

Theory of Condensed Matter Physics – Computational Methodologies

The Group



Website



Research lines

- Ground state properties (geometry, phonons.....)
- Excited state properties:
 - electronic band structures
 - optical properties
 - excitons
 - chiroptical spectroscopies
 - magnetic properties
- Plasmonics and Molecular Plasmonics

ab initio: DFT, PostDFT, PostHF

Multiscale QM/classical

The Projects



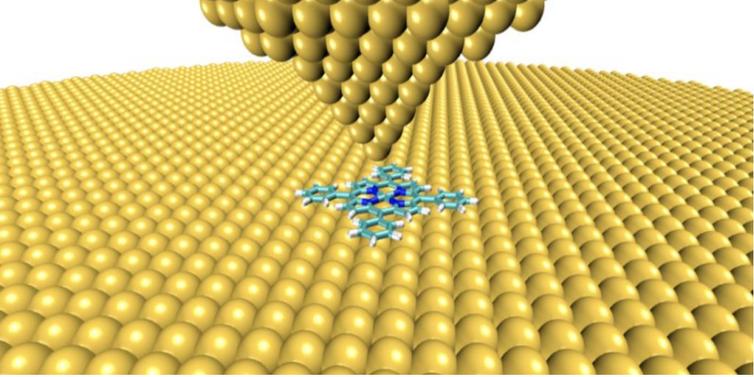
PRIN 2022 IRIDE

PRIN2022 HEROS

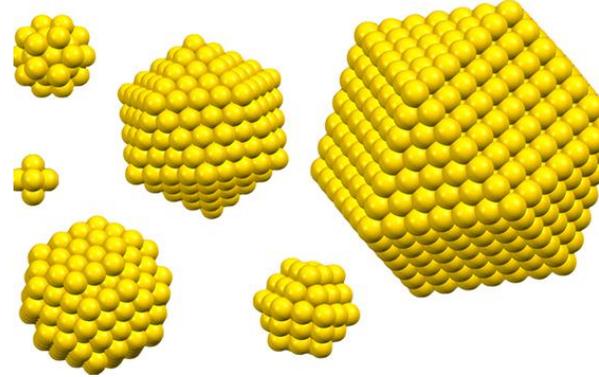


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UNIVERSITÀ DEGLI STUDI DI ROMA

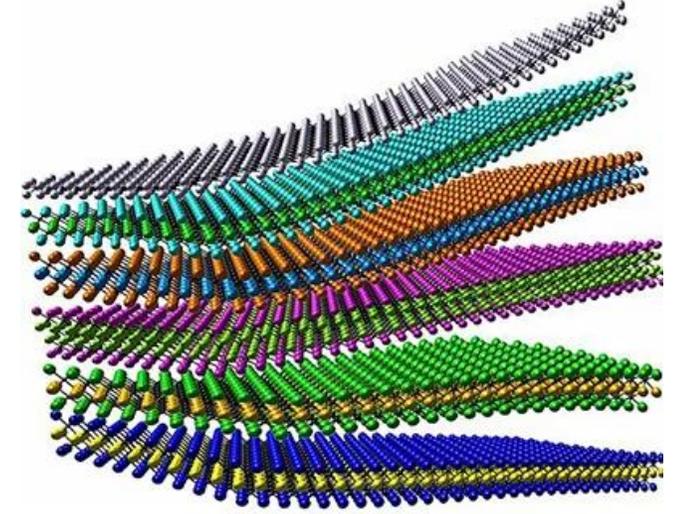
Light-Matter Interaction in Complex Systems



**0D Materials:
Molecules, Clusters, Nanoparticles**

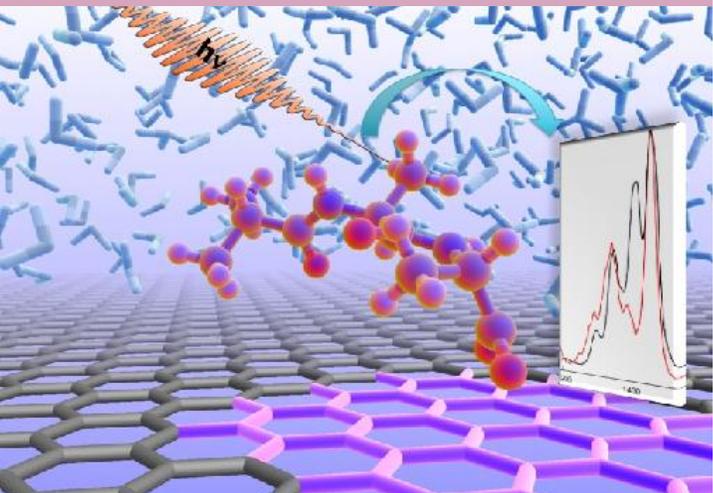


**2D Materials:
Graphene, XEnes, TMD and beyond**

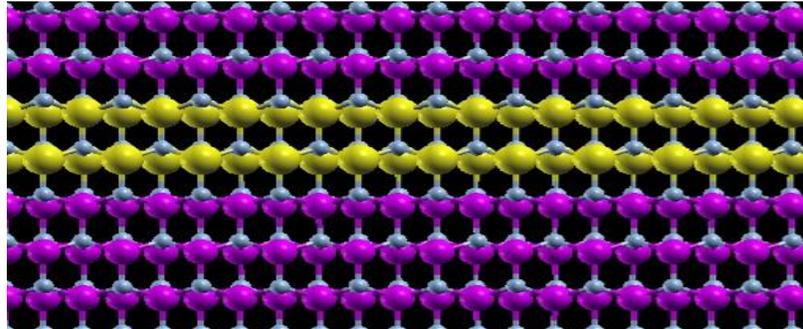
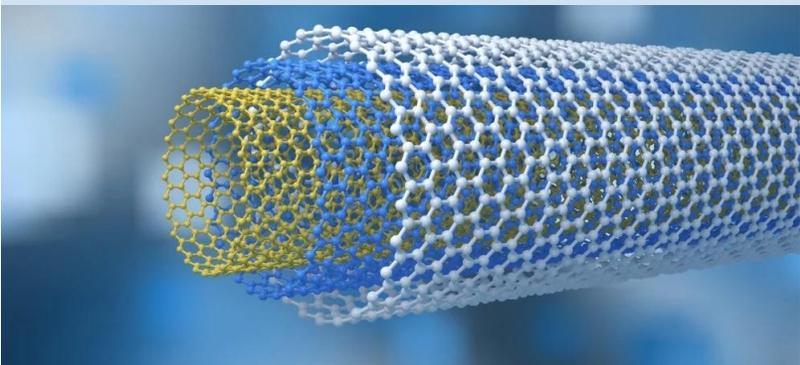


Computational Research of New Materials and Modeling of Complex Systems

**Soft Matter
Water, Organic, and Biological Systems**



**1D Materials:
Wires, Tubes, ...**



**3D Materials:
Crystals and Interfaces for Optoelectronic**

Nonequilibrium Theory and Simulations of Many-Body Quantum Systems

Group (from right): Enrico Perfetto, Gianluca Stefanucci, Alessandro Moreci (PhD),

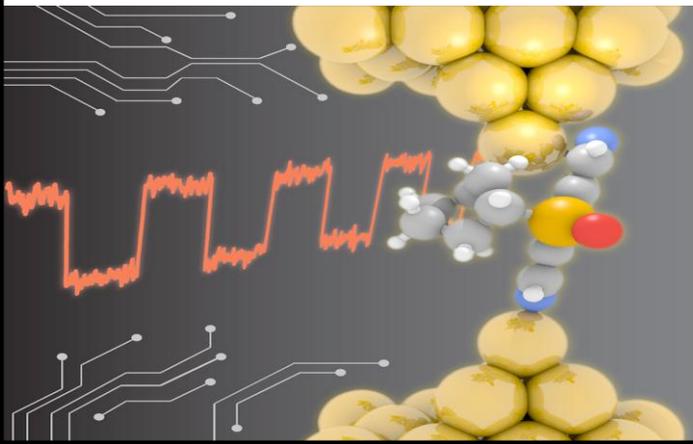
Carlos Bentacur (PhD), Zhenlin Zhang (visiting Phd), Kai Wu (PostDoc student)

Collaborations



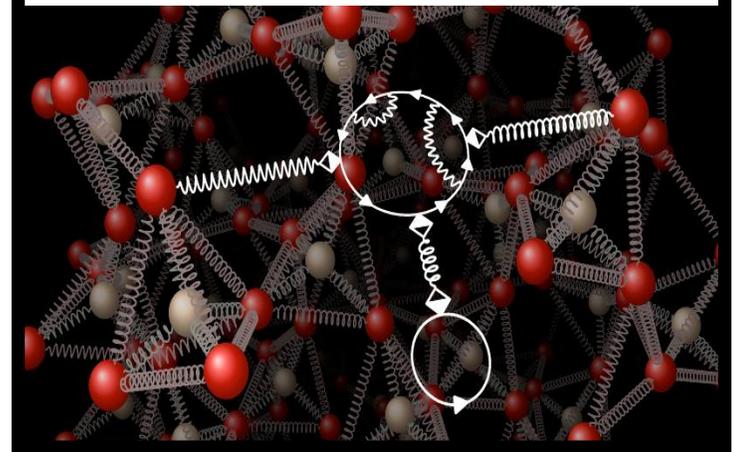
Nonequilibrium Theory and Simulations of Many-Body Quantum Systems

Molecular Electronics

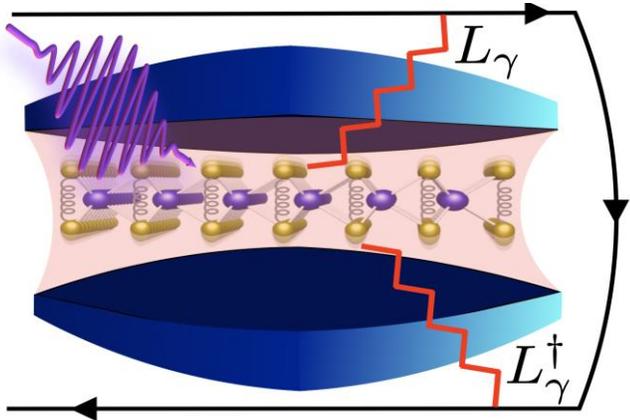


$$i\hbar \frac{d}{dt} \Psi = H \Psi$$

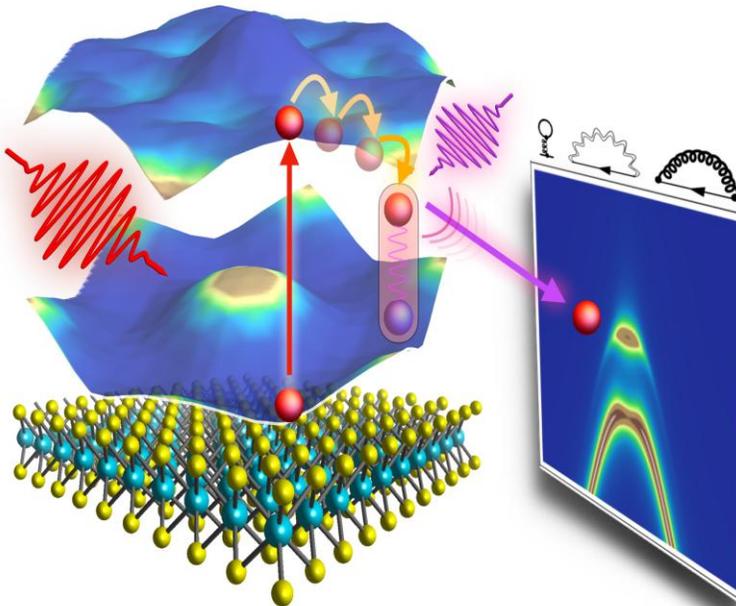
Nonequilibrium phonons



Dissipative Quantum Systems



Dynamics of Carriers and Excitons



Research on ultrafast quantum particles and their mutual interactions

Many-Body Theory Group

Contacts

Prof. Gianluca Stefanucci

Prof. Enrico Perfetto



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Nanomaterials for Photonics lab

Prof. Matteo Salvato

Prof. Paola Castrucci

Filippo Pierucci PhD Student

Riccardo Ciciotti Master Degree Student

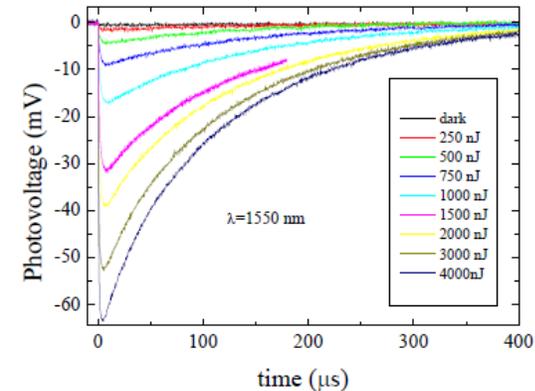
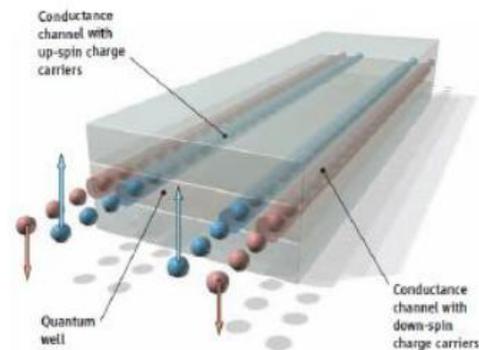
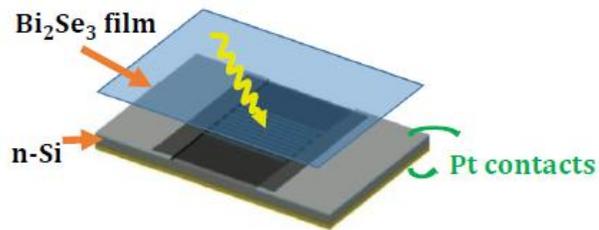
Elettra Meini Bachelor Degree Student



Research Activity

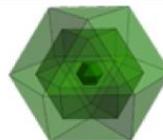
Physical and chemical vapour deposition growth and characterization of thin films and nanostructures of topological insulators

Investigation of heterojunctions based on topological insulators for Vis and IR photodetection



The Projects

- Regione Lazio, FOTONICS (2021-2023) – INFN, QUANTEP (2021-2023) - PRIN 2022 PNRR, SPIGA (2023-2025)
- University Project, ISTRICE (2022-2024), University Project – TESLA (2022-2024)

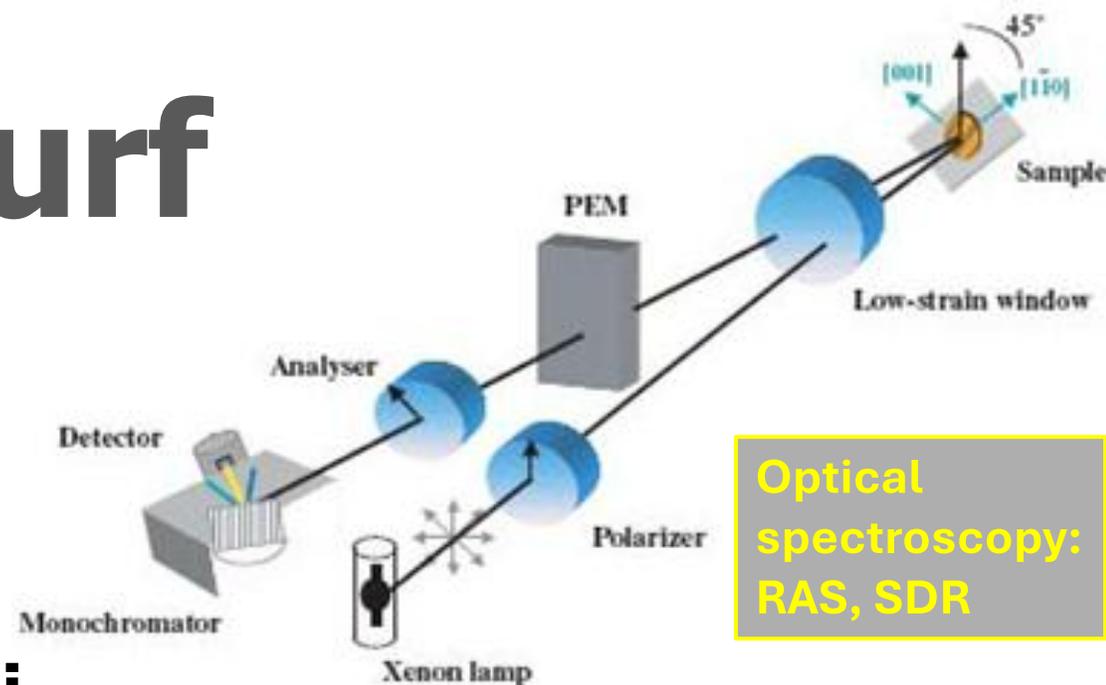


Nano@Surf



LT XPS Prebiotic Lab

Anna Sgarlata
Massimo Fanfoni
Beatrice Bonanni
Claudio Goletti
Ilaria Tomei
Valeria Battistelli
Raj Samnani



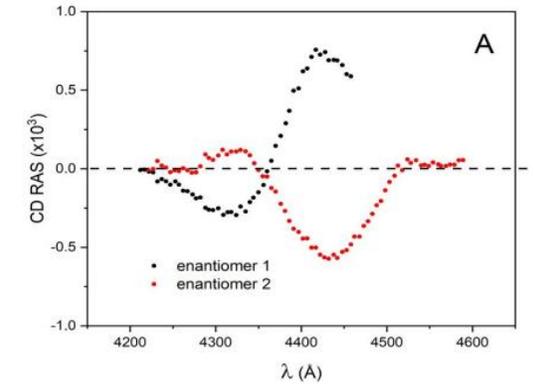
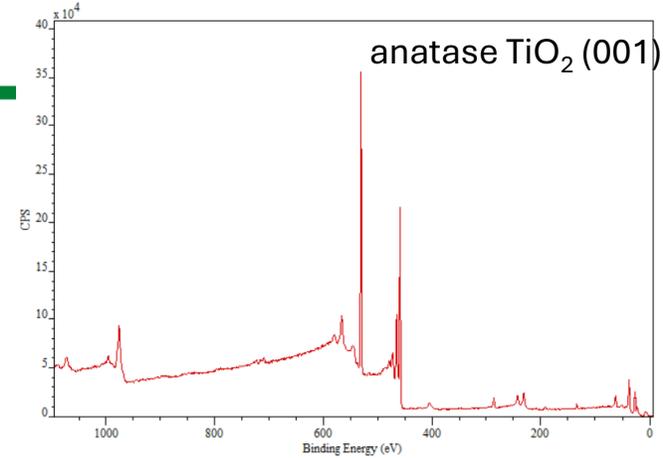
Optical spectroscopy:
RAS, SDR



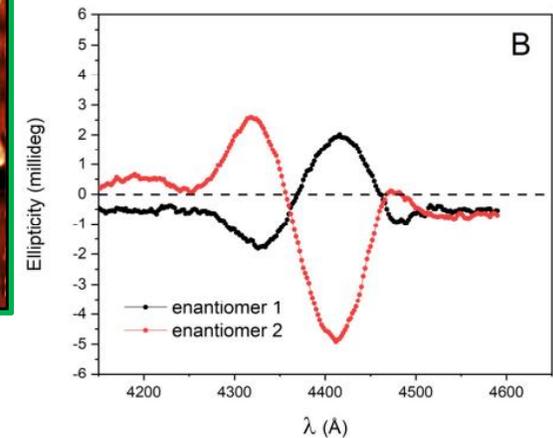
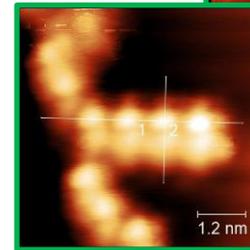
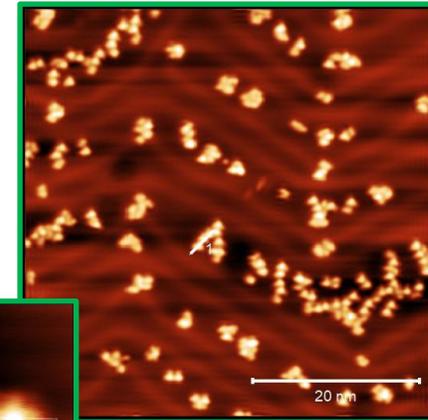
UHV STM

Research activities

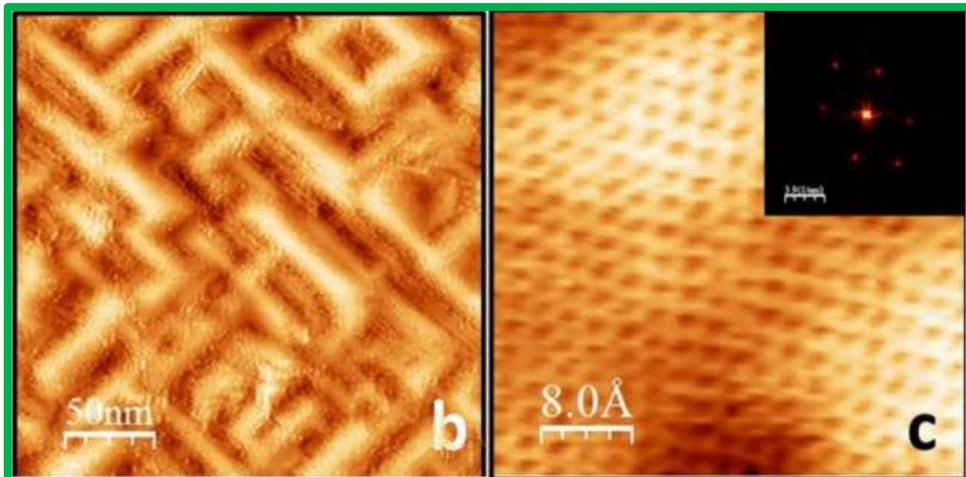
- **XPS** study of **prebiotic conditions** for the formation of peptide bonds in early Earth rocks or interstellar dust (**STILES project**)



- **Molecular films of porphyrins and/or corroles** for **sensing** applications. Study by **STM** and by **chiral symmetry-sensitive optical techniques (RAS and SDR)** (**GREEN project**)



- **2D materials**: growth and morphological and spectroscopic characterization with atomic resolution of **Graphene/Ge, Borophene, GeAs, ZrSe₂** (**HYBORON project**)



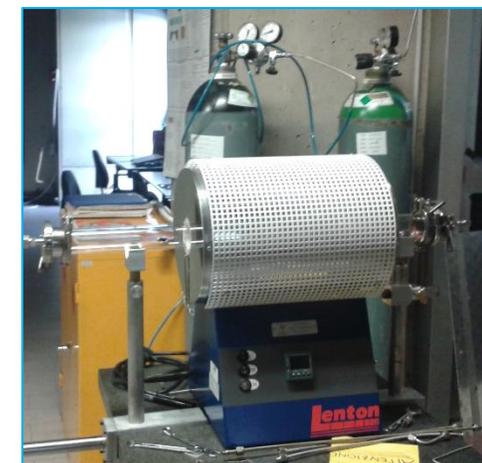


LowDLab

Prof. Manuela Scarselli
Dipartimento di Fisica



- Ultra high vacuum system equipped with
- scanning tunneling microscope (STM)
 - atomic force microscope (AFM)
 - x-ray photoelectron spectroscopy
 - low energy electron diffraction (LEED)
 - triple e-beam evaporator
 - e-gun

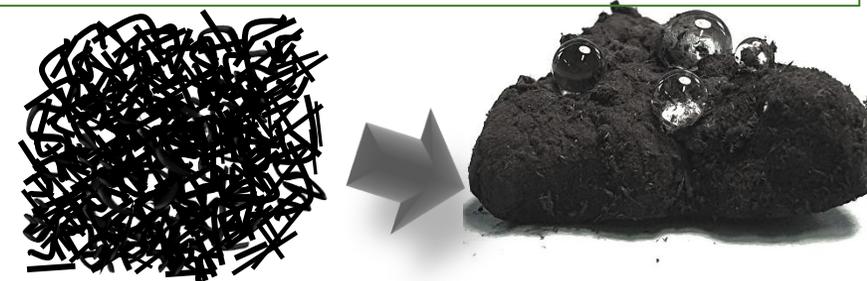


High vacuum system for thin film deposition on substrates

- 4 evaporators
- gas-line
- sample heater

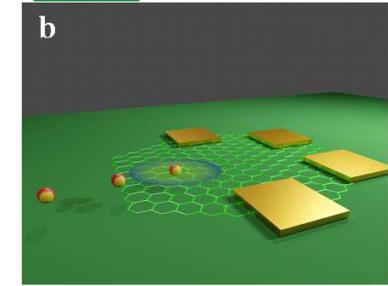
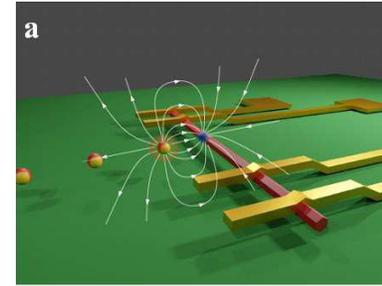


A system for the chemical vapor deposition growth of carbon nanostructures: carbon nanotubes (CNT) films or sponges, spheres

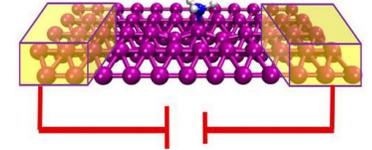


Funded projects:

Multidimensional nanodevice architectures For Low-perturbation Singlet Detection (INFN-MANIFOLD)



Metal clusters decoration of Borophene nanostructures with enhanced Hydrogen adsorption and release properties (PRIN 2022 - HYBORON)



Collaborations:

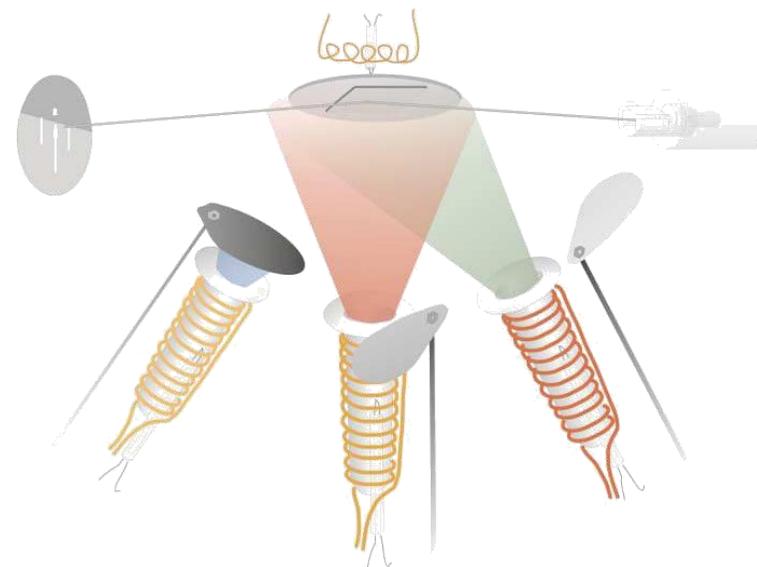
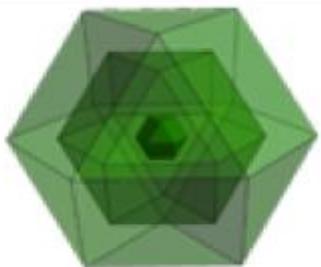
- INTEL: Synthesis and applications of Transition Metal Dichalcogenides (& prof. L. Camilli)
- Prof. Arduini, Dip. Scienze e Tecnologie Chimiche Tor Vergata => CNT sponges for water purification from heavy metals
- Prof. Gunnella, Dip. Fisica, Università di Camerino => Metal cluster for Borophene nanostructures for hydrogen storage
- Prof. Rosolen, Uni. Sao Paulo, Brazil => Development of electrochemical sensor with carbon nanomaterials



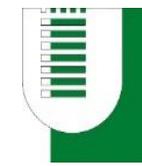
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Molecular beam epitaxy and electron spectroscopy lab

Prof. Fabrizio Arciprete
Dr Sabrina Calvi
Dr. Simone Prili
Dr. Adriano Diaz Fattorini
Dr. Christian Petrucci



Research activities

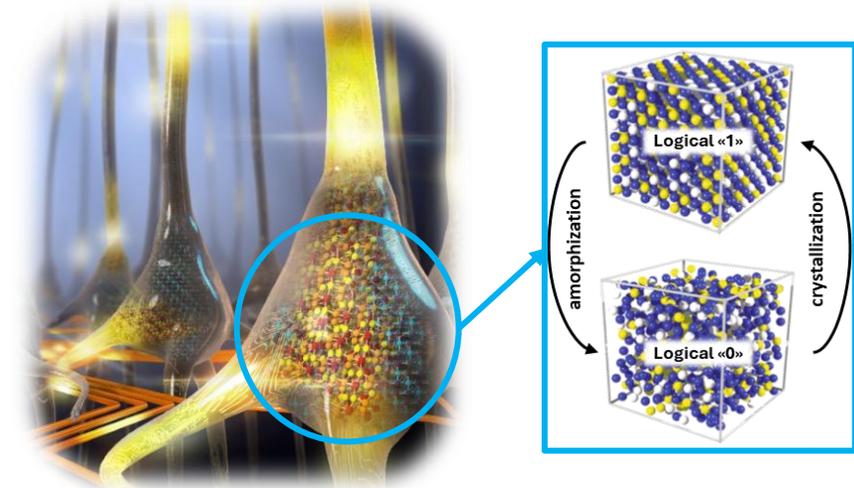


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Main activities:

Phase-change materials and heterostructures for memory and artificial intelligence applications:

- ❑ Growth via molecular beam epitaxy (MBE)
 - Ge-Sb-Te based alloys
 - 2D Materials with transition metals (Ti, Mo, W)
- ❑ Morphological, structural and electronic characterization
 - Atomic Force Microscopy (AFM)
 - Photoemission spectroscopies (XPS and UPS)
 - X-ray diffraction and Raman spectroscopy



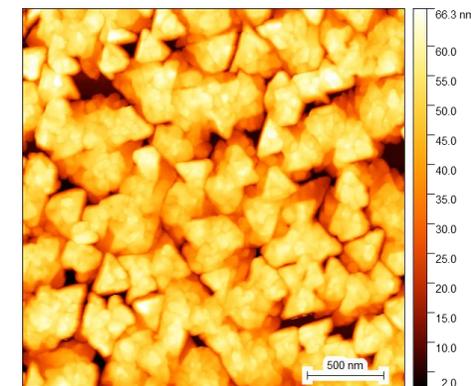
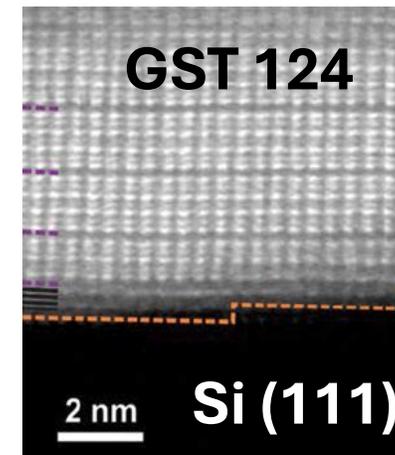
Funded projects:

- Horizon 2020 «BeforeHand»
- PRIN2020 «EMPHASIS»



Collaborations:

- CNR-IMM ARTOV
- IBM
- ST Microelectronics
- Sapienza Università di Roma





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Low-Temperature Microscopy and Spectroscopy lab

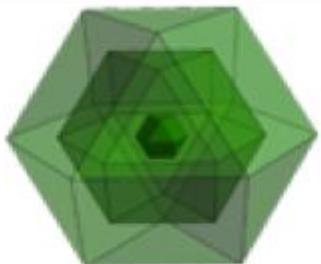
<https://www.camillilab.com/>

Prof. Luca Camilli

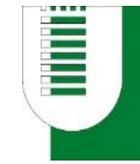
Prof. Luca Persichetti

PhD candidate: Antonio Caporale

PhD candidate: Gabriele Anselmi



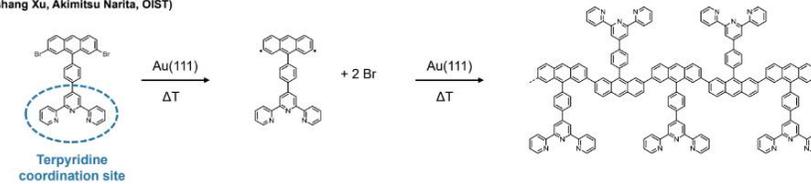
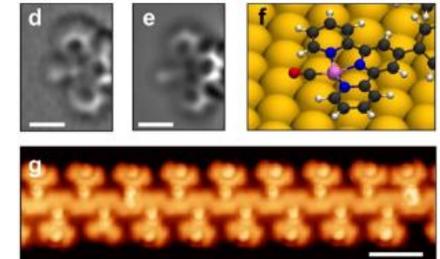
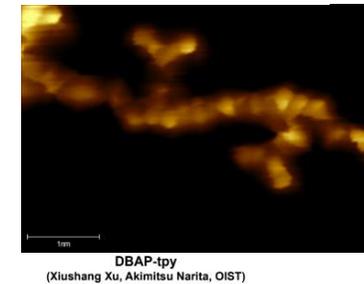
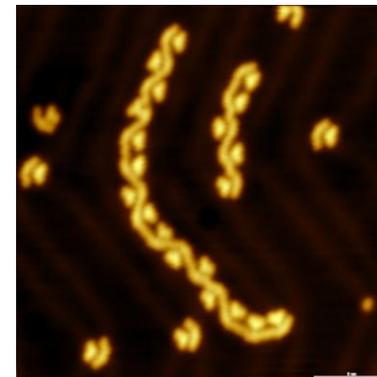
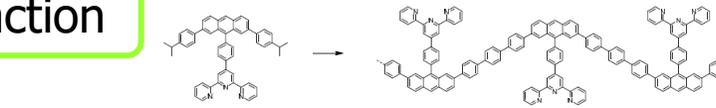
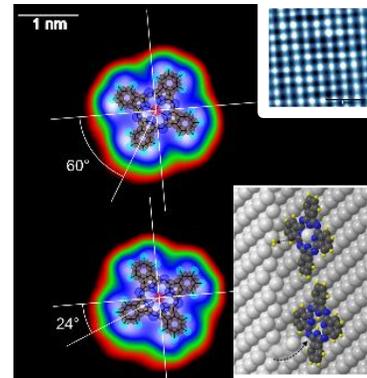
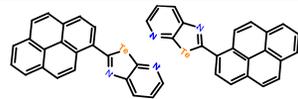
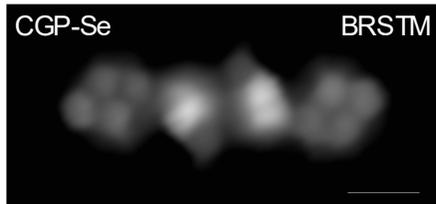
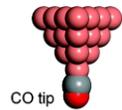
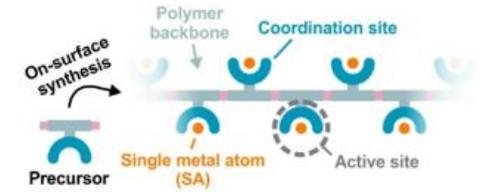
Research activities



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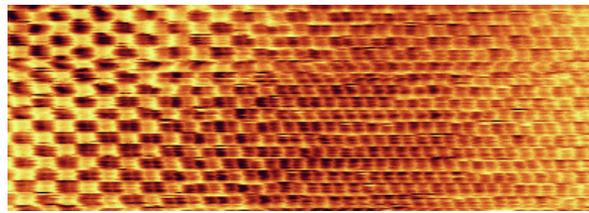
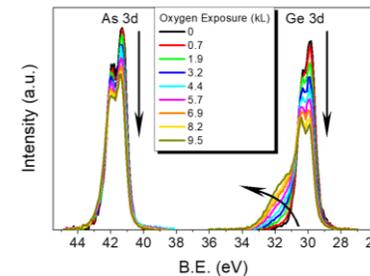
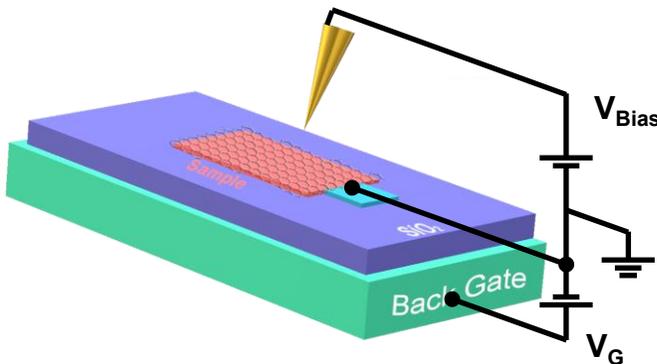
On-surface synthesis towards single metal atom platforms **PRIN 2020 Atypical**

On-surface molecular recognition via non-covalent interaction



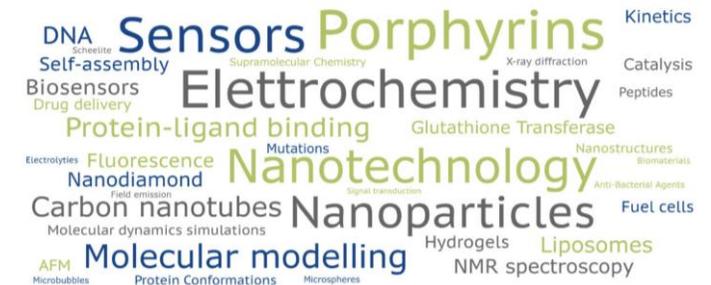
Chemical stability of 2D materials

STM on gate-tunable samples



Synthesis and characterization of topological insulators and 2D materials beyond graphene **PRIN 2022 PNRR Spiga & University grant SSITI**

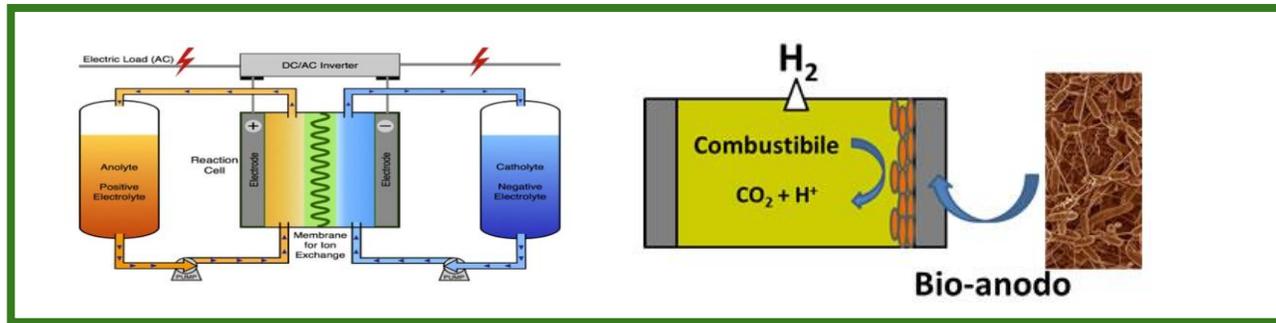
Department of Chemical Science and Technologies



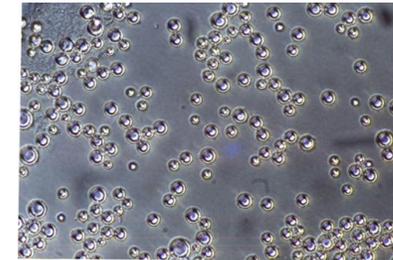
Research Activity

The Department of Chemical Science and Technologies has been selected as one of the 11 best Chemistry Departments in Italy.

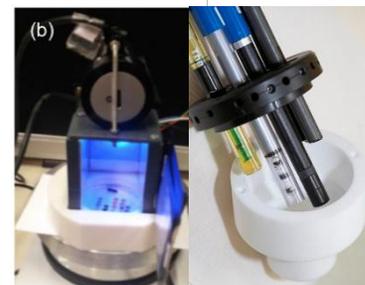
The X-Chem project involves the strengthening of three main lines of research:



Energy transition



Health

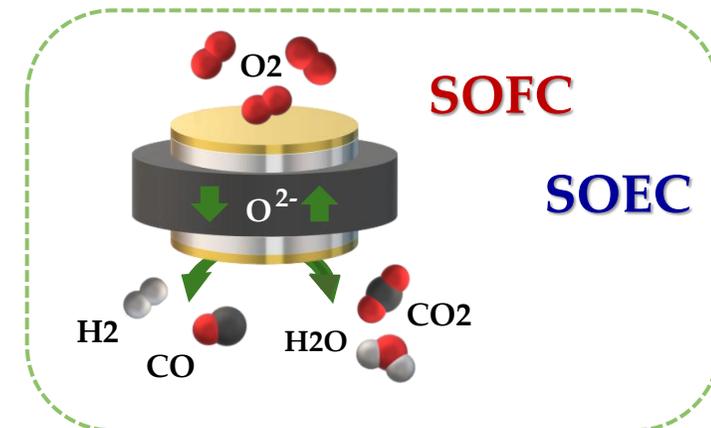


Environment



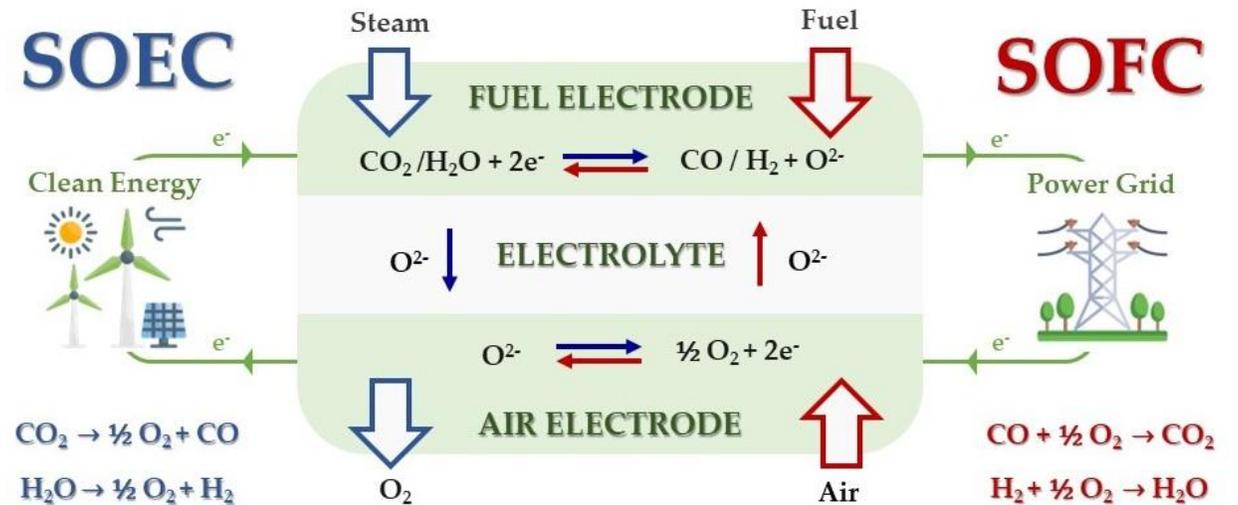
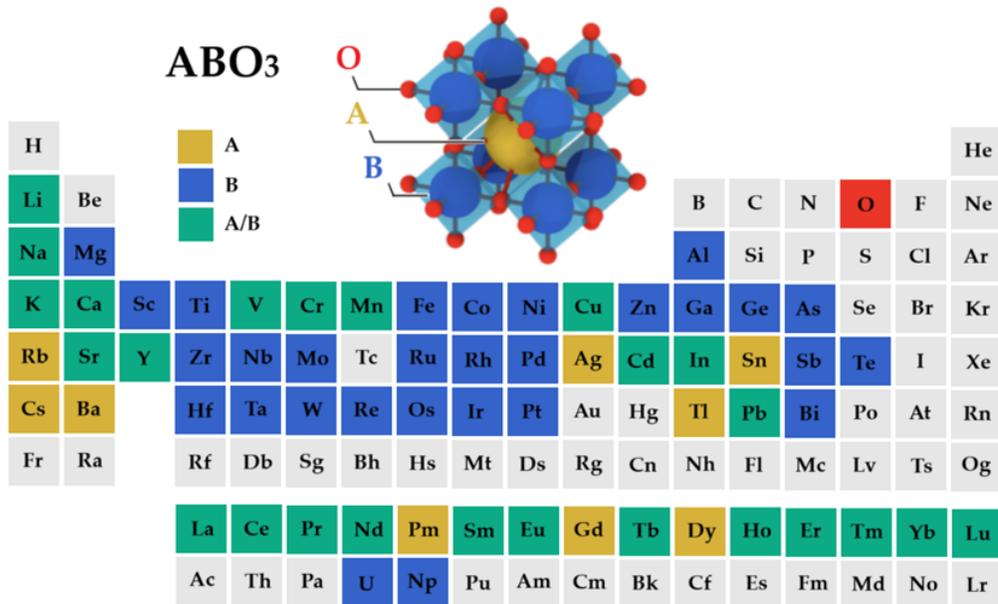
Solid Oxides Research Group (SORG)

Prof. Elisabetta Di Bartolomeo
Dr. Leonardo Duranti



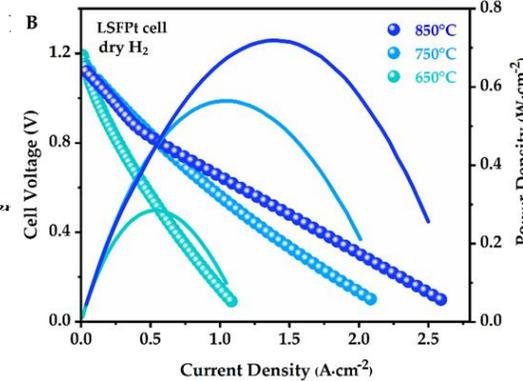
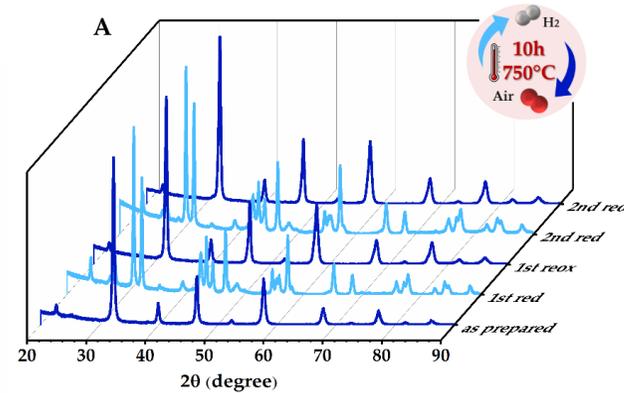
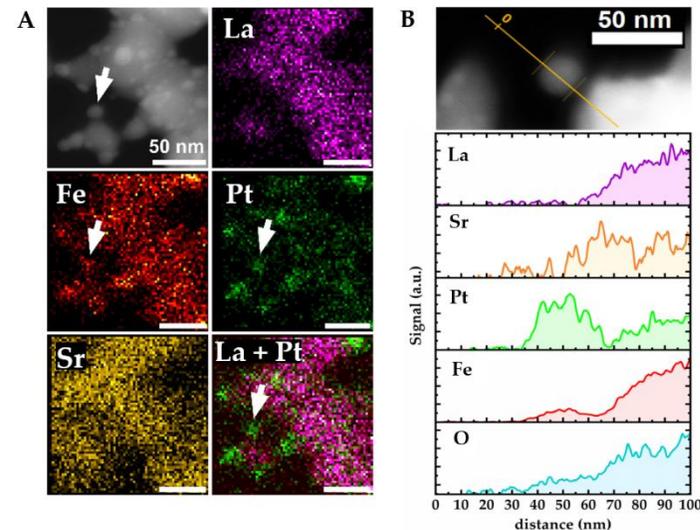
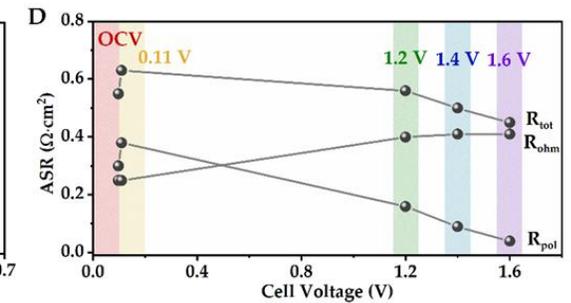
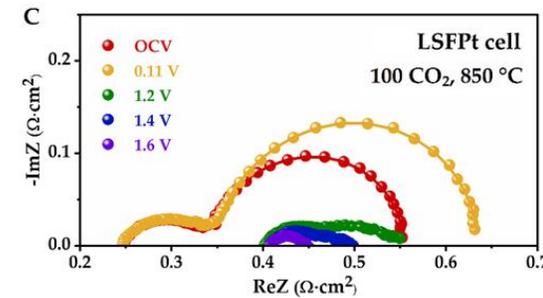
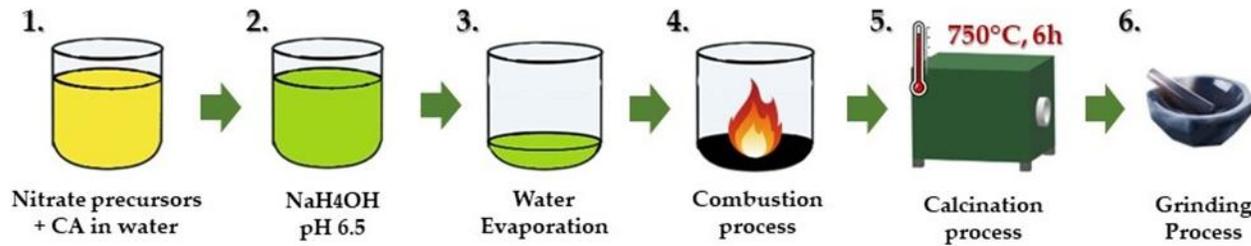
Research Activity

Development of mixed oxides for electrochemical devices for energy conversion and storage. The experimental activity concerns the chemical synthesis of powders, the structural and microstructural characterization, the fabrication of electrochemical cells operating at high temperature (SOFC/SOEC) and the electrochemical tests.

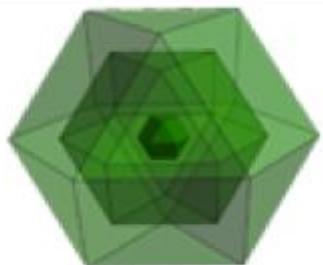


Research Topics

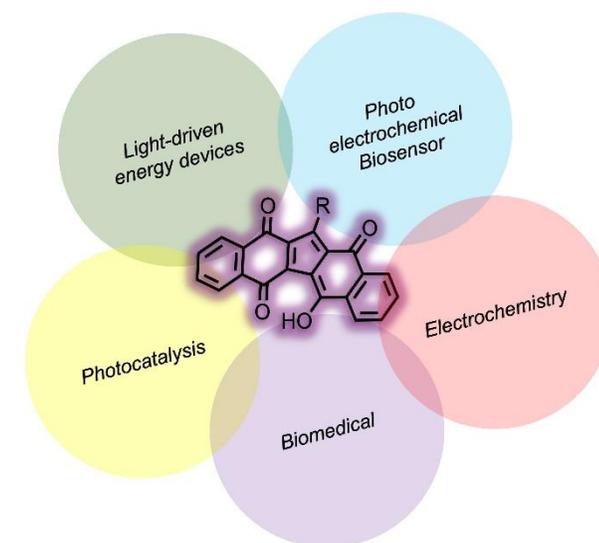
- Synthesis and characterization of oxides for oxygen electrocatalysis
- Development of oxides for high temperature electrolyzers/fuel cells



O2C Group – *Organic and Organometallic Chemistry*

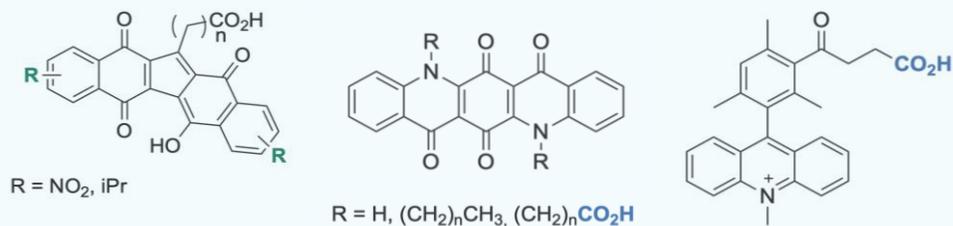


Dr. Federica Sabuzi
Prof. Pierluca Galloni
Prof. Valeria Conte

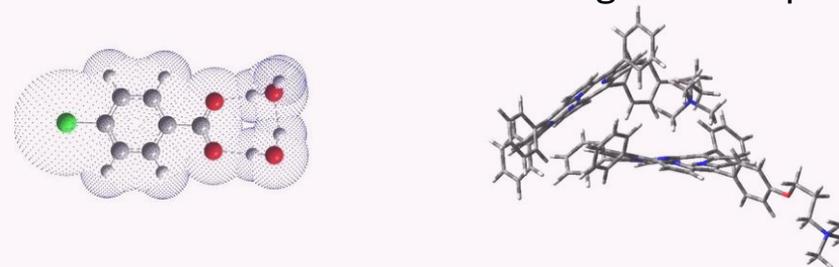


RESEARCH ACTIVITIES

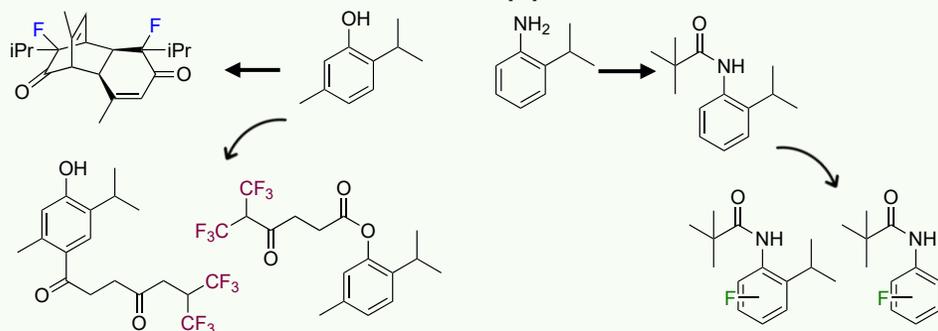
Synthesis and characterization of organic *dyes* for photo(electro)chemical applications



Computational study of molecular properties and intermolecular interactions of organic compounds



Tailored functionalization of natural compounds for biomedical applications



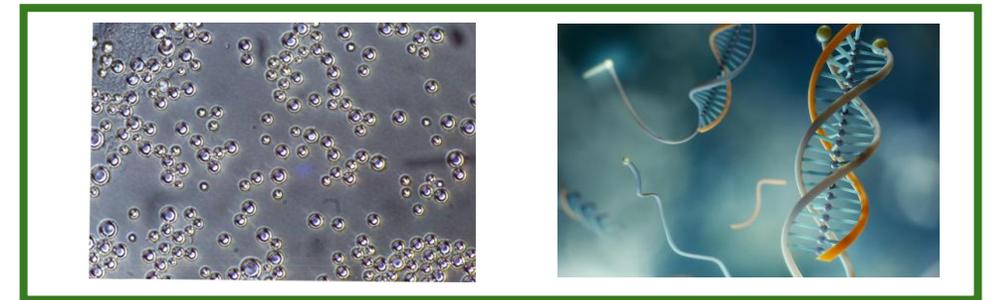
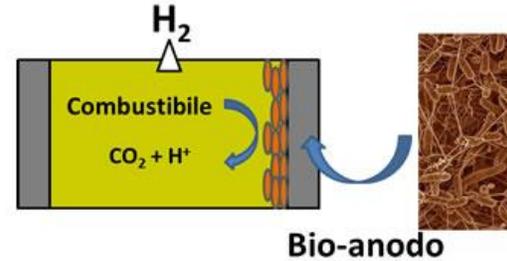
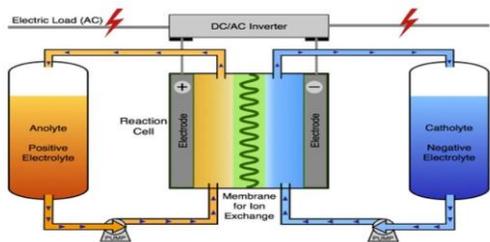
Collaborations: Prof. A. D'Epifanio (Università di Roma Tor Vergata); Prof. A. Sartorel (Università di Padova); Prof. A. Fontana (Università G. D'Annunzio di Chieti); Prof. S. Bettini (Università del Salento); Prof. X. Sala (Universitat Autònoma de Barcelona); Dr. N. Romero (Université de Toulouse); Prof. V. N. Nemykin (University of Tennessee).

Funded projects: NEST PNRR – NANOCARB High Surface Area Carbon Nanostructures as Electronic Transducers for Artificial Photosynthesis
PRIN 2022 – PROMETEO Photoelectrocatalytic modules for oxidative C-H activation

Research Activity

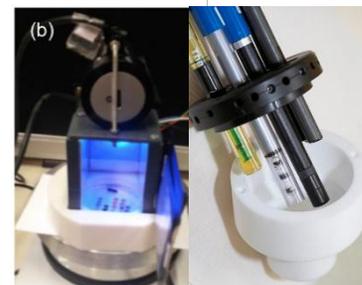
The Department of Chemical Science and Technologies has been selected as one of the 11 best Chemistry Departments in Italy.

The X-Chem project involves the strengthening of three main lines of research:



Energy transition

Health



Environment

Biochemistry and Biomaterials for Tissue Regeneration

Sonia Melino's team:

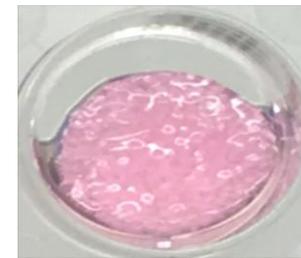
Dr.ssa Silvia Buonvino

Dr. Gabriele Feltrin



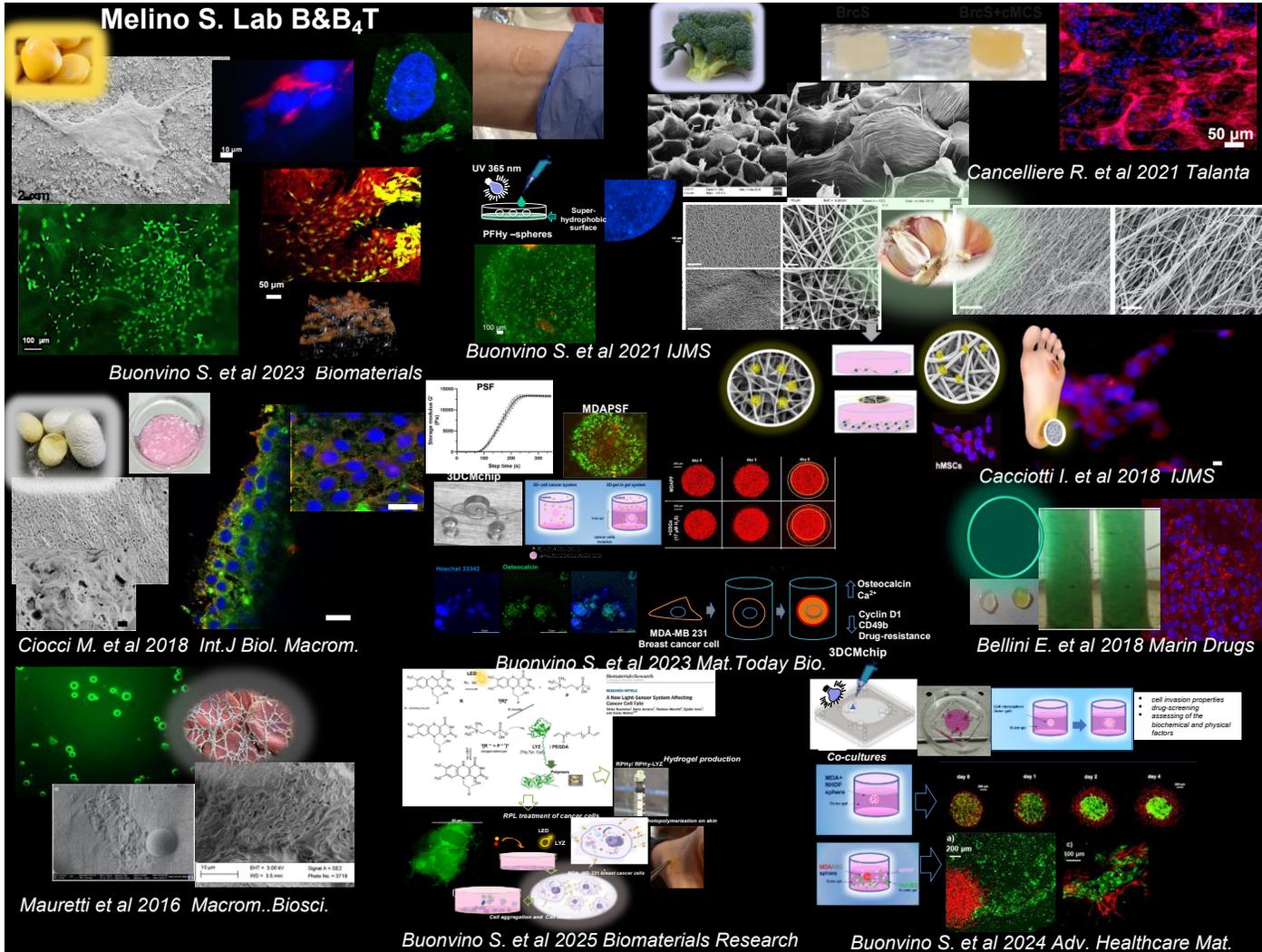
Prof.ssa Sonia Melino

B&B4T LAB



RESEARCH ACTIVITIES

- Fabrication and Characterization of 3D cellular models for regenerative medicine and cancer
- New biomaterials synthesis from wastes for cellular scaffold production



Projects

2022-2025 PI nel WP: *Modelling of 3D approaches of multicellular spheroids structures for estimating the risk of disease initiation and progression.* Progetto PNNR PE6 European Union Next Generation EU via MUR-PNNR HEAL ITALIA "Health Extended Alliance for Innovative Therapies, Advanced Lab-research, and Integrated Approaches of Precision Medicine

2023 **Principal Investigator** (PI) nel Progetto European Union Next Generation EU via Ministry of Health - HUB LIFE SCIENCE – Advanced Diagnostic- Italian network of excellence for advanced diagnosis (INNOVA)

Collaborations

Prof. D. Seliktar Technion Haifa

Prof. Ilaria Cacciotti University of Rome "Niccolo Cusano"

Department of Industrial Engineering

Prof. Giovanni Chillemi University of Rome Tor Vergata

Silvia Buonvino UniCamillus

Prof. M T Cambria University of Catania

Studenti e non solo



Physical Chemistry of Macromolecules

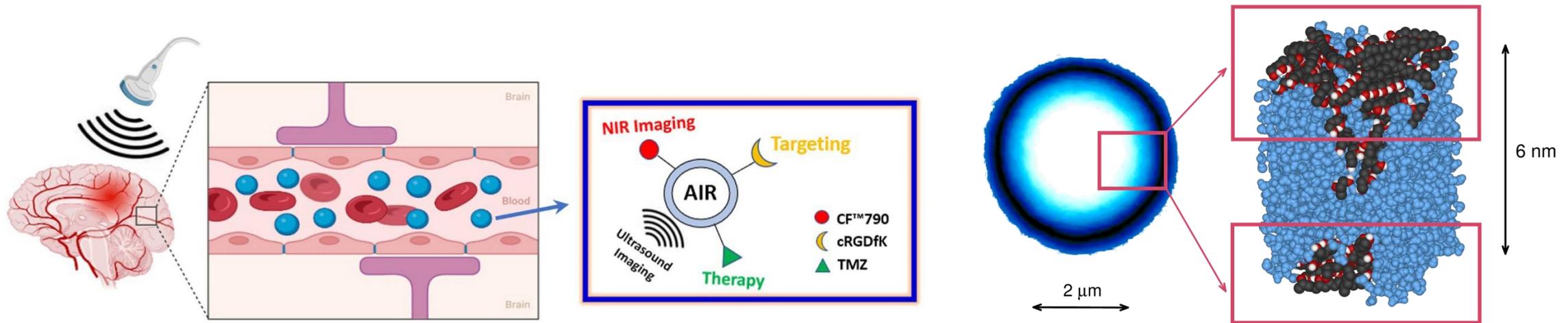


Gaio Paradossi
Ester Chiessi
Fabio Domenici



RESEARCH ACTIVITIES

Design and development of multi-responsive macromolecular systems for applications in biomedicine (imaging, drug delivery, tissue engineering), dosimetry, and conservation of cultural heritage



Multifunctional polymer-shelled microbubbles for selective targeting and elimination of brain tumors

European and Italian Projects: **EU:** - Microbubble driven multimodal imaging and theranostics for gliomas; - Acoustic markers for enhanced remote sensing of radiation doses; - Glioma Targeting by Drug Loaded Engineered Microbubbles; **IT:** - PRIN, Novel strategies for sensitized ultrasonic neuromodulation;

- BRiC: Study of cellular alterations induced by exposure to professional ultrasound; - INFN, Droplets as Injectable Dosimeters; - Umberto Veronesi Foundation: Engineered PVA-

RESEARCH ACTIVITIES

Collaborations: *Department of Cardiovascular Sciences KU Leuven; DIBRIS University of Genova; The National Center for Oncological Hadrontherapy (Pavia, IT); Health Physics of Complex Structures of Radiation Oncology «Sant'Orsola» (Bologna, IT); Harwell Science and Innovation Campus Oxfordshire, UK*



G. Paradossi E. Chiessi F. Domenici Y. Toumia A. Vitaliti G. Perilli M. Redi E. Bassotti O. Eslek M. Valenzuela A. Tani



TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA

Bachelor's Degree in Materials Science and Master's Degree in Science and Technology of Materials

University of Rome Tor Vergata

International Synergies in Photonics and Materials Science: Double Degree Dialogue 2025

June 12th 2025



Prof.ssa Silvia Orlanducci
Prof.ssa Emanuela Tamburri
Prof. Massimo Tomellini
Dott.ssa Valeria Guglielmotti
Dott. Massimo Longo

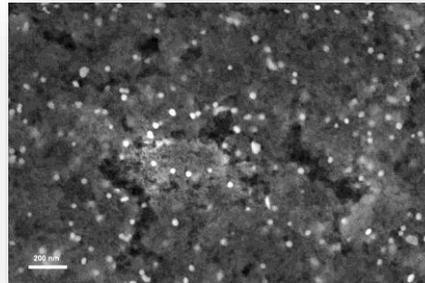


- ❖ The research activity focuses on the design, synthesis, and morphological–structural–functional characterization of materials for applications in the biomedical field, sensing technologies, environmental protection, cultural heritage preservation, microelectronics, energy, and catalysis.
- ❖ The materials of interest include innovative systems based on carbon, two-dimensional (2D) materials, conductive polymers, oxide and metal nanoparticles, as well as hybrid and composite materials.

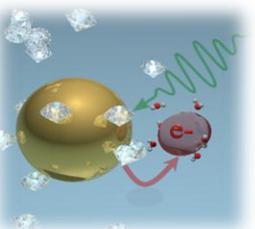
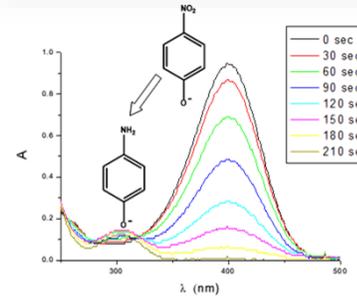
❖ Synthesis of nanodiamond/gold and nanodiamond/silver coupled particles for applications in plasmonics, catalysis, and sensing.



In collaboration with ISM-CNR
Dr Francesco Toschi
- Plasmonics -



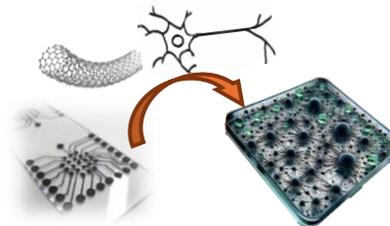
In collaboration with
Prof.ssa Laura Micheli
- Electrochemical Sensors -
Prof. Riccardo Salvio
- Catalysis -



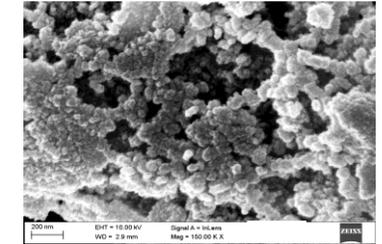
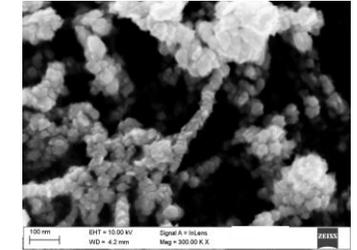
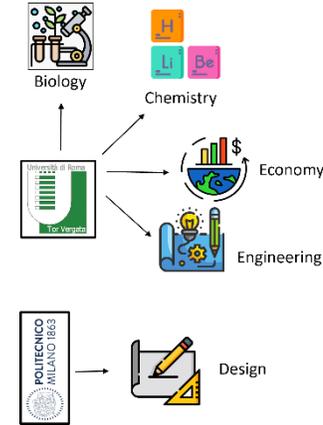
In collaboration with IMEM-CNR
Dr.ssa Silvia Battistoni

❖ Realization of CNT-based hybrid networks for cellular interfacing

CNT + cells



❖ Reuse and upcycling of domestic wastewater



Zero Mile[®] is the system already designed for the up-cycling of dishwasher wastewater

Nanodiamonds is the project to up-cycle the plastic microfibers from washing machine into nanodiamonds

Funding by the Italian Ministry of the Environment and Energy Security



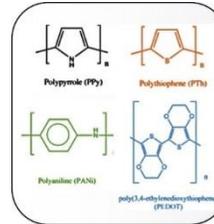
In collaboration with IMEM-CNR
Dr.ssa Silvia Battistoni

- ❖ *Synthesis and characterization of electrically conductive materials for 3D printing or inkjet for applications in organic electronics*
- ❖ *Printing and characterizations of flexible electronic circuits*

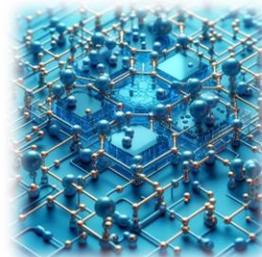
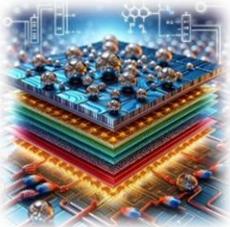


CNR
Istituto di Struttura
della Materia

In collaboration with ISM-CNR
Dr Francesco Toschi

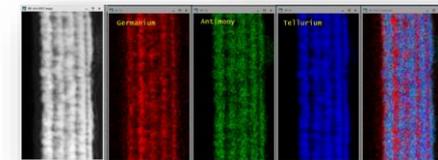


- ❖ *Conjugated Polymer Nanostructures for Organic Electronic Devices*
- ❖ *MXene-Based Systems for Batteries and Supercapacitors*
- ❖ *Synthesis and Characterization of Perovskite Nanostructures for Optoelectronic Devices*



In collaboration with IMM-CNR
Dr.ssa Raffaella Calarco

- ❖ *Sputtering-RF Deposition of Chalcogenide Thin Films and Multistructures for Phase Change Memory (PCM) Applications*
- *These systems enable neuromorphic computing with low consumption and are applicable to sustainable mobility (safety and energy efficiency)*

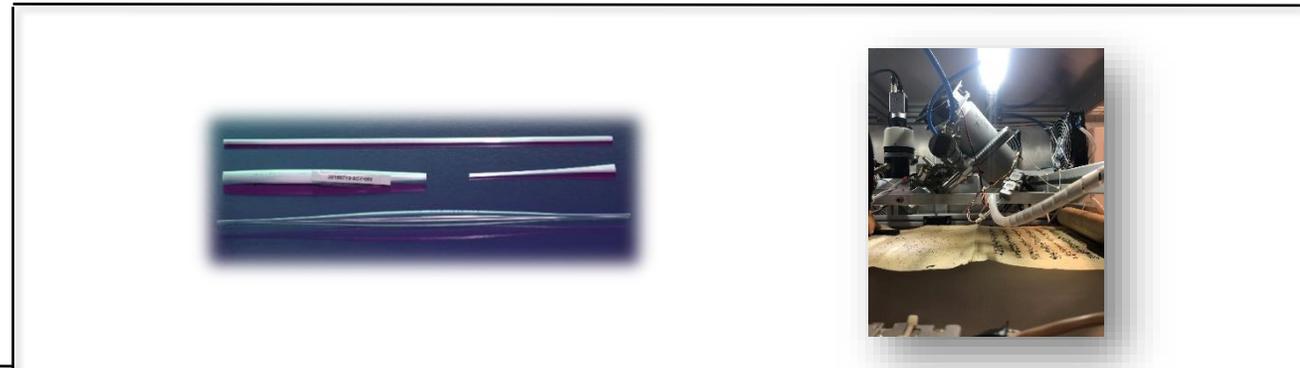
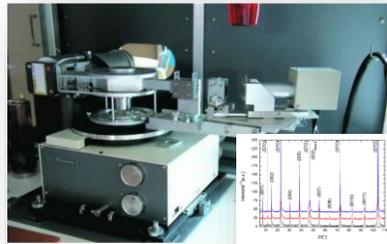
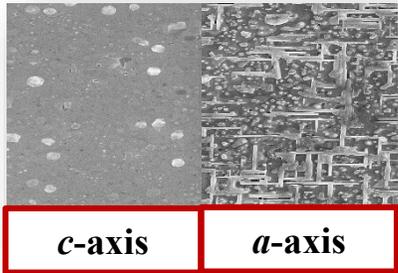
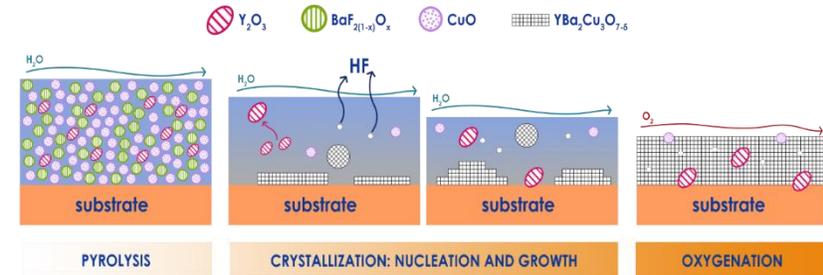




In collaboration with ENEA
Dr.ssa Valentina Pinto

- ❖ *Nucleation and Growth Study of High-Tc Superconductors*
- ❖ *Synthesis of YBCO by Solution Deposition Process, for Oriented Growth:*

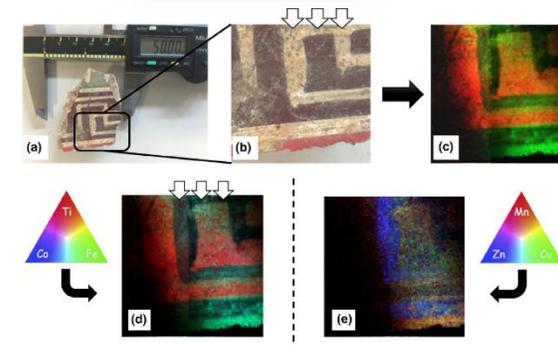
— *structural, morphological and superconducting characterization by XRD, SEM, optical microscopy and R(T) (Resistance-Temperature)*



Dott.ssa V. Guglielmotti

valeria.guglielmotti@uniroma2.it

In collaboration with XlabF (INFN-LNF)
Prof. Sultan Dabagov
Dr. Dariush Hampai

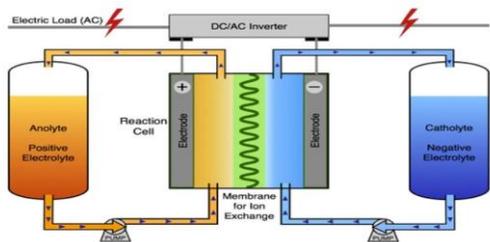


- ❖ *XRF and XRD maps using polycapillary focusing systems for the non-destructive analysis of pigments and paint layers in cultural heritage*

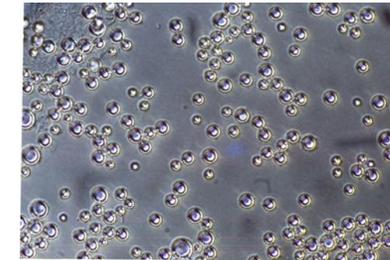
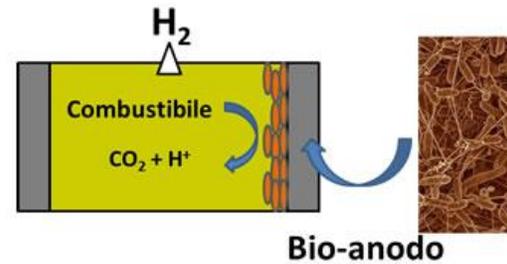
Research Activity

The Department of Chemical Science and Technologies has been selected as one of the 11 best Chemistry Departments in Italy.

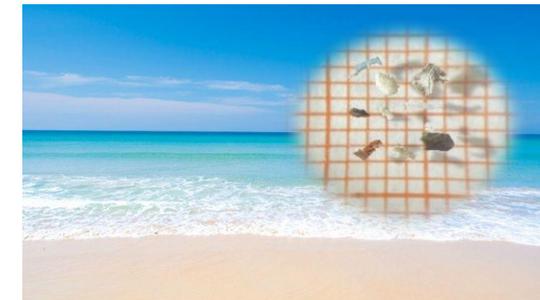
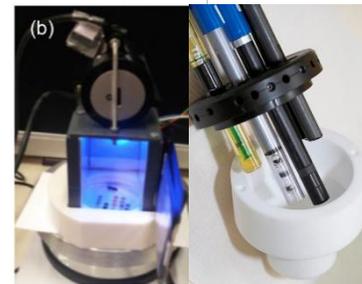
The X-Chem project involves the strengthening of three main lines of research:



Energy transition



Health



Environment

Nature-Inspired Functional Materials

Prof. Emanuela Gatto

Dott.ssa Raffaella Lettieri

Prof. Mariano Venanzi



Research Activity



TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA



Solar cells



Bioplastics



SPINOFF
UNIVERSITÀ DEGLI STUDI
DI ROMA TOR VERGATA

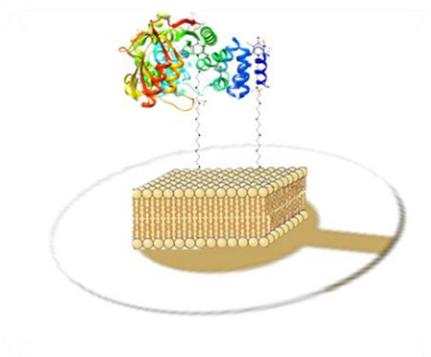
DNA

PROTEINS

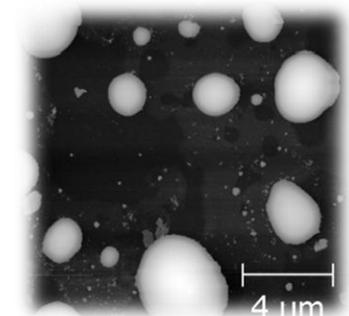
PHOSPHOLIPIDS

POLYSACCHARIDES

**Experts in natural polymers
for applications in the field of
sustainable materials**



Sensors



Medical
devices

Research Projects



Biopolymer-based organic solar cells

National Research Doctorate in Photoinduced Processes and Technologies

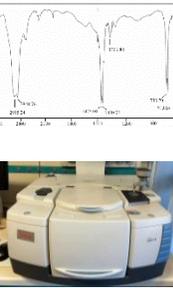
Prof. Aldo Di Carlo, dott. Luigi Vesce CHOSE
Dott.ssa Marta De Zotti, University of Padua



Use of wine waste for the production of sustainable materials

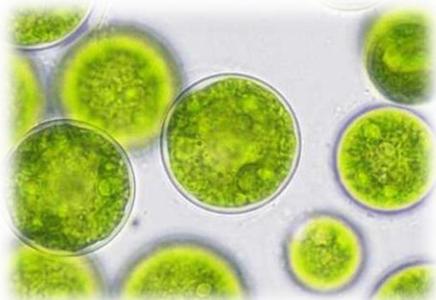
PON Doctorate RTDA PON- REACT EU-DM1062/2021

Prof. Silvia Licocchia, prof.ssa Elisabetta Di Bartolomeo,
Tor Vergata



Analysis and identification of micro- and nanoplastics in seawater samples

Dr. Raffaella Bullo, Polytechnic University of Marche
Prof. Susanna Dolce, Luisa Campagnolo, Nicola Toschi,
Medicine Department Tor Vergata



Synthesis and characterization of bioplastics from microalgae

Dr. Viviana Scognamiglio, dr. Amina Antonacci, CNR

PRIN 2022 project NanoGRAB



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UNIVERSITÀ DEGLI STUDI
DI ROMA TOR VERGATA





NEw Materials for Optoelectronics

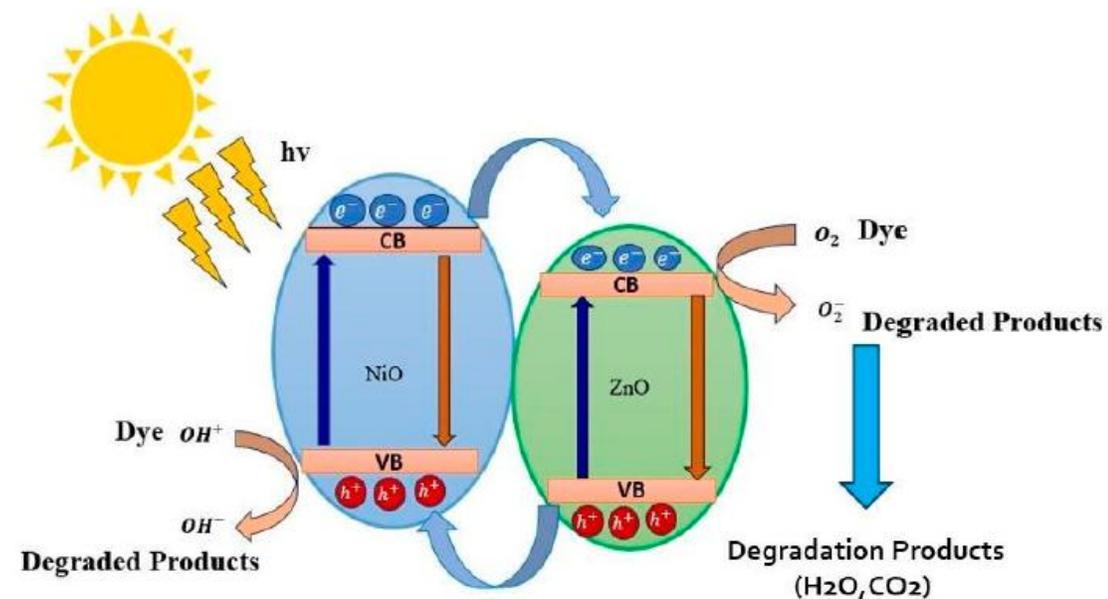
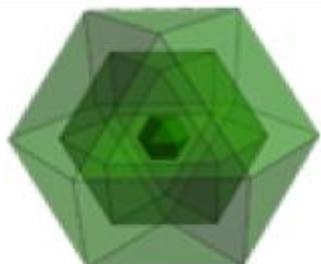
Prof. Paolo Proposito

paolo.proposito@uniroma2.it

Luca Burratti

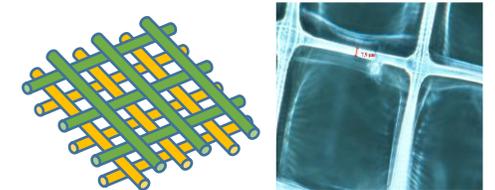
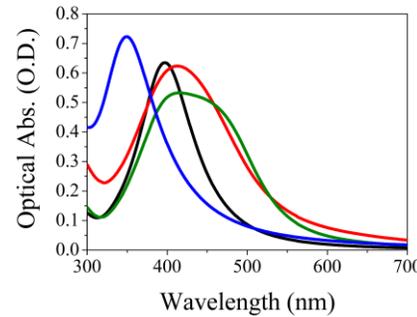
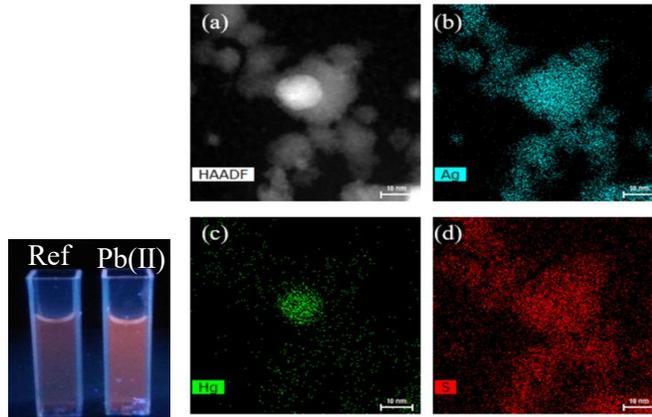
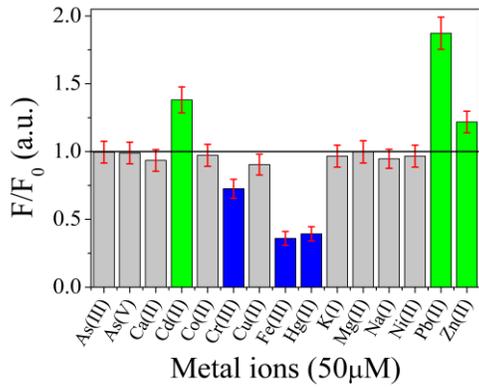
Sadaf Jasmine

Fabio De Matteis

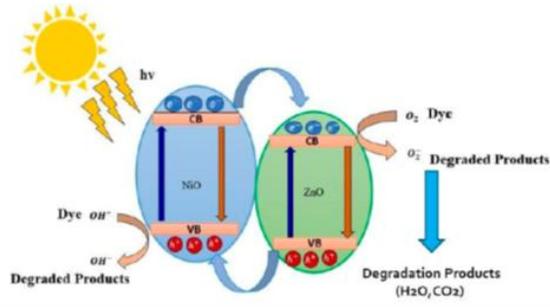
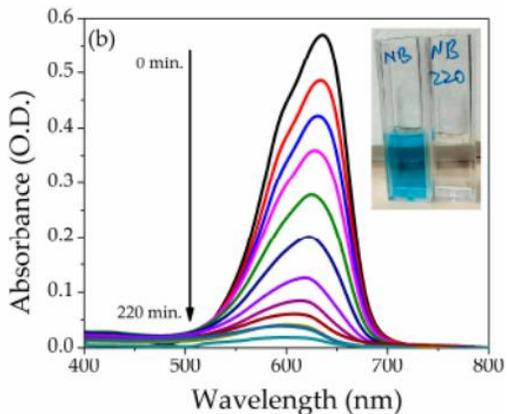




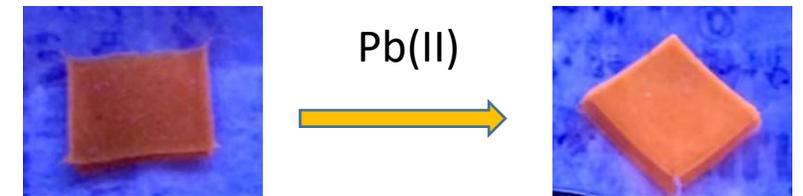
Heavy metal-ion optical sensors based on absorption and/or fluorescence by Silver nanostructures



Photocatalytic degradation of organic pollutants by means of metal oxides



Water filtration with 3D printed polymer filters



Prior to interaction

Following the interaction



TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA

**"International Synergies in Photonics and Materials Science:
Double Degree Dialogue 2025"**
Presentation of the scientific activities at Tor Vergata
June 12th, 2025



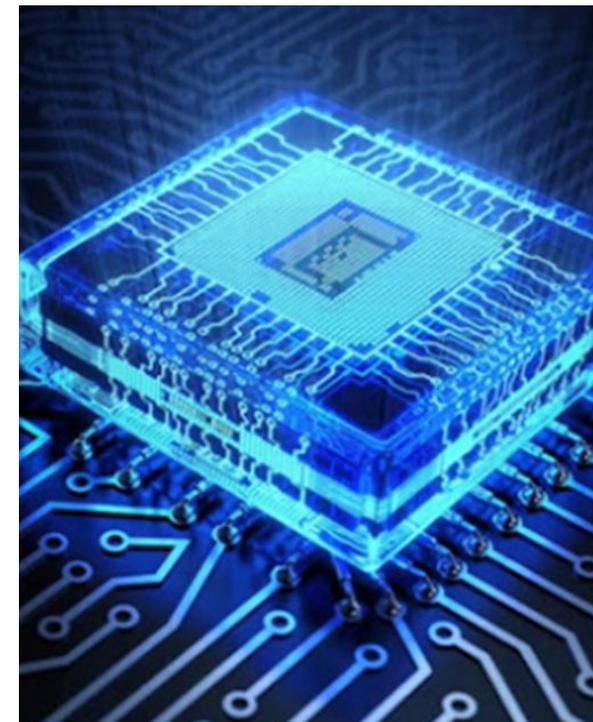
Prof. Fabio De Matteis

fabio.dematteis@uniroma2.it

Luca Burratti

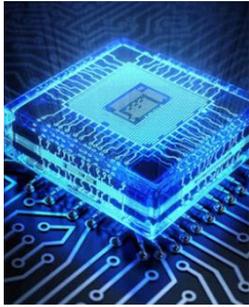
Andrea Salamon (INFN)

Thu Ha Dao (INFN)



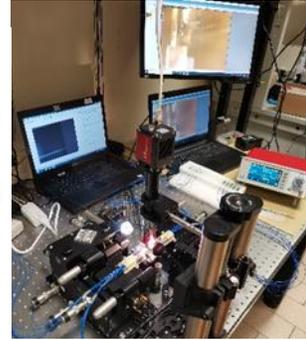
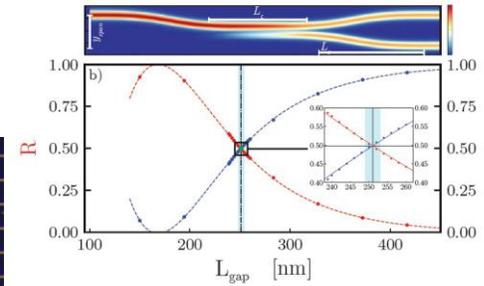
Silicon Photonics Lab

QUANTEP-Experimental Platform for Quantum Technologies



Creation of a platform based on Silicon Photonics for development and characterization of circuits for quantum computing in linear optics;

- Integration of SPD (single photon detectors);
- Integration of SPS (single photon sources);
- Integration of polarization control circuits.

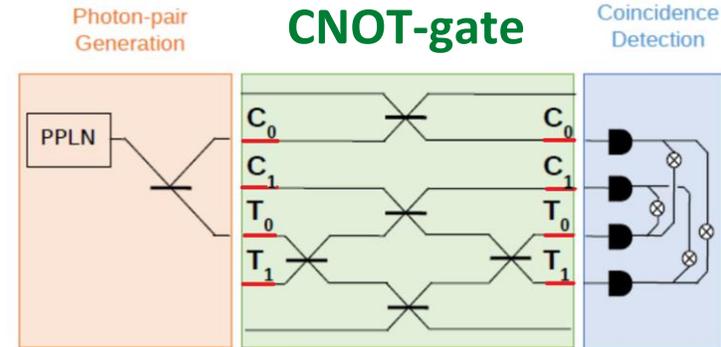
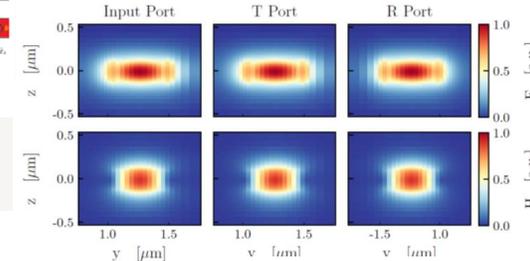
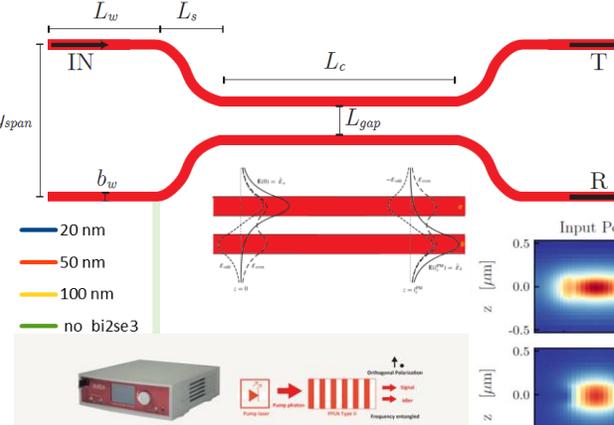
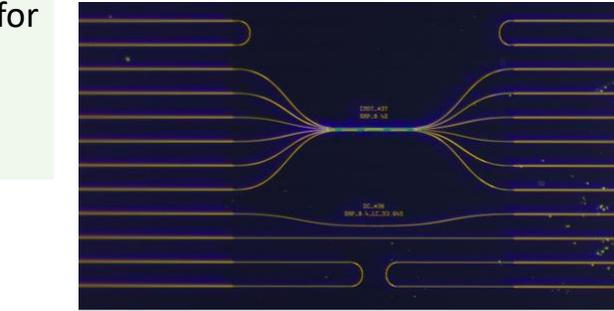
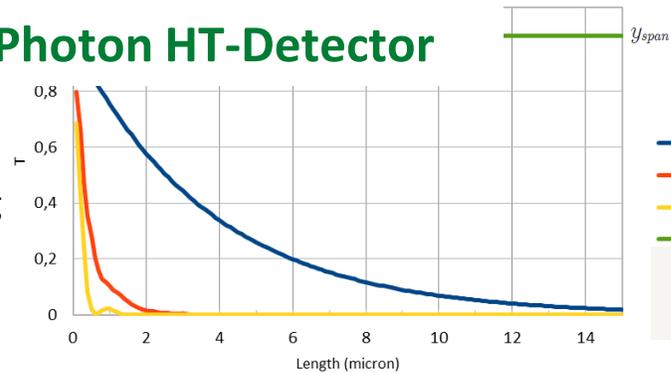


INFN CSN5 Project

Wavelength 1550.752 nm

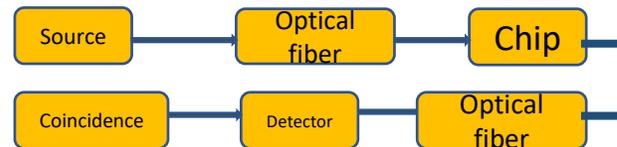
Integrated Single Photon HT-Detector

Si/Bi₂Se₃ and Si/Bi₂Se_xTe_y Heterojunction in evanescent wave coupling (M. Salvato)



Ansys Lumerical Software Package for Photonics Simulation & Design

FDTD – Finite Difference Time Domain solver
MODE - EigenMode Expansion (EME) solver



electrical contacts

cladding opening

Si wg



TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA

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CHOSE, Centre for Hybrid and Organic Solar Energy

Thomas M. Brown

Andrea Reale

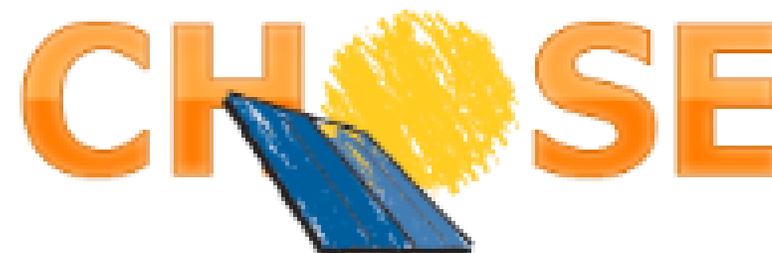
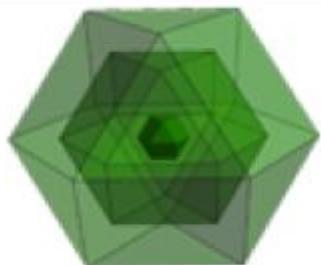
Francesca Brunetti

Matthias Auf Der Maur

Antonio Agresti

Fabio Matteocci

Aldo Di Carlo



Research Activities

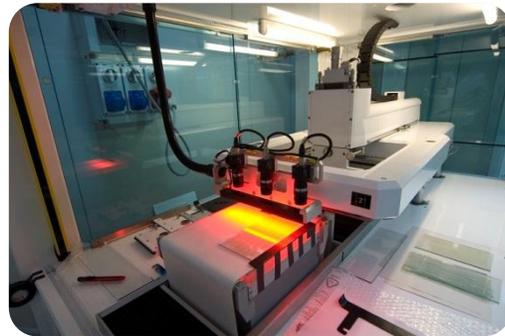
Materials and processes for new generation photovoltaics with organic and perovskite semiconductors

Deposition through printing techniques (but also thermoelectric devices, supercapacitors, artificial retinas...)

Inks



Printing Techniques



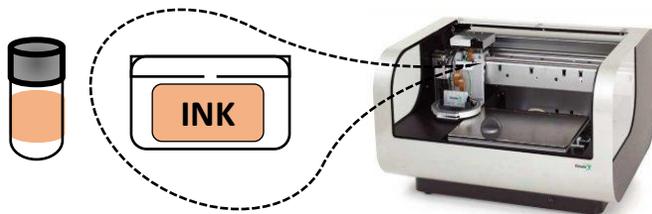
Solar cells & other devices



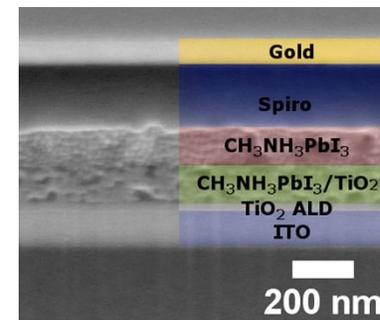
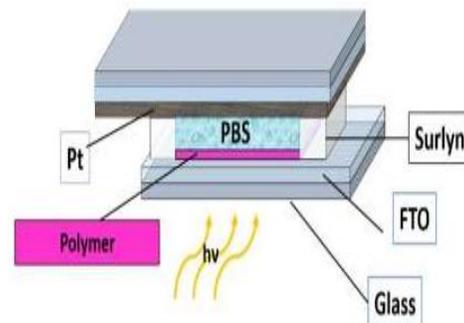
Photovoltaic modules



Biohybrid devices



Nanostructured Multilayers



Even flexible





Research Projects Available

Perovskite Photovoltaics

Organic Photovoltaics

Thermoelectric Devices

Bio-Hybrid Devices and Artificial Retina
Supercapacitors

Tandem Cells

Light Harvesting Outdoors, Indoors & in
Space

Flexible Solar Cells





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UNIVERSITÀ DEGLI STUDI DI ROMA

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Presentation of the scientific activities at Tor Vergata
June 12th, 2025

Metallurgy and Materials Science

Prof. Alessandra Varone

alessandra.varone@uniroma2.it

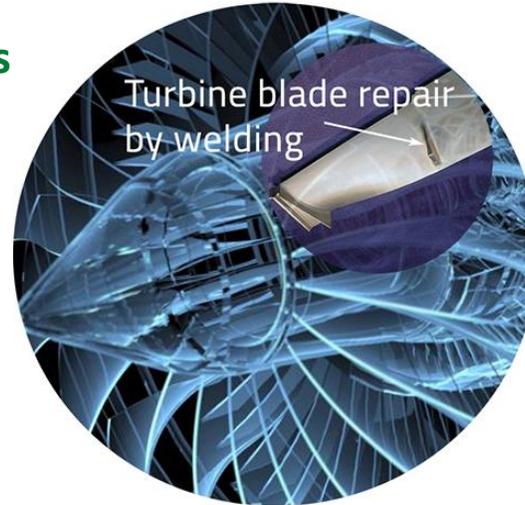
Prof. Maria Richetta
Alessandra Palombi



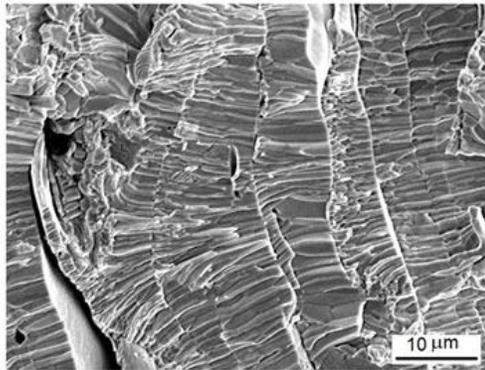
Research Activity

1) Welding and repair of Ni-Superalloys

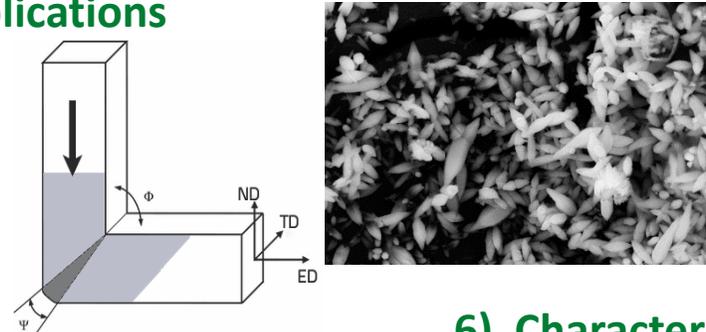
Laser welding of Ni-superalloys for aerospace applications.



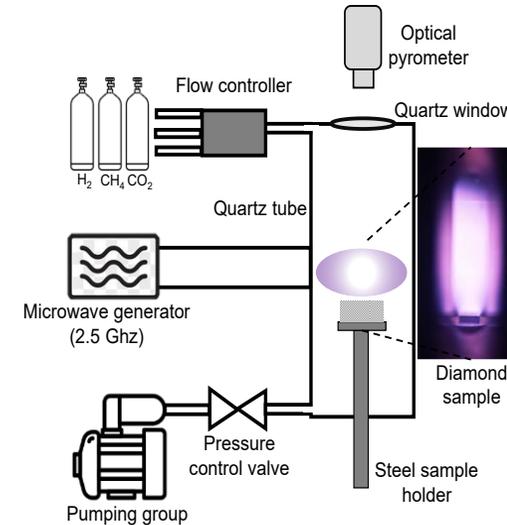
3) Materials for structural applications in fusion reactors



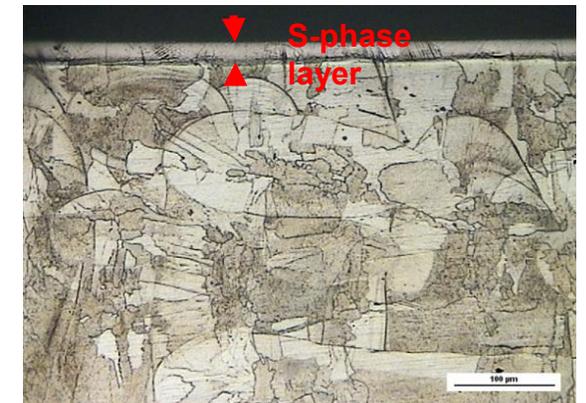
4) Metallic materials for biomedical applications



2) Plasma-assisted thermochemical treatment of austenitic stainless steels



Optimization of parameters (temperature, plasma atmosphere, duration) of the low-temperature ($T < 500\text{ }^{\circ}\text{C}$) thermochemical cementation treatment with plasma-assisted process for stainless steel 316L.



5) Additive manufacturing of metallic materials. Lattice structure.

6) Characterization of metallic materials by means of: XRD, optical and electronic microscopy, instrumented indentation, mechanical spectroscopy

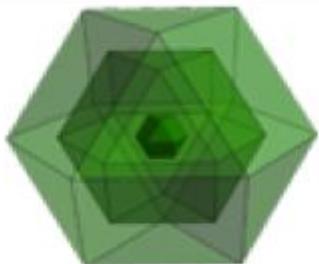


TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA

"International Synergies in Photonics and Materials Science:
Double Degree Dialogue 2025"
Presentation of the scientific activities at Tor Vergata
June 12th, 2025



Material Science and Technology group



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Dott. Ing. Lorenzo Paleari

Dott. Elisa Pizzi



Research Activity



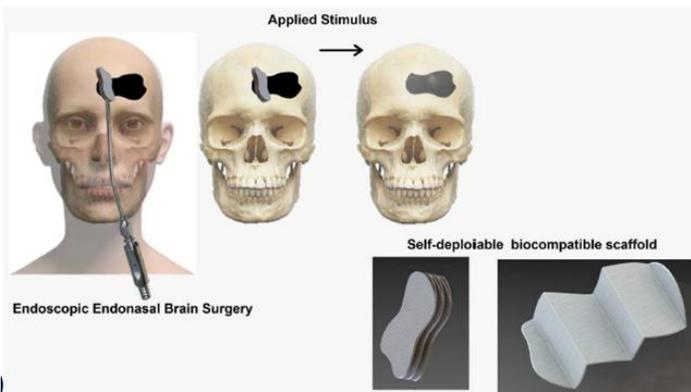
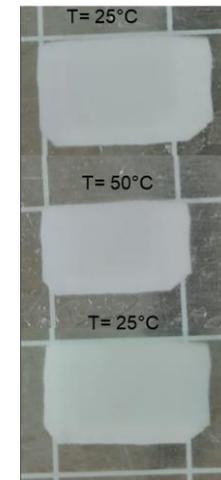
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R&D and technological transfer
in the field of Material Science
and Technology.

Polymers, composites,
elastomers, ceramic, metallic
and cement materials, with
particular emphasis on
multifunctionality, additive
manufacturing (3D printing)
and sustainability.



Temperature
responsive
material
(PCM)



- 3D printing of shape-memory materials (4D Printing)
- 3D printing of biobased scaffolds
- Innovative Hosts for Phase Changing Material (PCM) (Thermal applications)



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