-quadruplex nella sequenza telomerica e dei meccanismi di stabilizzazione con scopo terapeutico	L. Comez	Perugia	25.000,00
IOM Start-up Project	CNR-IOM	Determinazione della Densità di stati elettronici del DNA – D^3	E. Magnano	Trieste-Area Science Park	50.000,00
IOM Start-up Project	CNR-IOM	Development and testing of a reliable pseudopotential set for electronic structure calculation	L. Martin-Samos	Trieste SISSA	23.000,00



Title	***SUPERBAD** – Understanding Superconductivity from the foundations*
Source of funding	*European Research Council (ERC)*
Cordinator	*CNR IOM, IT*
IOM coordinator	*Massimo Capone*

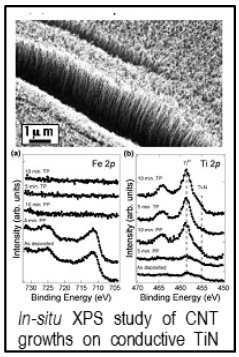
Objectives



The aim of the project is to exploit modern advances in material science and in the theoretical description of correlated solids to address the main question raised by the high-temperature suerpconductors, namely “Ehat makes the critical temperature high and, more importantly, how can we control it and raise it?”. The main deliverable of the project will be the implementation of a complete theoretical scheme for the quantitative calculation of the superconducting properties of strongly correlated superconductors. The main idea that we will explore is that an optimal distance from a Mott insulator is the key for high-temperature superconductivity in a wide range of superconductors, including cuprates, fullerenes and iron-based superconductors. Supercomductivity appears has a cure that “heals” the anomalies of the strongly correlated metallic state. The project has achieved all its goals, in particular we have strengthened our understanding of strongly correlated superconductiivty in the fullerides, we have identified the hidden role of strong correlations in iron-based superconductors, and we have demonstrated how the non-equilibrium dynamics in the cuprates is dominated by Mott physics. We have published several papers in important journals, including one Nature Communications, one Science, and four Physical Review Lettes.

Title	***TECHNOTUBES** –Technology for Wafer-Scale Carbon Nanotube Applications*
Source of funding	*FP7, Theme 4, Large-Scale Integrating Project*
Coordinator	*University of Cambridge, UK*
IOM coordinator	*Cinzia Cepek*

Objectives

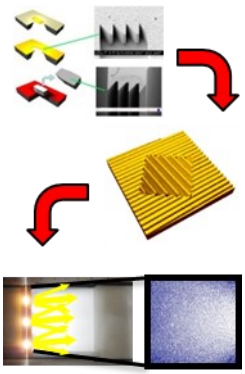


In-situ XPS study of CNT growths on conductive TiN

The aim of this 3-year project was to develop growth processes, automated equipment, quality control/monitoring and a variety of end-applications based on carbon nanotubes (CNTs). It has bring together world-class partners from industry and research, to create a CNT value chain, from growth equipment to material production to exploitable devices. The key applications that emerged from this project include interconnects, thermal interface materials, medical and security X-ray sources, gas detectors, biological probes, microfluidics and novel energy storage devices. Inside Technotubes, IOM has studied test systems finding out the best protocols for the controlled synthesis of CNTs on oxide and conductive substrates, compatible with industrial processes. All CVD steps was studied using in situ XPS, to determine the chemical effects on the substrate and catalyst due to different pre-treatments and to CVD gasses exposures. This work allowed understanding in detail the mechanisms driving the CNTs synthesis, helping to find the best protocols to optimize the process.

Title	***NAPANIL**—Nanopatterning, Production and Applications based on Nanoimprinting Lithography*
Source of funding	*European Community (FP7)*
Coordinator	*VTT Technical Research Centre of Finland , FIN*
IOM coordinator	*Massimo Tormen*

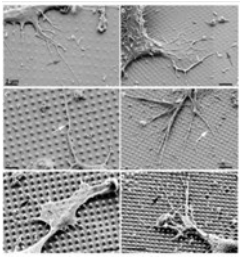
Objectives



The concept of the project is based on identified application fields with very high potential impact but with no mature production processes developed yet. We have readily identified potential target applications for large scale implementation and upscaling to industrial production of tools, materials, processes and knowhow developed in the nanoimprinting lithography (NIL). The applications chosen are based on the idea of controlling light at surfaces using nanoscale 3dimensional surface structures. At the moment there is no efficient production method available for this kind of surfaces and the aim in this project is to develop and qualify processes that can produce such surfaces in small scale production environments. The focus of this project is driven by our end-user partners, on applications with surface areas in the range from a few mm to tens of cm. These include mobile applications, automotive applications, housing and spot lighting.

Title	***NANOSCALE**—Understanding interactions between cells and nanopatterned surfaces*
Source of funding	*European Community (FP7)*
Coordinator	*SISSA, IT*
IOM coordinator	*Massimo Tormen*

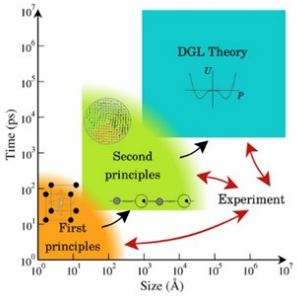
Objectives



The study of biological processes occurring at the nanoscale is becoming a new discipline at the border between Physics and Biology with major scientific challenges and new technological applications. In fact, interactions at the nanoscale between cells/neurons and surfaces with specific nanopatterns appear to control several major biological processes, such as cell proliferation and differentiation. The aim of the present NanoScale proposal is therefore to explore interactions between stem cells, neurons, neuronal networks and surfaces with specific geometrical nanopatterns and nanoprints of specific proteins and molecules. The NanoScale project has produce and develop a variety of nanodevices for growing, guiding, manipulating cells, neurons and neuronal cultures. It is composed of two major ingredients: i - the combination of a MicroElectrode Arrays (MEAs) with chemical and topographic micro/nanosubstrates controlling the network growth; ii – the coupling with external measuring and/or manipulating devices such as Electron Microscopes and Optical Tweezers.

Title	***ATHENA**—Advanced Theories for functional oxides: New routes for handling the devices of the future.*
Source of funding	*E.U. – Republic of India*
Coordinator	*Trinity college., Dublin, IRL*
IOM coordinator	*Alessio Filippetti*

Objectives

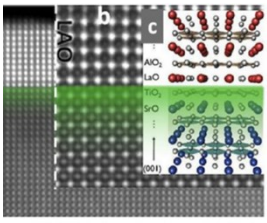


The ATHENA project aimed at refining and unifying the computational methods used in the study of functional oxides over a wide range of sizes and time scales. The first goal, mainly undertaken by European partners, was the assessment of beyond-DFT methods for the ab-initio treatment of strong electronic correlation and magnetism in oxides. To achieve this goal the Variational Self Interaction Corrected Scheme (VpSIC) was implemented and its accuracy, compared with results from hybrid functional HSE, was positively assessed [1,2]. As a second milestone, the project pointed to devise and implement techniques for extracting, from total energy ab-initio calculations, parametric quantities to be feeded to large scale model computations which had been, in the while, implemented by the Indian partners of the project. The extraction of exchange coupling constants from ab-initio calculation has been demonstrated and successfully used for Monte-Carlo and Tight-Binding empirical calculations. A full paradigm for a multi-scale and progressive accuracy study of oxides has been achieved. A disseminative school was held in march 2012 in Kolkata, India.

[1] Phys. Rev. B. 84,195127— [2] Phys. Rev. B. 84,115124

Title	***OxIDes**—Engineering exotic phenomena at oxide interfaces*
Source of funding	*E.U.*
Coordinator	*Université de Liege , B*
IOM coordinator	*Alessandro Mattoni*

Objectives



The OxIDes project (Oxide Interface Design) was targeting the engineering of exotic phenomena at oxide interfaces. It was a theory-driven project, also relying on strong and continuous interactions with experimentalists. The main objectives were (i) the development of advanced theoretical and simulation techniques to model the most relevant types of oxide interfaces and (ii) the use of these tools to design, in close collaboration with experimentalists a new generation of layered materials with unique experimentally-confirmed properties.

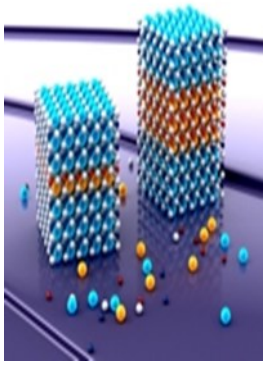
OxIDes considered ABO3 perovskites that can exhibit a wide range of properties and many different orders. They can also be combined in hetero-structures.

Artificial multilayers and superlattices allow to tune and couple different degrees of freedom through various effects like charge transfer, electrostatic coupling, symmetry breaking; combining oxide intrinsic properties but also inducing totally new phenomena.

The project achieved many of these goals. The CNR-IOM group contributed by demonstrating the validity of VpSIC as a valid alternative to usual LDA+U correction for the study of oxide interfaces and for investigating with this technique many interfaces based on SrTiO3 and characterizing their electric and thermoelectric properties.

Title	***IFOX**- Interfacing oxides*
Source of funding	*European Community (FP7)*
Coordinator	*Stichting Katholieke Universiteit, NL*
IOM coordinator	*Giancarlo Panaccione*

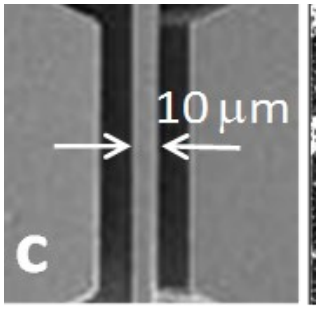
Objectives



The goal of IFOX is to explore, create and control novel electronic and magnetic functionalities, with focus on interfaces, in complex transition metal oxide heterostructures to develop the material platform for novel 'More than Moore' (MtM) and 'beyond CMOS' electronics, VLSI integratable with performance and functionality far beyond the state of the art.
Investigations include ferroelectric and ferromagnetic oxides as well as artificial multiferroic heterostructures (deposited on large area silicon substrates) with as final deliverable concepts for multifunctional magneto-electronics devices controlled by electric and magnetic fields and ultimately by ultra short light pulses.
The role of CNR (two insititutes, ISMN-Bologna and IOM-Trieste) is Grow oxide films on commercial substrates with a quality comparable to state-of-the-art semiconductor growth and characterize their structural, electronic and magnetic properties.

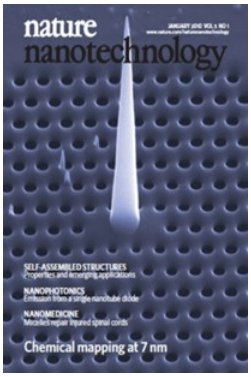
Title	***CHIPCAT—**Design of thin-film nano catalysts for on-chip fuel cell technology*
Source of funding	*EU FP7-NMP-2012*
Coordinator	*Charles University of Prague , CZ*
IOM coordinator	*Stefano Fabris*

Objectives



The chipCAT project focus at knowledge-driven development of novel thin-film catalysts for proton exchange membrane fuel cells (PEMFCs). The state-of-the-art thin film technology, particularly the plasma assisted physical vapor deposition (PVD) methods, has already achieved a cutting-edge level in the field on novel material synthesis. Co-deposition of materials at equilibrium or non-equilibrium conditions leads to easy and fast preparation of new compounds. This way a virtually unlimited number of combinations of functional materials can be created including nanoalloys, mixed oxides, and nanostructured porous materials. The ground-breaking potential of these thin film technologies in catalysis, however, has not been exploited yet. While scaling up of thin film processes has issues that limit the techniques to relatively small areas (less than a few square meters), in the case of fuel cells for mobile applications - ranging from automotive to micro-device electronic systems - size is not a critical parameter, however.

Title	***SMD**—Single Molecule Detection*
Source of funding	*UE – FP7-NMP-2008-SMALL-2*
Coordinator	*CBM S.c.a.r.l. IT*
IOM coordinator	*Marco Lazzarino*



The understanding of fundamental biological processes and of molecular events causing major diseases require a miniaturized chemical probe or microscope, which could be moved around and inside a cell, able to detect and identify a single or a small number of molecules. The SingleMoleculeDetection (SMD) proposal was aimed at the integration on the same device an atomic force microscope (AFM) or an optical tweezers (OT, with Raman/SERS/IR/TeraHertz microscopy so to perform simultaneously - and in a dynamic way - force and spectroscopic measurements.
The main result of the project was the design and fabrication of novel devices for the generation of Plasmon Polariton (PP) combined with photonic crystals (PC) and novel plasmonic nanolenses and their use in chemical nanoscopy.
Chemical mapping with spatial resolution down to 7nm was demonstrated during the project.

Title	***ORION**—Optimization of sisolar cells plastic materials and technologies for the development of more efficient concentration photovoltaic system*
Source of funding	FP7 – SMART COMPANIES -
Coordinator	INTEGRA Renewable Energies Srl , IT
IOM coordinator	*Filippo Romanato*

Objectives

The MAIN OBJECTIVE of the project is the **optimization of materials and technologies involved in Concentration PhotoVoltaic System production** in order to reduce the systems' cost/watt and increase the system efficiency.

The **reduction of system cost/watt**, that reflects in a reduction of the PV-generated electricity, will be achieved by: developing an all-plastic system by using recycled plastic compounds; developing Si solar cells for automatic assembling technology; implementing and industrializing automated high-throughput technologies for cell assembly and optics production.

2. The **increase of system efficiency** will be achieved by: increasing Si concentration cell efficiency by using surface plasmonic crystal structures; developing plastic materials doped with down-converting nanoparticles for modification of the solar spectrum in order to enhance the absorption efficiency of cells.

Title	***NFFA—****Nanoscience Foundries and Fine Analysis*
Source of funding	*EC FP7 - Capacities Specific Programme Research Infrastructures*
Coordinator	*CNR-IOM, IT*
IOM coordinator	*Giorgio Rossi*

Objectives

NFFA - Nanoscience Foundries and Fine Analysis is a Design Study for a European Distributed Research Infrastructure, that will co-locate Nanoscience Centres with the LSFs, enabling access to nanoscience, atomic precision and fine analysis with a unified metrology. The NFFA Centres will:

•provide an infrastructure, with open access to academic, industry and civil services, for the integration of research efforts in nanoscience made by advanced nanofabrication methods and a fuller exploitation of atomic-precision metrology of the European LSF;

•create a common technical platform for advanced nanofabrication and characterization of nanostructures, providing a well defined metrology for synthesis and nanofabrication protocols, atomic resolution analysis, modeling and simulation methods;

•develop the first Repository of Nanoscience Data and Protocols for Metrology, Synthesis and Analysis on systems selected by the research community;

•maximize the impact of LSFs by raising the standard of sample definition and characterization for advanced experiments with ultrafast, nanofocused and high energy resolution probes available at Synchrotrons, FELs and Neutron facilities;

•strengthening the use and scientific return of all relevant RI of the ESFRI roadmap for nanoscience and nanotechnology.

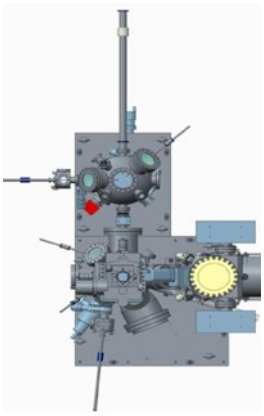
Title	**EXPROREL** - EXcitation PROcesses and RELaxation in condensed matter and nanostructures
Source of funding	PIK ELETTRA
Coordinator	*University of Bologna, IT*
IOM coordinator	*M. Pedio, F. D'Acapito, M Malvestuto*

Objectives

This project aims to develop specific instrumentation along with methods and protocols to perform pump and probe spectroscopy measurements of excitation/ relaxation processes in condensed matter and nanostructures. In fact, the FEL pulse duration (1-100f s) is ideally suited to probe relaxation processes due to electron–electron and electron–phonon scattering. The challenge is to extend to the VUV–X-ray region techniques currently used in the UV, VIS and IR ranges. The implementation of the project consists in three main tasks: development of instrumentation, execution of selected pilot/exploratory measurements and progress in computational spectroscopy. The instrumental development includes the pre – design of a UHV chamber appropriate for measurements at XFEL (see Figure). We plan to use existing storage ring and lower energy FEL sources to develop novel instrumentation and the necessary expertise. The proposal brings together scientists with a background in synchrotron radiation techniques, experts in sample growth and surface science and a theory component.

Title	***ULTRASPIN**—Utrafast spectroscopy with SPIN polarization*
Source of funding	*MIUR-Sincrotrone Trieste*
Coordinator	*CNR-IOM, IT*
IOM coordinator	*Giancarlo Panaccione*

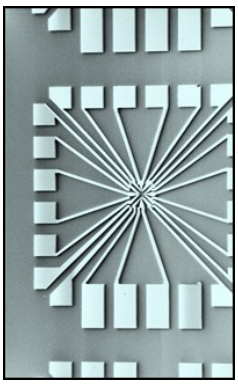
Objectives



The proposal addresses the need to design and build an experimental station dedicated to ultrafast spin polarization dynamics from nanostructured-solids and surfaces with capability of measuring the spin polarization (SP) of the photoelectron yield as excited by individual Free Electron Laser radiation pulses. The core instrument of the experimental station is a four-axis Mott scattering device allowing for full vectorial reconstruction of the SP both in the static and dynamic (pump-probe) modes.
The complete experimental station will make available to future users an advanced sample environment (EM field pulses from lasers, localized magnetic fields, electric fields, temperature control from cryogenic temperatures to relevant Curie temperatures) as well as in situ sample synthesis and characterization by complementary electronic and magneto-optical methods.
The Ultraspin station will be instrumental to many experiments on magnetization dynamics, including pump-probe experiments, in operando experiments (during growth, vs. temperature, vs. applied electric field), spectroscopy experiments (photon-in photon-out XAS at L2,3 and M4,5 core level thresholds), combination with magneto-optic effects (time-resolved Kerr), and with electron spectroscopy (Time of flight and pump-probe photoemission experiments).

Title	*Nanotechnological approaches toward tumor theragnostic*
Source of funding	*MIUR – FIRB accordi di programma*
Coordinator	*University of Trieste , IT*
IOM coordinator	*Marco Lazzarino*

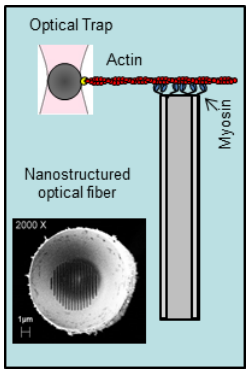
Objectives



The project is aimed at introducing innovative devices and therapeutic protocols based on the nanomechanical response of biomolecular nanostructures, with the ultimate goal of performing high-throughput, high sensitivity and low-cost measurements on large, predetermined diagnostically relevant, subsets of the proteome obtained from very small samples down to the single cell level. In few words: protein expression fingerprinting assays.
The project targets particularly to cancer, as it represents the second cause of death in western countries. Rather than scouting new drugs, the project directs major efforts toward targeting existing drugs to specific tumor types, not only by increasing the efficacy but also by reducing the side effects. The main current problems that the project aim at solving are related to 1) the difficulties in early tumor detection with the related problem of identify characterize and treat metastatic tumors; 2) the lack of selectivity of existing drugs and 3) the intrinsic or acquired drug resistance of tumor cells.
The project created a strong Italian theranostics networking in which different disciplines are mixed together and chemists, physicists, biologists and clinicians work in close contact with each other shortening the time necessary for the safe transfer of knowledge from the laboratory to the clinical practice.

Title	***MYOMAC**— Myosin based machines*
Source of funding	*Italian Insitute of Technology IIT- SEED projects*
Coordinator	*University of Florence, IT*
IOM coordinator	*Dan Cojoc*

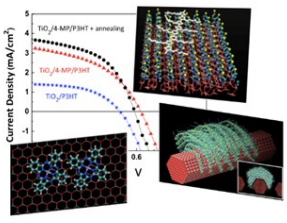
Objectives



Goal: development of a synthetic sarcomere-like machine based on a nanostructured array of myosin II motor proteins. Objectives: 1) interfacing motor proteins and inorganic devices, 2) design and fabrication of nanostructures to control the geometry of the motor protein array, 3) application of optical tweezers to measure and control the mechanical outputs (force and length) of the synthetic machine.
Results. A simplified version of the machine able to deliver steady force and power has been realized and tested limiting the number of motors interacting with the actin filaments by the size of the support (tip of etched optical fibre between 3 and 8 μm. This machine generates steady force in a physiological like condition. Actually, due to the compliance of the trap acting as force transducer (7 nm/pN), the steady level force (50 pN) is achieved in an interval of time four time slower than in an "isometric" contraction in vivo. The myosin ensemble induces a filament sliding of 350 nm during the rise of force. Considering the size of the working stroke of the myosin motor (10 nm at most), this means that the motor ensemble undergoes several cycles af ATP driven interactions, simulating what is known in muscle physiology as an "auxotonic" contraction, in which the load increases during the movement induced by muscle contraction.

Title	***POLYPHEMO**—Polymer based hYbrid nanomaterials for photovoltaics: improving efficiency by iheoretical modeling*
Source of funding	*Italian Insitute of Technology IIT- SEED projects*
Coordinator	*CNR-IOM, IT*
IOM coordinator	*Alessandro Mattoni*

Objectives



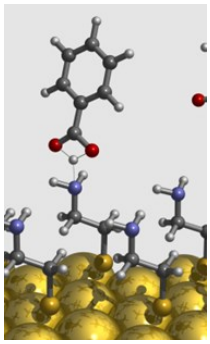
The POLYPHEMO project aims at developing a multiscale theoretical framework based on a hierarchic combination atomistic and mesoscopic methods to model predictively and to improve the relevant physical properties of hybrid nanomaterials for photovoltaics; the theoretical framework has been tuned, validated and applied to improve the photoconversion properties of polymer based nanomaterials; the activity focused on dye sensitized polymer-metaloxyde nanostructure considered as a promising route for a cheap and efficient solid state photovoltaic solar cells. The central idea being that by a suitable design of the molecule it is possible to improve the polymer/ inorganic structure and optoelectronic properties of interfaces. The Project has successfully developed a theoretical framework able to model predictively and support the experimental realization of polymer-based hybrid solar cells made of prototypical materials, namely, poly(3-hexylthiophene) (P3HT) infiltrated in a TiO2 scaffold or blended with ZnO nanoparticles. Step-change improvements of in the device performances have been enabled by engineering the hybrid interface by the insertion of suitable molecular interlayer (pyridine derivatives [1] or phthalocyanines[2]).

[1] Energy Environ. Sci. 5, 9068 (2012) doi:10.1039/c2ee22212d
[2] Adv. Energy Materials (2014) doi:10.1002/aenm.201301694

Main Projects

Title	***ANCHOR**—Anchoring of molecules through the interaction Cooh-NH2 on functionalized surface*
Source of funding	*MIUR – FIRB 2010 Futuro In Ricerca*
Coordinator	*CNR-IOM, IT*
IOM coordinator	*Albano Cossaro*

Objectives



The ANCHOR project aims at studying the amino-carboxylic interaction at surfaces, as a possible route to the formation in-situ of complex hetero-organic architectures. In order to have the description of both the chemistry and the morphology of the systems, the combination of the X-Ray Spectroscopies (photoemission, adsorption, resonant photoemission) with Scanning Tunneling Microscopy is exploited. A growth protocol has been developed, where first a metal surface is functionalized with an amino-terminated molecule and then a carboxylic-terminated molecule is grown ontop. The morphology of the systems can be tuned by varying the number of carboxylic terminations as well as their mutual position in the molecules. Moreover, the proper choice of the amino-terminated molecules allow to obtain different templating schemes of the substrates. The next objectives of the research activity are to improve the thermal stability of the architectures, which are based on hydrogen bonds, and to study their electronic transport properties for possible applications in the design of nanodevices.

Main Collaborations

The following list shows the CNR-IOM **main partners** involved in the realization of International, European, National and Local **R&D Projects**.

from A- **AUSTRIA**

OEAW - Austrian Academy of Sciences, Institute of Biophysics and Nanosystems Research
Universitat Wien

from B- **BELGIUM**

Université de Liege
Interuniversity Microelectronics Centre—IMEC

from CH- **SWITZERLAND**:

Paul Scherrer Institut
EPFL
ETHZuerich
PSI - Paul Scherrer Institute, Laboratory for Micro- and Nanotechnology
Université de Geneve
PHASIS, Geneve
Swiss Federal Institute of Technology Zurich

Istituto Officina dei Materiali

Main Collaborations

from CZ– **CZECH REPUBLIC**

Charles University of Prague
L.E.T. optomechanika Praha

from D– **GERMANY**

AMO GmbH
Max Planck-Halle
Forschungz.Juelich
University of Goettngen
Martin-Luther University of Halle
University of Regensburg
Universitat Augsburg
Ruhr-University Bochum
Technical University of Dortmund
Universitat Erlangen Nurnberg
SOLVICORE GMBH & CO KG
AIXTRON
Philips GmbH
Fritz Haber Institute
Technical University of Berlin
Micro resist technology GmbH

from DK– **DENMARK**

Technical University of Denmark
Naturwissenschaftliches und Medizinisches Institut
MultiChannelSystems GmbH

from E– **SPAIN**

Fundacio Privada Institut Catala de Nanotecnologia
Fundacion Inasmet
Universidad de Cantabria
ICMAB-Barcellona
Nanotec Electronica S.L.
Universitat the Barcelona

from F– **FRANCE**

Unité Mixte CNRS/Saint Gobain
SET SAS
CNRS LTM
LETI Commissariat à l'Energie Atomique
CognoScens
Ecole Normale Supérieure
Synchrotron SOLEIL
UNIVERSITE DE BOURGOGNE
Thales Research and Technology
Thales Electron devices

Main Collaborations

from F– **FINLAND**

VTT Technical Research Centre of Finland
Modines Oy Modines Ltd
University of Helsinki

from IND– **INDIA**

S.N. Bose National Center, Kolkata
J.Nehru Center, Bangalore
Harish-Chandra Research Institute, Allahabad

from IRE– **IRELAND**

Trinity College Dublin

from I– **ITALY**

Centro Ricerche FIAT
Organic Spintronics
C.R.F. Societa' Consortile per Azioni
Scuola Internazionale Superiore di Studi Avanzati (SISSA)
Promoscience Srl
University of Rome III
Elettra Sincrotrone Trieste
CNR-SPIN Genova
CNR-ISC,
CNR-ISM
CBM S.c.a.r.l.
University of Magna Græcia
University of Trieste
University of Florence
University of Padua
University of Genoa
University of Udine
INSTM
Centro di Riferimento Oncologico di Aviano
Istituto di Oncologia molecolare
Azienda Complesso Ospedaliero San Filippo Neri
PROTOS Research Institute
Fondazione IRCCS Ospedale Maggiore
Policlinico Mangiagalli e Regina Elena
ThunderNIL srl
EUROTECH

Istituto Officina dei Materiali

Main Collaborations

from NL– **THE NETHERLANDS**

Stichting Katholieke Universiteit
University of Twente
Twente Solid State Technology

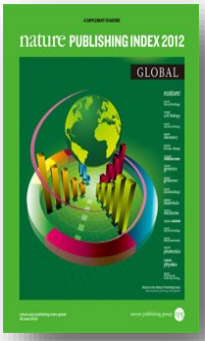
from UK– **UNITED KINGDOM**

University of Glasgow
Impattern Solutions
University of Glasgow
CSIC-CNM - Consejo Superior de Investigaciones Cientificas - Centro Nacional de Microelectronica
University of Strathclyde
University of Cambridge
Cambridge CMOS sensor
STFC - Science and Technology Facility Council

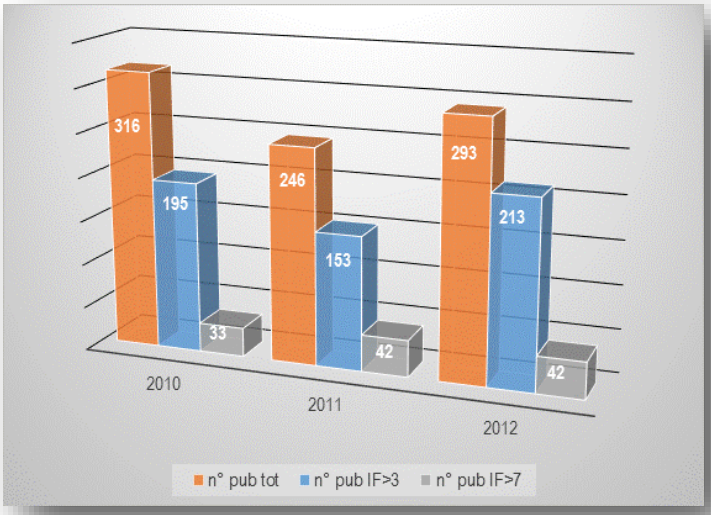
The IOM Insitute carried out several R**&D collaboration agreements** with the folloqing partnrs:

Publications

The results achieved in the period 2010-2012, covering a very broad spectrum of activity that produced 855 international publications, include 3 Nature Nanotechnology, 6 Nature Materials, 1 Nature Photonics, 1 Nature Chemistry, 2 Physics Reports and 2 Nature Physics.
The journals in which appears the most number of publications are Physical Review Letters (46), The Journal of Physical Chemistry C (49) and Physical Review B (170). 561 publications (65.6%) had IF greater than 3 and 117 (13.7%) had IF greater than 7.



As appeared on the Nature Publishing Index 2012, the only Italian institution present in the ranking of the 100 international institutions that have contributed the most in 2012 with publications in journals of the group of Nature was CNR. It placed at the 95th position of the ranking and among the CNR institutes that contributed to this result, IOM was the one that gave the highest score.



Main Events

Main Event

Istituto Officina dei Materiali

2010

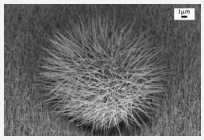
Trieste , 5-9 July

Workshop ICTP
Emergence of new states of matter in magnetic systems and beyond: frustrated magnets, topological insulators and cold atoms in optical lattices

Losinj, 23-27 August

10th ECSAC Conference on Sustainable Energy: Challenges and Opportunities

Roma, 4-5 November



5th Nanowire Growth Workshop NWG

Valencia, 6-10 September

25th EuPvSE Conference and Exhibition
Nanomodules and light trapping systems for high voltage organic

Trieste, 30 Sept.—01 Oct.

IOM Workshop

Berlin, 16-19 November

Psi_k Conference Symposium Catalysis from first principles: Energy conversion and storage

2011

Trieste , 13-15 January

15th Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

Trieste , 4-8 September

WIRMS: Workshop on Infrared Spectroscopy and Microscopy with Accelerator-Based Sources

Roma , 10-11 March

Workshop italiano sulla crescita di strati epitassiali e di nanostrutture di semiconduttori

Trieste , 4-29 July

Summer School on 'Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics

Trieste , 28 September

Nanomoduli fotovoltaici per celle solari organiche

Trieste Next

S.Giovanni in Valle Aurina (BZ), 25–30 June

Giornate didattiche SISN
Società Italiana di Spettroscopia Neutronica

Istituto Officina dei Materiali

Main Events

Trieste , 17-21 October

Workshop on New Materials for Renewable Energy

Saxa Rubra (RM) , 26 December

Rai 1 una MATTINA

Nanomoduli fotovoltaici per celle solari organiche

2012

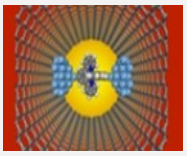
Lausanne, 23-25 April

CECAM Workshop Chemical and topological functionalization of graphitic surfaces: open challenges for computational modeling

Trieste, 23 January—3 February

Winter School on Quantum Monte Carlo Methods at Work for Novel Phases of Matter'

Parma, 20-22 June



Workshop SINFO Surfaces, INterfaces and Functionalization Processes in Organic Compounds and Applications

Trieste, 9-27 Julne

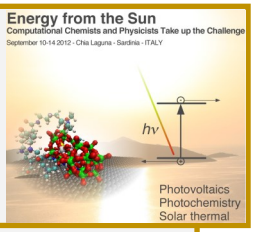
Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics

S. Margherita Ligure (GE), 3-7 September

Magnonics Conference

Chia Lugana (CA), 10-14 September

CECAM Conference Energy from the Sun: Computational Chemists and Physicists Take up the Challenge



Perugia, 23-26 September

International conference Frontiers in Water Biophysics

Trieste, 26-30 November

ICTP School on Numerical Methods for

Istituto Officina dei Materiali

Area Science Park - Basovizza
Ed.MM, Strada Statale 14 Km 163,5
I-34149 Trieste, Italy
www.iom.cnr.it