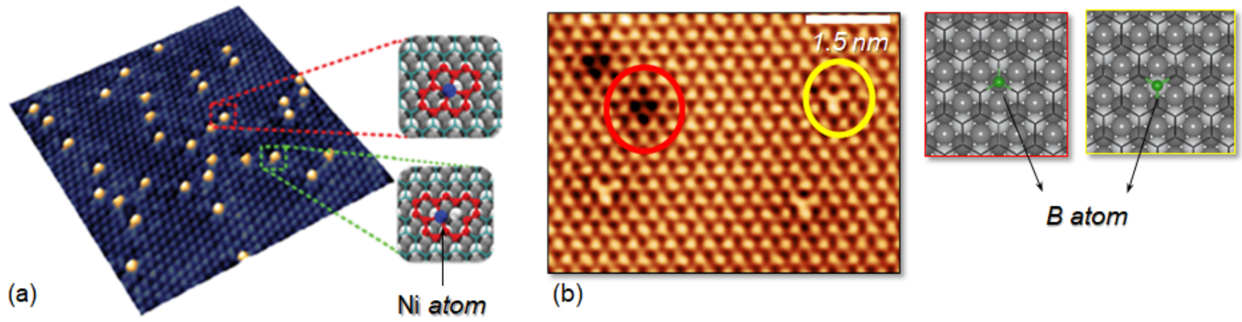
NOTE

Candidates applying for the scholarship 8 may carry out their activity in any of the research area active within the PhD program in Nanotechnology. These can be found here.

There are also specific research projects available for candidates applying for this scholarship. These are presented in the following pages.

Synthesis and characterization of functionalized 2D nanomaterials: an in-situ microscopy and spectroscopy study

Host Surface Structure and Reactivity at the Atomic Scale group, Istituto Officina dei Materiali of the Italian National Research Council, Trieste



STM images and models of graphene with substitutional Ni (a) and B (b) atoms.

The synthesis of stable tailored 2D nanostructured systems has become of paramount importance in catalysis, energy conversion and sensing applications. For instance, the functionalization of low dimensional materials, *i.e.*, through substitutional atoms or adatoms (see the figure), may result in an increased chemical reactivity, offering a valid alternative to conventional catalysts. Among the surface sensitive techniques, scanning tunneling microscopy (STM) has the potential to explore the structural and electronic properties of (functionalized) 2D nanostructured materials, offering real-space imaging with atomic scale resolution. When combined with photoemission spectroscopies, owning chemical and reciprocal space sensitivity, within the same (or a UHV-connected) experimental setup, a full in-situ material characterization is possible.

This project will focus on the synthesis of functionalized 2D nanostructured systems, and their characterization through STM and photoemission spectroscopies, providing proof of their enhanced physical and chemical properties. The experimental activity will be based on the expertise of the hosting research group. In particular, the project will rely on the complementarity between a "low temperature" and a "variable temperature" STM, LT- and VT-STM, respectively. In the study of the structural and electronic properties of the synthetized nanomaterials, as well as of their reactivity upon exposure to selected gases, LT-STM will allow cryogenic measurements, down to 4.2K, while VT-STM will complement the low temperature data with video-rate imaging, in realistic thermodynamic conditions, and in a temperature range up to 900 K. The use of XPS/UPS to characterize chemical properties, and LEEM/PEEM to access electronic structure and surface composition, will complement the microscopy data. Furthermore, the upgrade of the sample hosting plates and sample holders of both LT- and VT-STM will guarantee a full exchangeability of samples among LT-STM, VT-STM, XPS/UPS and LEEM/PEEM, preventing detrimental exposition of the material to the air.

The experimental results will be supported by ab-initio calculations performed through external collaborations. Beamtime application to external synchrotron radiation facilities will also be encouraged and supported.

The ideal PhD candidate is expected to have a Master degree in Physics, Chemistry or Materials Science, previous experience with vacuum technology and surface science techniques, high drive to solve challenges independently, attitude to work in an international research environment with collaboration spirit, and good English skills. Skills in scripting and analysis using programming languages as well as in the building/maintenance of experimental setups will be added values.

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Fiori S. et al. Carbon 11(20), 8887-8892 (2020) 10.1016/j.carbon.2020.09.056
Patera L.L. et al. Science, 359-6381:1243-1246 (2018) 10.1126/science.aan8782

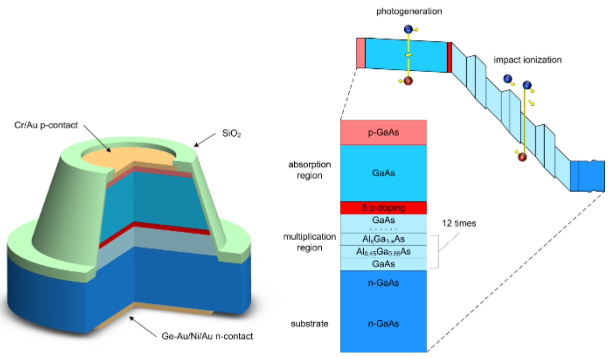
Supervisor	**Dr. Cristina Africh**	**africh@iom.cnr.it**
Co-Supervisor	*Dr. Cinzia Di Giorgio*	*digiorgio@iom.cnr.it*

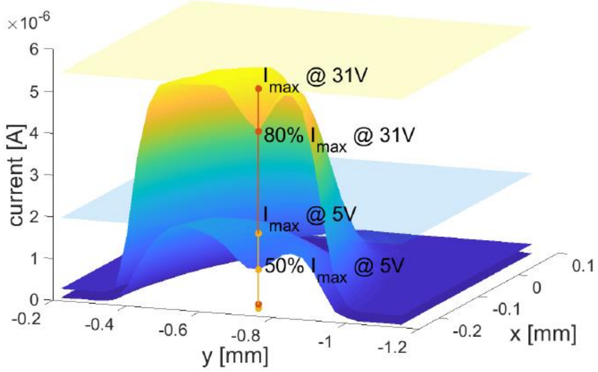
3D radiation detectors based on engineered quantum semiconductors

Dr. Giorgio Biasiol, Istituto Officina dei Materiali, Consiglio Nazionale delle Ricerche, AREA Science Park Basovizza, Trieste

The study of time-resolved ultrafast phenomena with radiation ranging from the infrared to the hard X-rays will be one of the research fields in frontier science in the coming years. Detectors are an indispensable element for any experiment with photon sources. Research in detectors is therefore continuously stimulated by increasingly stringent requirements, both on the source side and on the experimental needs one. Among the aspects that need to be improved are quantum efficiency, which is very poor for silicon-based detectors in the case of hard X-rays, and temporal resolution.

This project aims to develop single-photon detectors that cover frequencies ranging from the infrared to the hard X-rays with 3D (x-y-time) resolution. Avalanche photodiodes with separate absorption and multiplication regions (SAM-APD), based on III-As semiconductors, will be used (right) [1]. Thanks to the higher atomic number they are considerably more efficient and faster than silicon in absorbing hard X-rays and possibly pushing the temporal resolution in the range of 10 ps. The activity carried out so far has allowed the demonstration and optimization of prototypes of SAM-APD with state-of-the-art performance for absorption, response speed and signal-to-noise ratio (left) [2]. Starting from these results, the project aims to develop single-photon multiband detectors with unprecedented spatio-temporal resolution by improving the structures already made, and applying local functionalizations with ion beams and hard X-ray irradiation.





The involvement of research centers in the definition of the training path also in the context of broader collaborations with the University will be one of the strengths of this doctoral proposal, as detailed below. These collaborations will ensure that the PhD student can take advantage of qualified and specific operational and scientific structures for study and research activities.

Low-dimensional, band-engineered quantum structures will be synthesized by molecular beam epitaxy and lithographically fabricated by the student at CNR-IOM in Trieste. Spatial resolution at the sub-µm scale will be achieved by local functionalization by ion beam implantation through an electrostatic accelerator, which allows the localized alteration of the quantum mechanical properties of matter, at the Legnaro National Laboratories of INFN. A collaboration with Elettra-Sincrotrone Trieste and the University of Trieste, besides the development of measurement electronics, will allow the student to measure the device performance in terms of gain, noise and time response both with conventional and synchrotron radiation light sources. The activities will also be carried out in close collaboration with the Department of Engineering of the University of Udine, which will provide theoretical modeling of the devices. Finally, the student will benefit from a collaboration with the CNR-IOM LISA beamline at ESRF Grenoble, capable of generating bunches of beams lasting a few tens of ps and energies up to 90 keV (not reachable at Elettra).

References:

[1] J. Lauter et al 1995 NIMPR A 356 324, DOI: 10.1016/0168-9002(94)01237-7

[2] C. Nichetti et al 2020 JINST 15 C02013, DOI: 10.1088/1748-0221/15/02/C02013

NANOTECHNOLOGY PhD program @ UniTS

Exploring the *nano-bio interface* with SERS spectroscopy

Biofluids on metal nanostructures

Prof. Alois Bonifacio – abonifacio@units.it – https://orcid.org/0000-0002-2251-7786

A better understanding of the interaction between metal nanostructures, such as metal nanoparticles, and biological fluids (e.g. serum, urine, saliva) is a necessary step toward the **application of nanotechnology to biological systems**, and in particular to humans. **Gold and silver nanoparticles**, as well as other nanostructured surfaces, are promising for a variety of applications, from photo-thermal therapy to drug delivery, from drug monitoring to diagnostics, as antibacterial agents or as sensors. Many of these application require the direct contact between these nanomaterials and a biofluid, so that a better insight on how there nano-objects interact with these complex biological samples is crucial. While most studies on the "nano-bio interface" concerned the role of proteins, especially in the formation of an adsorbed layer ("protein corona") on gold and silver nanoparticles, the interaction of small-molecules, such as metabolites, with metal nanostructures ("non-protein corona") still needs to be studied. The reason of this delay has been the lack of experimental techniques able to investigate small molecules adsorbed on these metal surfaces in the context of chemically complex samples, such as biofluids. **Surface-Enhanced Raman Spectroscopy (SERS)** is an analytical technique capable of detecting the **vibrational spectra** of species adsorbed on nanostructured metal surfaces, and thus to identify adsorbed metabolites.

In this project between nanotechnology and photonics, candidates will use SERS to study the interaction of different biofluids, starting from model solutions of proteins and metabolites, with gold and silver nanoparticles and nanostructured surfaces. Besides SERS, other techniques will be used to characterize the nanostructures and the nano-bio interface, also in collaboration with other centers, such as electron microscopy (TEM, SEM), Dynamic Light Scattering (DLS), fluorescence, and FT-IR among others. Raman spectroscopy will be extensively used, also using Raman microscopes to get images. While studying the nano-bio interface, candidates will be also encouraged to explore and develop possible bioanalytical or clinical applications relying on their findings. Candidates will also have the chance to learn and apply advanced data analytics (including machine learning) to fully exploit the information present in their spectroscopic datasets.

KEYWORDS: metal nanoparticles, nanostructured metal surfaces, surface enhanced Raman scattering, SERS, metabolomics, nano-bio interface, bioanalytical spectroscopy

KEY PUBLICATIONS

Biomedical SERS–the current state and future trends, 2024, Chemical Society Reviews, 53, 8957-8979

Label-free surface-enhanced Raman spectroscopy of biofluids: fundamental aspects and diagnostic applications, 2015 Analytical and bioanalytical chemistry 407, 8265-8277

Direct comparison of different protocols to obtain surface enhanced Raman spectra of human serum, 2024, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 317, 124390

Project title: Thermodynamic non-equilibrium probes of cells metabolism

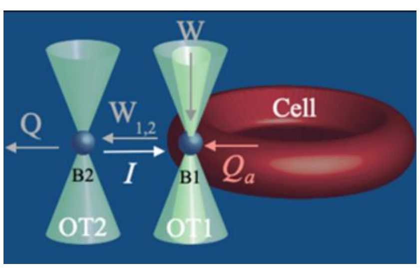
Supervisors: Dan Cojoc, (CNR-IOM cojoc@iom.cnr.it) and Edgar Roldan, (ICTP-QLS, edgar@ictp.it)

Cell metabolism is crucial for life because it's the set of chemical reactions that enable cells to obtain energy from nutrients and build the necessary structures for survival and reproduction. Dysregulation of metabolism is implicated in various diseases, including diabetes, cancer, and other metabolic disorders, therefore understanding how cellular metabolism is affected in disease states is crucial for developing new therapies.

Characterizing the thermodynamic properties intrinsic to life is among the central goals of current theoretical and experimental research in nonequilibrium statistical physics, active matter, nanotechnology and biophysics. Over the last decade, researchers have developed accurate numerical schemes to quantify nonequilibrium properties of small biological systems as living cells in several experiments, opening new avenues for applications of the emerging field of stochastic thermodynamics in a broad biological context. However, quantifying *in concert* heat, work and information fluxes in living cells is a research direction still to be explored.

Over the last few years, membrane fluctuations of living red blood cells (RBCs) have been established as a paradigmatic case study of nonequilibrium fluctuations in cells. Stochastic-thermodynamics concepts applied to optical-microscopy experiments have suggested that the entropy flow along the RBC membrane equatorial cell contour is spatially heterogeneous, with correlation lengths of about a micron. However, it remains unclear, for example, whether RBCs dissipate more heat around their central region (where the cell is more rigid and contains most of its hemoglobin) or around their peripheral region (where the membrane is more flexible).

In this project, we will combine optical tweezers microscopy **experiments** with stochastic thermodynamics **theory** by joining together the expertise of two leading groups in optical tweezers (Cojoc) and statistical thermodynamics (Roldan), both based in Trieste.



Schematic of a dual-trap (beads B1 B2) experiment which allows access to thermodynamic fluxes (heat Q, work W, information I) in the vicinity of a cell membrane, resulting from their nonequilibrium activity.

Key goals of the project:

(1) establish theoretical estimates for how the heat dissipation across RBC stochastic models depends on their local mechanical (e.g. friction) and chemical (e.g. active temperature) properties;

(2) perform dual-trap experiments with optically-trapped colloidal particles near the RBC membranes under different levels of activity (see Figure at the left);

(3) analyze the experimental data in the light of stochastic thermodynamics in order to access heat and information flows between the beads that are intrinsic to RBC's inhomogeneous activity;

(4) extend this approach to cancer cells characterization.

Smart therapeutic drug-delivery system
for neurological diseases

Supervisor: Prof. Tatiana Da Ros (daros@units.it)

Project highlights:

- Multidisciplinarity: research on the intersection of nanotechnology, chemistry and pharmaceutical technology, microelectronics, and biomedical engineering
- Focus on innovation: find scientific solutions to the most urgent challenges in neurology
- Collaboration: with academic and business partners (INSTM, UNIMORE, SISSA, Future Needs, SINDREL Medtech s.r.l)

Motivation:

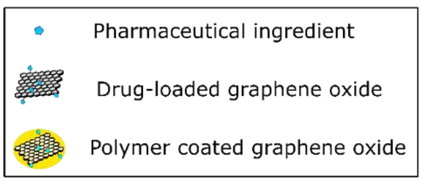
We aim to deliver innovative solutions for urgent neurological conditions affecting millions worldwide, including status epilepticus, seizure clusters, and Sudden Unexpected Nocturnal Death in Epilepsy (SUDEP). Currently, no effective treatment fully meets the needs of patients with drug-resistant epilepsy. Our goal is to address this gap by developing a smart medical device with controlled drug release.

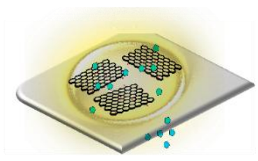
Project scope:

The goal of the current PhD Fellowship is to develop an effective drug-delivery system based on molecular (including drugs) and nanomaterial components to meet the needs of patients suffering from neurological diseases.

To achieve this aim, the candidate will synthesize functionalized carbon-based nanomaterials and characterize them using spectroscopic and microscopic methods. In particular, the candidate will gain knowledge of interactions between the drugs and nanomaterials and get practical experience on Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), UV-vis and fluorescence spectroscopy, Raman spectroscopy, Thermal Gravimetric Analysis (TGA) and Dynamic Light Scattering (DLS), among others.

During different stages of the project, the candidate will closely collaborate with scientific research teams with expertise in animal testing and bioengineering manufacturing to succeed in smart device fabrication.





Drug release

Patent "Graphene-based drug delivery device for mucosal and transmucosal administration" (PCT/EP2023/056424)

References:

*M. Ochoa-Urrea et.al Seizure Clusters, Seizure Severity Markers, and SUDEP Risk. Front. Neurol (**2021**) 12:643916*

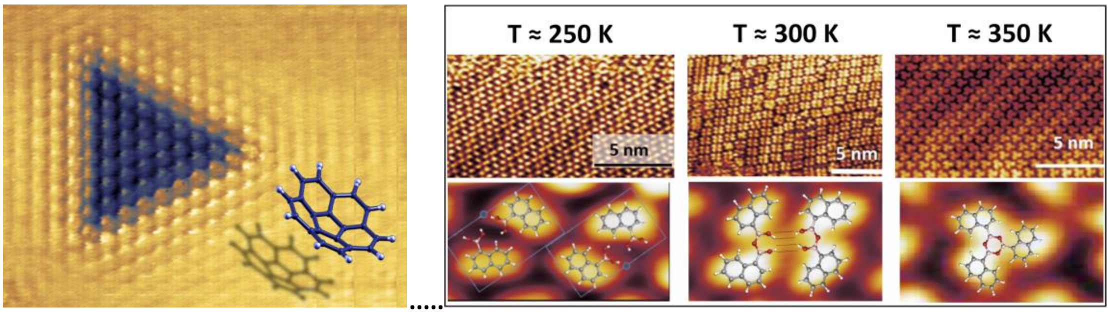
ON-SURFACE MODIFICATION OF ORGANIC SEMICONDUCTORS
(OSMOS)

Study of the synthesis and modification of molecules on metals and metal oxides in UHV environment with the aim of improving the charge transport properties at the interface and/or enhancing the catalytic properties of the reaction products. The research activity is performed at Sincrotrone-Elettra in the OSMOS lab and ALOISA (https://www.elettra.eu/elettra-beamlines/aloisa.html) beamline.

RESEARCH LINES

RL1: Morphological and structural characterization of self assembled layers of organic molecules, namely polyconjugated and heteroaromatic compounds (oligomers, polyacenes, perylenes, porphyrins and their derivatives). Study of the charge transfer and molecular bonding to the substrate, the on-surface molecular modifications, as well as the chemical interactions and linking in hetero-molecular systems, both in 2D and 2D+1 architectures.

RL2: Synthesis of 2D frameworks on surfaces, using small molecular precursors, aimed at modifying the chemical and morphological properties of the substrate. The main goal is to build 2D templates with specific chemical properties, able to selectively anchor guest species via molecular recognition.



LEFT: bowl-shaped corannulene molecules are trapped inside an artificially created triangular hole (8 nm side) on Ag(111); the fading intensity of the molecules on the upper terrace originates from the decrease of residence time due to molecular mobility. RIGHT: the pathway to 2D boronic condensation on Au(111) of naphtalene boronic acid through intermediate precursor stages: paired monomers at 250 K, partially condensed paired dimers at 300 K, and fully condensed trimers at 350 K.

EQUIPMENT

- The OSMOS laboratory for microscopy (joint project between CNR-IOM and Sincrotrone-Elettra) is composed of three interconnected experimental chambers, including i) variable temperature STM chamber (SPECS Aahrus), ii) sample preparation chamber equipped with LEED and quartz microbalance, iii) X-ray spectroscopy chamber equipped with an Al/Mg X-ray source PSP Tx-400 and a monochromatized Gamma Data VUV 5k source (He I, II), which are coupled to a Scienta R3000 (150mm) electron spectrometer with CCD detector, and a closed-circuit liquid He cryostat (11 K on sample) for in-situ XPS and angle-resolved UPS analysis.
- The project takes advantage of direct access to the Synchrotron beamline ALOISA (responsible Luca Floreano) for performing high resolution fast-photoemission, resonant photoemission and X-ray absorption spectroscopy (NEXAFS) at variable scattering and polarization geometries.

CONTACTS

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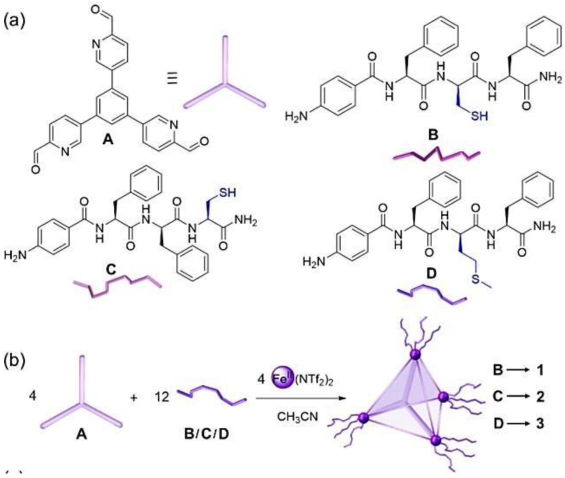
PEPTIDES FOR FUNCTIONAL SUPRAMOLECULAR NANOSTRUCTURES

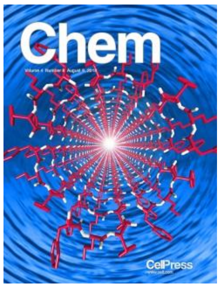
Supervisor: Prof. S. Marchesan email: smarchesan@units.it www.marchesan-lab.com

Our research group's expertise lies at the interface between supramolecular chemistry and nanotechnology, pertaining the organization and bioactivity of simple peptides and their assemblies, through the modulation of their intra- and inter-molecular interactions. These biomolecules are green building blocks that do not persist in the environment and can exert various functions for diverse green uses. They can mimic biological structures, such as the extracellular matrix, encode messages to deliver to cells, to guide them towards adhesion or differentiation for regenerative medicine and wound healing. Their assemblies can mimic enzymes, whereby catalytic functions are protected within pockets, and can be switched on/off with assembly/disassembly cycles. For example, they were designed for organo-, photo-, or bio-catalysis. Alternatively, self-assembling peptides have been designed to yield hydrogels for targeted drug delivery, also through the use of responsive linkers for cancer therapy. Thanks to the understanding of their interactions, short peptides were developed also for cosmetics and anti-age, to stabilize biotherapeutics such as insulin, or to inhibit amyloid fibrillation relevant to neurodegeneration. Finally, they proved to be excellent dispersants of poorly soluble nanomaterials, such as carbon nanotubes, to yield functional nanocomposites that could find use in the regeneration of conductive tissues (*e.g.*, heart and nerve tissues), or cancer diagnostics.



Recent studies focus on more complex systems with internal cavities to guide molecular guests, entrap them or release them as needed. On one hand, short peptides have been embedded in metal-organic cages that were applied to remove pollutants through the use of peptide functionalities. Cages have also been designed to bear opposite charge and form a salt that yields a porous ionic liquid, where different guests can be entrapped within the different cages. This research line is in collaboration with Prof. Nitschke at the University of Cambridge and is exploring the synergy between assembling peptides and cages to control supramolecular organization all the way to macroscopic, yet nanostructured, smart materials.

On the other hand, we are mapping the sequence space of heterochiral dipeptides and tripeptides to produce peptide nanotubes, with tunable diameter (form 0.4 nm to 22 nm) and surface properties, thanks to a combination of approaches, including out-of-equilibrium and dynamic covalent chemistries. These nanotubes can find diverse applications, such as smart antimicrobials, channels for selective transport across cell membranes, and many more thanks to their peculiar physico-chemical properties, electronic properties, and responsive behavior.



The PhD candidate will be offered a highly multidisciplinary environment, a modern office space, training also on cutting-edge techniques and advanced characterization methods through collaborations with the nearby Elettra synchrotron, and the possibility to enjoy international collaborations and periods abroad. We ask for commitment and passion for research, an open mind, good team-working skills, care for equipment and shared spaces. A positive attitude is very welcome and encouraged. Interested candidates are encouraged to email Prof. Marchesan.

Selected References: S. Adorinni, *et al. Chem. Sci.* **2026**, doi:10.1039/D5SC08607H. M. Li , *et al. Angew. Chem. Int. Ed.* **2024**, *63*, e202406909. S. Marchesan, *Nature* **2024**, *630*, 308. S. Adorinni, *et al. ACS Nano* **2024**, *18*, 3011. O. Bellotto, *et al. J. Mater. Chem. B* **2023**, 11, 5378. I. Jahovic, *et al. Matter* **2021**, *4*, 2123. A. M. Garcia, *et al. ACS Nano* **2021**, *15*, 3015. S. Piovesana, *et al. Nano Res.* **2020**, 13, 380. D. Iglesias, *et al. ACS Nano* **2018**, *12*, 5530. A. M. Garcia, *et al. Chem* **2018**, *4*, 1862. S. Marchesan, *et al. Science* **2017**, 356, 10109.

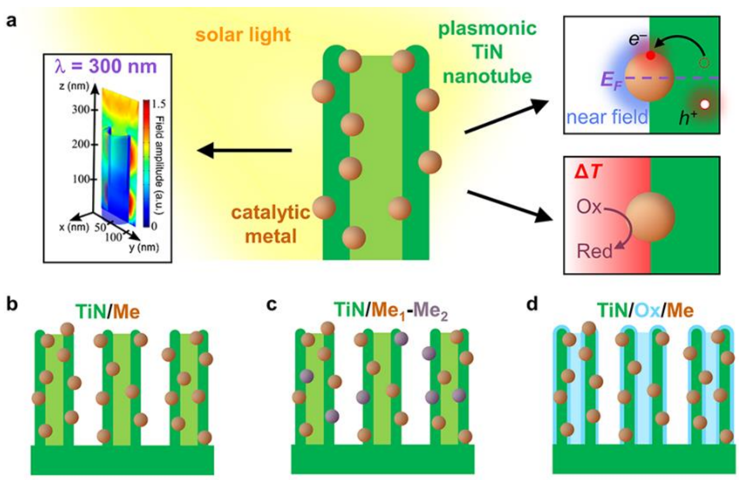
Photothermal heterogenous catalysts for energy-related applications

Supervisor: Prof. Tiziano Montini (University of Trieste), tmontini@untis.it

Co-supervisor: Prof. Paolo Fornasiero (University of Trieste), Prof. Alberto Naldoni (University of Turin).

Concentrated solar power (CSP) enables storing energy in high-temperature heat, which later can be converted to electricity. While such technology is already commercially available, a similar architecture has been explored to produce fuels (such as CO, CH_4 or H_2) using thermochemical pathways. Recent studies have demonstrated the generation of fuels or chemicals under moderate concentration regimes by exploiting catalysts including plasmonic nanoparticles. The latter can significantly alter the reaction mechanisms and, therefore, product selectivity by means of non-thermal plasmonic effects, which occur simultaneously with purely thermal ones, making sustainable an energy-demanding production process.

In this project, TiN plasmonic nanostructures will be decorated with metal nanoparticles by sputtering or wet impregnation. Both monometallic or bimetallic systems will be investigated, to investigate the role of metal-metal interaction on the catalytic activity. For specific applications, TiN plasmonic materials will be covered with an oxidic layer by ALD before metal nanoparticles deposition (i.e. Al_2O_3 as inert layer to discriminate thermal and electronic activation of the catalytic metal nanoparticles; CeO_2 or Fe_2O_3 as redox promoter in the formulation of the photocatalysts). The obtained materials will be employed as heterogeneous catalysts in reactions relevant for sustainable energy production: CO_2 reduction to CO or CH_4 and H_2 production from alcohol reforming (methanol or ethanol). The nanostructure of the active photocatalysts will be investigated in detail by means of state-of-the-art techniques offered by the modern nanotechnology, such as electron microscopy (SEM, TEM), spectroscopy (XPS, XANES/EXAFS, FT-IR) and diffraction (gracing incidence XRD).



Research Topic: Charge transfer process in complex interfaces

Supervision:

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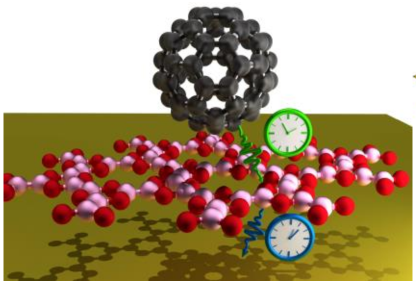
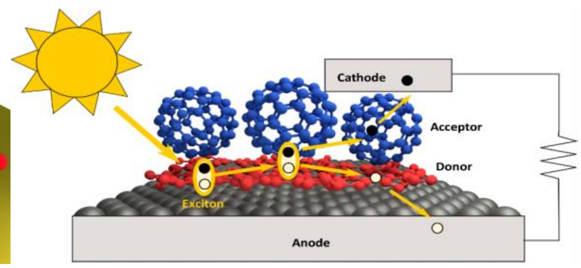
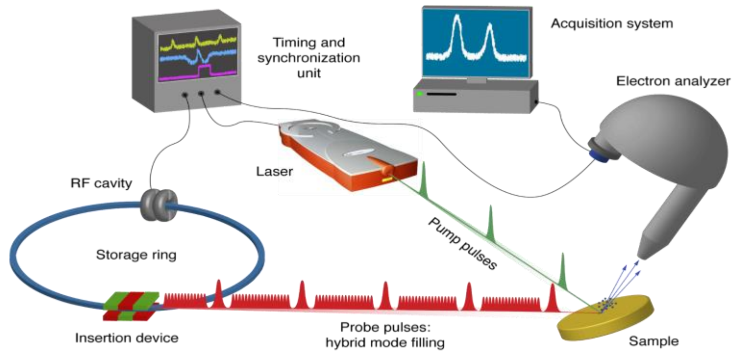
Martina Dell'Angela (CNR-IOM Laboratorio TASC) e-mail: dellangela@iom.cnr.it
Alberto Morgante (Physics Department, University of Trieste, and CNR-IOM Laboratorio TASC), e-mail:amorgante@units.it





There is a dramatic raise in the scientific and technological interest for new complex 2D materials that extend substantially the graphene family (2D dichalcogenides, phosphorene, hexagonal boron nitride hBN etc), their combination in stacked heterostructures, 2D Covalent Organic Frameworks (COF) and more complex hybrid materials that incorporate also organic molecules. In devices based on these materials, interface processes are ubiquitous and critical for the efficiency much more than when traditional materials are employed. Furthermore the interposition of a 2D templating architecture between electrodes and the organic layers represents a powerful tool for the improvement of the overall device performances. Therefore, there is an increasing interest in the synthesis and characterization of possible 2D templates able to tailor the electronic properties of complex Metal/Template/Organic (MTO) architectures. Possible templates we are interested in range from functionalized 2D materials, to Covalent Organic Frameworks, to self-assembled monolayers of organic molecules. Major efforts have been made in last years to study the morphology of these systems, while their electronic properties are in most cases only partially described. There is a need therefore for a deeper understanding and control of processes like charge transfer at interfaces between the different components in complex materials and in MTO architectures. Charge injection across molecular junctions can occur at the femto- to nanosecond time scales. We combine different time resolved spectroscopic techniques (pump-probe spectroscopy using femto laser or Free Electron Lasers, X-ray Resonant Photoemission spectroscopy) to investigate the electronic properties in MTO hetero-structures, revealing the charge dynamics in both directions (to/from the molecule) at these complex interfaces.
The research program is part of the recently financed project MIUR PRIN: FERMAT Fast ElectRon dynamics in novel hybrid organic-2D MATerials and will be carried out in collaboration with various international research groups based in USA (Columbia University), Slovenia etc.
The student will have access to newly installed experimental apparatuses for Time resolved spectroscopies and Synchrotron radiation experiments.



Timing and
synchronization
unit
Acquisition system
Electron analyzer
Laser
RF cavity
Storage ring
Pump pulses
Insertion device
Probe pulses:
hybrid mode filling
Sample

DYNAMICS NANOMATERIALS WITH FUNCTIONAL PROPERTIES

Supervisor: Paola Posocco (University of Trieste)

The research activity will focus on studying self-assembling dynamic nanomaterials in equilibrium and out-of-equilibrium conditions to understand key molecular factors, forces and properties that control self-assembly, structure, reaction, adaptability, and recognition properties. Two main classes will be investigated by computational techniques and machine-learning approaches: peptide-based systems and organo-modified metal nanoparticles. Via the integration of classical atomistic and coarse-grained molecular simulations, advanced molecular simulation methodologies and data-driven models, the candidate will explore structure, dynamic and functional behavior of these fascinating nanomaterials on a wide spatio-temporal scale. The activity will be carried out in collaboration with national and international experimental groups. The research project can be adapted and tailored based on the candidate developing skills, interests, and the results achieved throughout the course of the research.

The ideal candidate has a Master Degree in Chemistry, Physics or Materials Science. Basic experience with common molecular simulation packages (e.g. LAMMPS, GROMACS, AMBER) is required, along with reasonable programming skills (Python or Fortran). Strong motivation and enthusiasm for research, good attitude to work in team, good written and spoken English is also an asset.

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