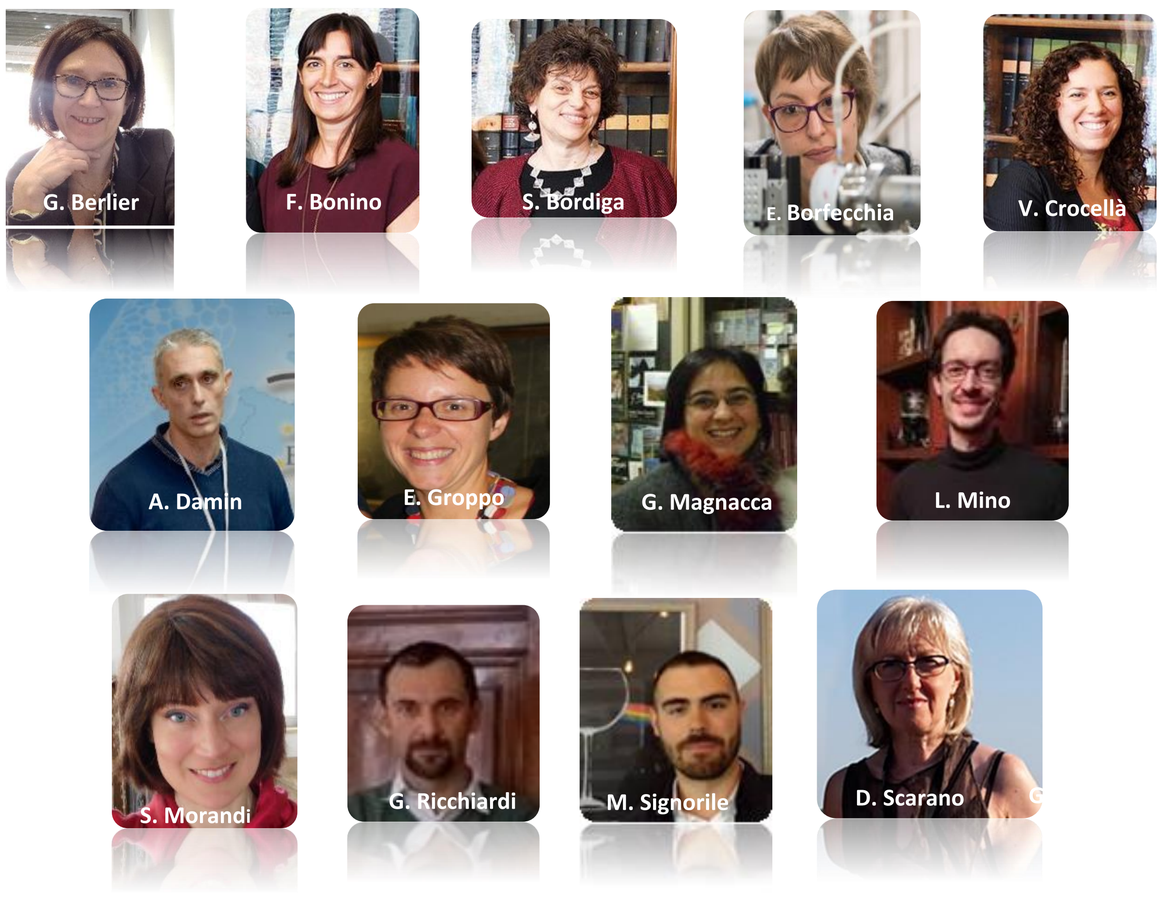
Dipartimento di Chimica – Università di Torino

Thesis topics: the SURFIN group
Experimental physical chemistry

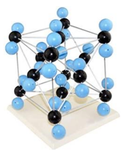
2023 - 2027 DIPARTIMENTO DI ECCELLENZA
Ministero dell'Università e della Ricerca

UNIVERSITÀ DI TORINO — Dipartimento Chimica — chimica

The research group

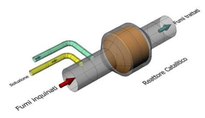


Overview



BULK AND SURFACE CHARACTERIZATION

SYNTHESIS



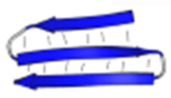
STUDY OF MATERIALS

MULTIDISCIPLINARY APPROACH

CATALYTIC ENVIRONMENTAL AND BIOMEDICAL APPLICATIONS

STUDY OF PROCESSES

INSTRUMENTAL MULTITECHNIQUE APPROACH



COLLABORATIONS WITH EXTERNAL INSTITUTIONS

POSSIBLE COLLABORATIONS ABROAD

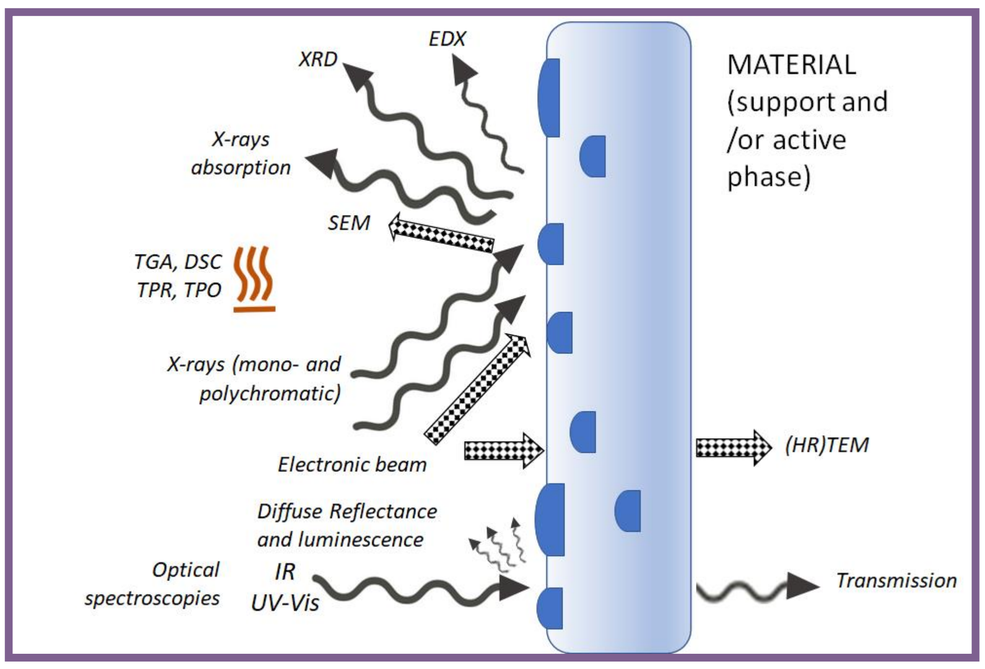
General approach

Synthesis, characterization and testing for applications in:

- heterogeneous catalysis and photocatalysis
- sensors for gas and volatile compounds
- selective adsorption/separation/entrapment of molecules for the energy sector

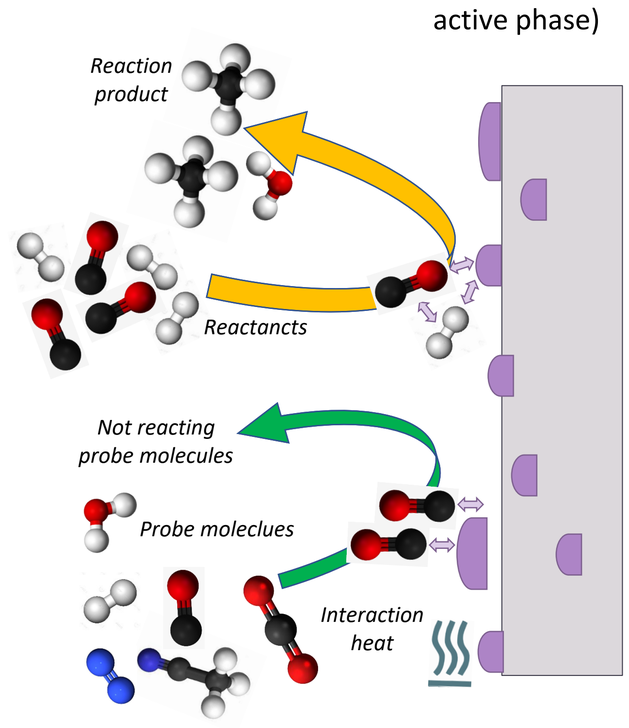
Multi-technique approach:

Powder X-ray Diffraction / Inelastic Neutron Scattering / Microscopies (HRTEM; SEM; AFM); Infrared spectroscopy; Raman Spectroscopy, UV-Vis-NIR spectroscopy; X-Ray Absorption and emission spectroscopies (XAS and XES); Volumetric and gravimetric measurements



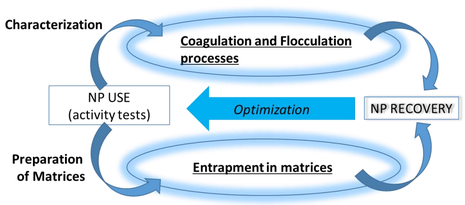
TECHNIQUES "MOLECULE-BASED" FOR SURFACE CHARACTERIZATION AND REACTIVITY STUDIES

Depicted molecules can be probes for surface characterization (**green arrow**) or reactants followed in operando conditions (**yellow arrow**)

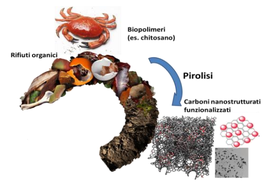


Materials for environment: synthesis, characterization and applications

Materials for the **recovery of nanoparticles** from aqueous systems: synthesis, characterization and testing of hybrid system after capture: functionalized oxidic systems, fibers from electrospinning, graphene oxide (in collaboration with Pierangiola Bracco, Mery Malandrino and Federico Cesano).



High surface area **carbon materials for adsorption** obtained from biomasses pyrolisis: synthesis and characterization (in collaboration with Federico Cesano)



Study of physico-chemical and thermocatalytic properties of systems based on perovskites for the abatement of pollutants in aqueous solutions (in collaboration with Alessandra Bianco Prevot, M.Cristina Paganini, Enzo Laurenti, CNR-ISMN Palermo)

The communication of science: alternative systems for the involvement of the general public (in collaboration with Elisa Borfecchia)

Possibilities for thesis abroad

Contact: Giuliana Magnacca, e-mail: giuliana.magnacca@unito.it

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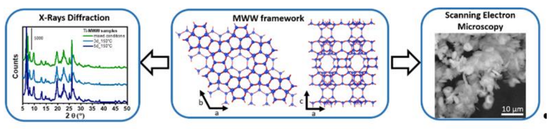
Ti-zeolites for partial oxidation reactions of bulky substrates

From an industrial point of view, partial oxidation reactions (e.g. alkenes epoxidation and phenol hydroxylation) are often catalyzed by Ti-substituted zeolites, that allow the use of hydrogen peroxide as oxidizing agent. The first and most important catalyst of this family is titanium silicalite-1 (TS-1), with MFI framework. Its utilization is however limited to linear alkene and small cycloalkene substrates, due to its limited pore openings. Ti-zeolites like Ti-MWW zeolite can be a valuable alternative for bulkier substrates instead, thanks to its double pore system.

GOALS

- Synthesis of Ti-MWW by adopting different methods for Ti insertion, also with DoE approach
- Multi-technique characterization of the synthesized Ti-MWW
- Study of the catalytic properties of the synthesized Ti-MWW

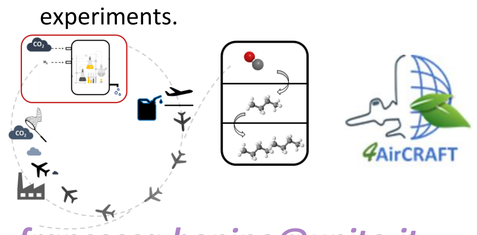


Advanced characterization of materials for air carbon recycling

From 1800 and particularly in the last 50 years a constant increase of CO2 emissions due to anthropogenic activities has been registered, reaching an excess of 922 metric Gt with respect to pre-industrial levels in 2019. Among the different strategies applied in order to contrast this steep increment and to reach the limit settled by the Paris Agreement, Carbon Capture and Utilization (CCU) and Carbon Capture and Storage (CCS) technologies are expected to contribute to nearly 20% of total reduction.

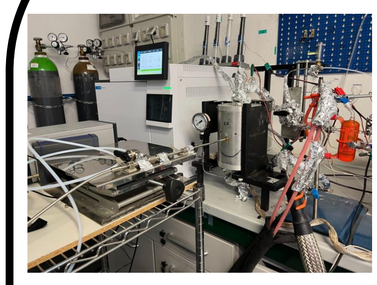
GOALS

- Synthesis, functionalization, modification of materials for CO_2 conversion.
- Multi-technique advanced characterization to study the materials, their reactivity towards CO_2, mainly employing in situ IR spectroscopy, volumetric approaches and microcalorimetric experiments.

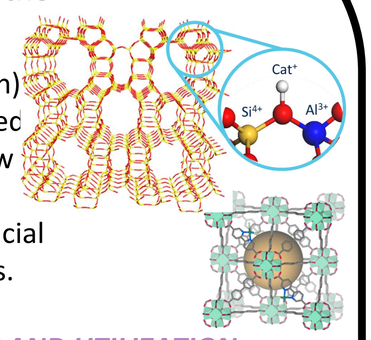


Contact: Francesca Bonino -E-mail: francesca.bonino@unito.it

Heterogeneous catalysts for the synthesis of sustainable chemicals



Use of in situ and operando spectroscopies (UV-Vis; IR; Raman) on well defined catalysts combined with GC and MS analysis to follow target reaction, devoted to the synthesis of simple molecules crucial for the development of chemicals.



FUNCTIONAL MATERIALS FOR CARBON DIOXIDE CAPTURE AND UTILIZATION

objectives: Synthesis, functionalization, modification and advanced characterization of materials (zeolites, Metal-organic-frameworks, oxides, mixed oxides) for CO_2 capture and conversion.

UNRAVELLING THE SECRETS OF CU-BASED CATALYST FOR C-H ACTIVATION (CUBE)

Cu-based catalysts are excellent candidates for the direct conversion of alkanes to the corresponding alcohols, a process that could shift the paradigm of alcohols production toward a more sustainable and bio-economical route.

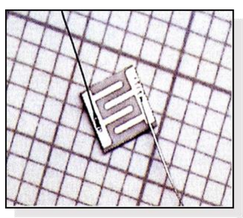
objectives: i) to make Cu-MOFs, ii) to propose the local environment of the Cu species; iii) to see the effects upon interaction with the oxidant/reductant agents. iv) to quantify the amount of Cu species involved in the reaction.

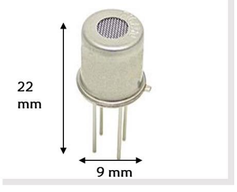
Possibility to combine molecular modelling

Contact: Silvia Bordiga -E-mail: silvia.bordiga@unito.it

Semiconducting oxides for gas sensors

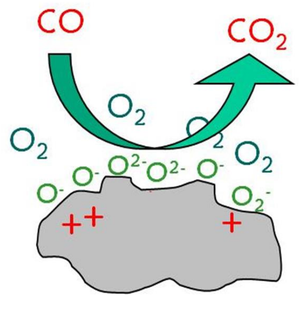
Study of the surface and electronic properties of semiconducting oxides during the interaction with oxidizing and reducing gases by means of the combined use of UV-Vis and IR spectroscopies.

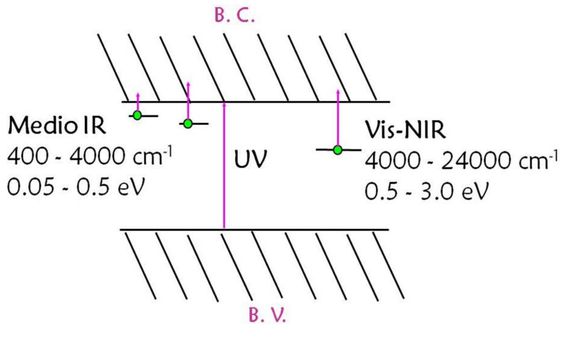




GOALS

- Characterization of the electronic properties and their variations during the interaction with gases
- Determination of the surface reactions related to the sensing mechanism
- Sensitivity toward specific gases

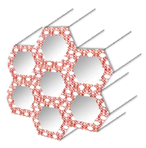




Contact: Sara Morandi, e-mail: sara.morandi@unito.it

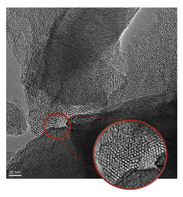
Zeolites for Catalysis: Tailoring new Hierarchical Structures and Active Sites

The new frontier in the synthesis of heterogeneous catalysts is represented by the production of hierarchical zeolites, able to overcome the major drawbacks of standard zeolites, related to the dimensions of the their micropores.



GOALS

- Synthesis of new zeolites with multiple level of porosity.
- Advanced characterization of the hierarchical porous system and of the active sites.
- Study of the catalytic properties of the new multi-level porous zeolite.

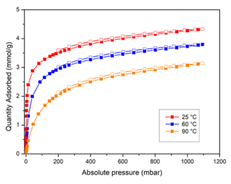


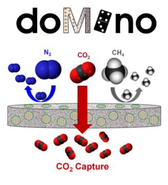
Porous Materials for Carbon Dioxide Capture

The presence of a large amount of carbon dioxide (CO_2) in the atmosphere is one of the most important environmental problem for our generation. CO_2 is a greenhouse gas and its presence causes and increase in the earth average temperature with serious consequences for life. In order to reduce its emissions in atmosphere, Carbon Capture and Storage (CCS) has been proposed as a solution.

GOALS

- Synthesis and advanced characterization of materials for CO_2 capture and separation (zeolites, metal-organic-frameworks, hydrotalcites and composites).
- Evaluation of their adsorption capacity through volumetric approaches, breakthrough measurements, *in situ* and *operando* IR spectroscopy and microcalorimetric experiments.

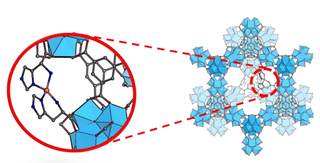


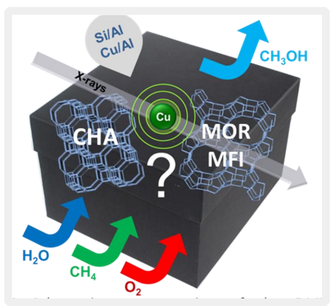


Contact: Valentina Crocellà, e-mail: valentina.crocella@unito.it

Investigating Cu-based porous catalysts by X-ray spectroscopy and modelling

Due to the dispersed nature of Cu sites within porous catalysts, their structural investigation via conventional approaches (e.g. XRD) is challenging. The combination of element selective X-ray spectroscopy methods at synchrotrons and quantum mechanical simulation represent a powerful alternative to reveal structural and electronic properties of active sites.





TOPICS

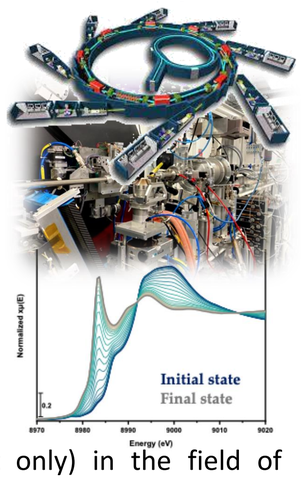
- XAS-XES investigation of Cu-MOFs under reaction conditions
- Operando XAS on Cu-zeolites during hydrocarbons conversion
- Inferring Cu distribution from Al siting via XAS and simulation

Beamtimes at Synchrotron Radiation Facilities (ESRF & SLS) are available on each topic during next semester.

Contacts: Matteo Signorile, e-mail: matteo.signorile@unito.it
Elisa Borfecchia, e-mail: elisa.borfecchia@unito.it

Understanding functional materials by in situ/operando synchrotron-based techniques

X-ray characterization techniques carried out at synchrotron radiation facilities represent powerful tools to reveal local structure and electronic properties of selected active sites in functional materials. Our group actively exploits ***in situ/operando*** **X-ray spectroscopy** (XAS, XES, NEXAFS), eventually in combination with diffraction/scattering techniques, frequently using the **ESRF** (Grenoble, France) and the **Elettra** (Trieste, Italy) synchrotron sources. We also develop & implement **advanced data analysis methods**, e.g., based on statistical/multivariate or machine-learning approaches.



- Applications to different research cases, mostly (but not only) in the field of functional materials and heterogeneous catalysis, depending on approved synchrotron experiments every semester.
- Detailed information on specific thesis projects typically avaialble at the **end of June** (*experiments in the September-February period*) and **end of January** (*experiments in the March-July period*): if interested, get in touch at the contact email in due time!

Contacts: Elisa Borfecchia, e-mail: elisa.borfecchia@unito.it

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Catalysts for production of (functional) polyolefins

Description: In the world of catalysis for olefin polymerization, chromium and titanium have both a leading role. The challenge in this field is to develop catalysts able to produce functional polyolefins with high performance and increased durability. A molecular-level understanding of the active site structure is essential.

Objectives: correlating the molecular level properties of homogeneous and heterogeneous Cr-based catalysts and Ziegler-Natta catalysts, to their performances in the homo- and co-polymerization of olefins.

Approaches: *In-situ* and operando IR and UV-Vis spectroscopies / lab scale kinetics experiments

Collaboration with: SCITEC-CNR / UNINA / JAIST

Metal nanoparticles for catalysis

Description: Heterogeneous catalysts based on Platinum-group-metals are the workhorses of industrial scale production of fine and bulk chemicals and intermediates.

Objectives: Determination of the nature of the active site / surface and bulk reconstruction affecting nanoparticles in the presence of adsorbates / disclosure of the reaction mechanisms.

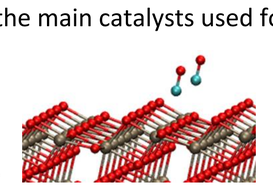
Approaches: *In-situ* and *operando* techniques: Infrared spectroscopy (IR); X-Ray Absorption spectroscopy (XAS); Neutron inelastic scattering; catalytic tests; microcalorimetry of adsorbed probes.

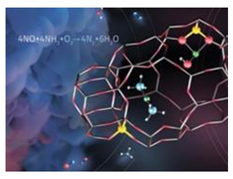
Collaboration with: SChimet A.p.A. / ESRF / ILL

Contact: Elena Groppo, e-mail: elena.groppo@unito.it

Catalysts for removal of NOx from exhaust gases

Description: The selective catalytic reduction of NOx to N_2 by ammonia (**NH_3-SCR**) plays an important role in the abatement of NOx emissions in the exhausts of diesel engines and power plants. **Cu-CHA zeolite and VOx-TiO2** are the main catalysts used for the reaction.





Objectives: improve catalytic activity and resistance to deactivation

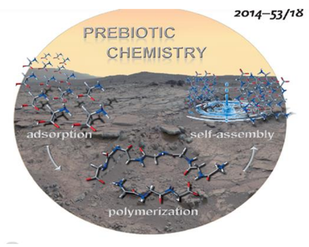
Approaches: synthesis of VOx-TiO_2, i*n-situ* and operando IR and UV-Vis spectroscopies, EPR, Raman

Collaborations

Origin of life

Description: Study of the formation and/or reactivity of aminoacids and small molecules on the surface of oxides

Objectives: Role of mineral surfaces in the formation of first polypeptides at the origin of life on earth in prebiotic conditions or in space



Approaches: Use of model oxide materials; Chemical Vapour Deposition or Selective adsorption; *In-situ* infrared spectroscopy

Collaborations: Sorbonne Université

Contact: Gloria Berlier -e-mail: gloria.berlier@unito.it

Characterization of porous materials for I_2 uptake

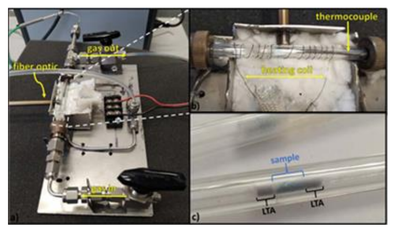
The activity is inserted in the frame of radioactive I_2 uptake for the treatment nuclear wastes.

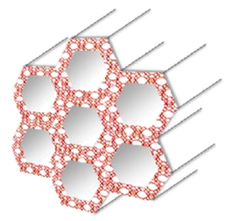
Commercial porous materials (MOFs and/or porous polymers) obtained through several synthetic approach (COFs, Covalent Organic Frameworks) will be characterized through several physico-chemical techniques and tested through UV-Vis and Raman spectroscopy in order to investigate: a) their ability in I_2 uptake; b) the adsorbed I_2 species.

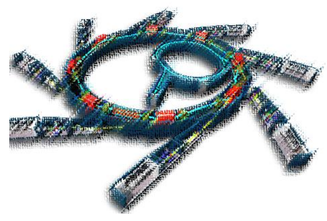
The experimental activity would be eventually supported by the modeling one (Gaussian and CRYSTAL code will be used) in order to get more clues about the energetical features of the I_2 uptake.

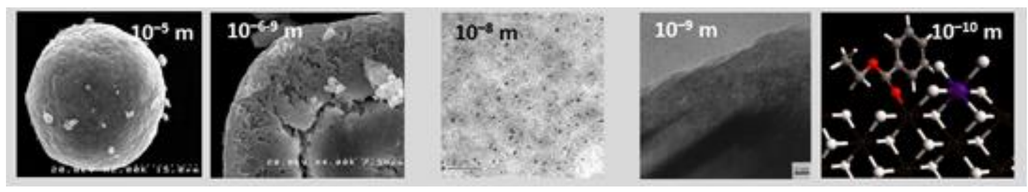
Contact: Alessandro Damin, e-mail: alessandro.damin@unito.it

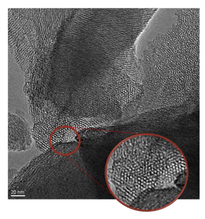
Some examples of equipment and materials





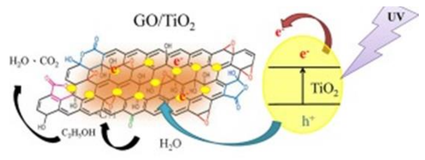






Photocatalysts for energy and green chemistry

Semiconductor oxide nanoparticles (e.g. TiO_2, ZnO) under irradiation can generate electron-hole pairs which can be exploited in different photocatalytic reactions. The functionalization with metal nanoparticles or low-dimensional carbon structures (e.g. graphene) can considerably improve their performance. A molecular-level understanding of the active sites coupling *in situ* spectroscopy and quantum-chemical calculations can guide the synthesis of improved photocatalysts.



Possible target applications:

- Photocatalytic H_2 production
- CO_2 photoreduction
- Green photocatalytic processes for salicylic acid production

Collaborations: Universitat de Barcelona, Università di Palermo

Functionalized synthetic nanohydroxyapatites

Hydroxyapatites are intrinsically biomimetic nanomaterials with engineerable shape, size and composition, comparable to the apatite particles in the bone mineral phase. Functionalization with different metals can optimize their properties for specific target applications.

Objectives: nanohydroxyapatites synthesis and functionalization by exchange or «one-pot» methods and their characterization for applications in catalysis and in nanomedicine (anticancer, antifungal and antibacterial).

Collaborations: CNR-ISTEC

Contact: Lorenzo Mino, e-mail: lorenzo.mino@unito.it;
Domenica Scarano, e-mail:domenica.scarano@unito.it

Collaborations abroad and with industry

Erasmus and other (not exhaustive.. Ask!)

- Institut Charles Gerhardt (Montpellier, France, **Erasmus**, gloria.berlier@unito.it)
- Universitat de les Illes Baleares (Mallorca, Spain, **Erasmus**, gloria.berlier@unito.it)
- Université Sorbonne (Paris, France, , **Erasmus**, gloria.berlier@unito.it)
- Queen's University (Belfast, Ireland, **Erasmus Traineeship**, gloria.berlier@unito.it)
- La Plata University and Comahue University, Argentina, **Bando Overseas**, giuliana.magnacca@unito.it)
- Aalborg University (Aalborg, Denmark, **Erasmus Traineeship**, giuliana.magnacca@unito.it)