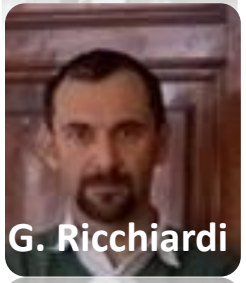
SURFIN

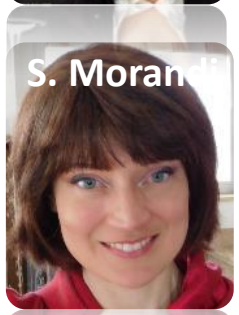
Synthesis, characterization and testing of functional materials mostly applied in the area of:

- heterogeneous catalysis and photo-catalysis
- sensors for gases and volatile species
- selective adsorption/separation/storage of molecules for the energy sector
- surface-related problems in industrial manufacturing

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 , gravimetric

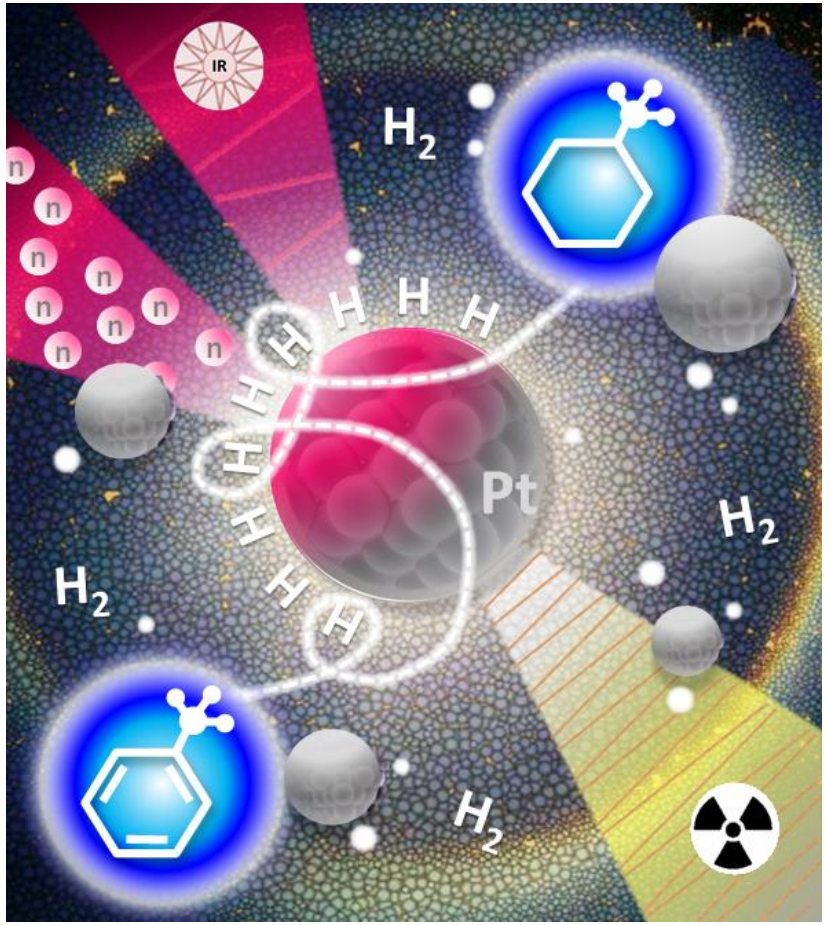




METAL NANOPARTICLES FOR CATALYSIS

Supervisor: E. Groppo
Number of available positions : 1
When: from September 2021
Where: Chemistry Department (Via Quarello 15)
In collaboration with: Chimet / ESRF / ILL

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.



ESRF
NEUTRONS FOR SCIENCE
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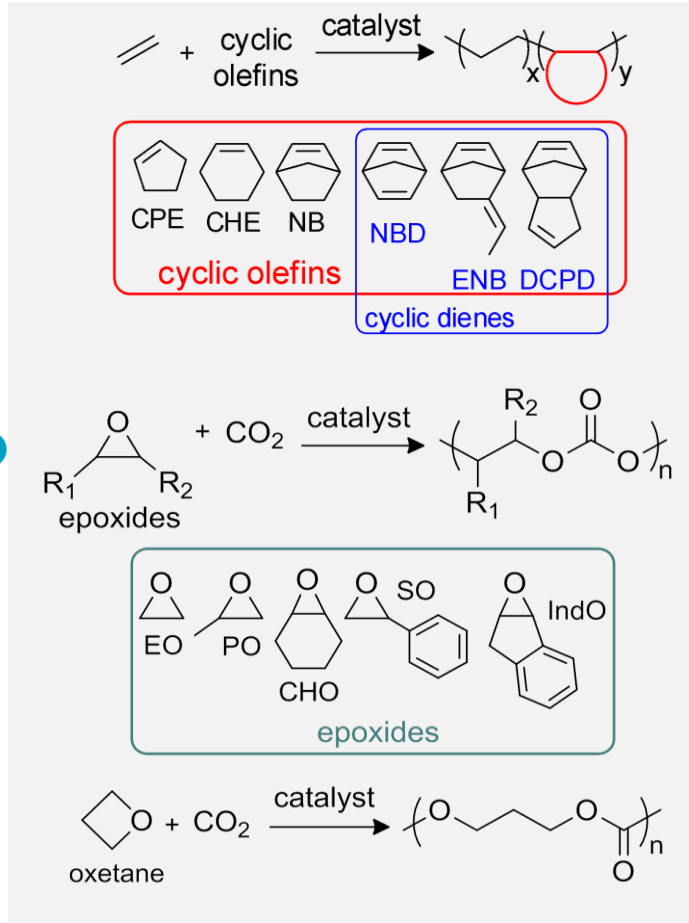
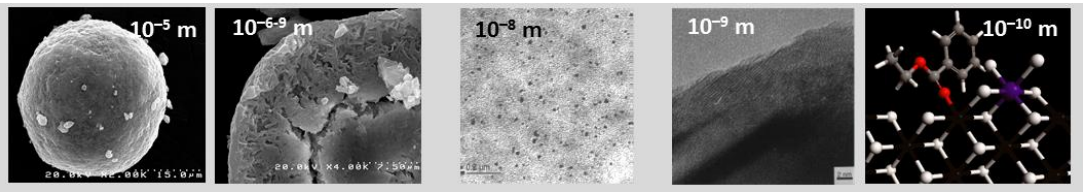
CATALYSTS FOR PRODUCTION OF (FUNCTIONAL) POLYOLEFINS

Supervisor: E. Groppo
Number of available positions : 2
When : from September 2021
Where: Chemistry Department (Via Quarello 15)
In collaboration with : SCITEC-CNR / UNINA / JAIST

PRIN2017

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





CATALYTIC RECYCLING OF POLYOLEFINS TO OLEFINS

Supervisor: E. Groppo, V. Crocellà, G. Ricchiardi
Number of available positions : 1
When: from September 2021
Where: Chemistry Department (Via Quarello 15)

Description: Plastic solid waste (PSW) is an ever-growing environmental challenge for our society. A key strategy to overcome this problem while also preserving carbon resources is to use PSW as a feedstock,
evolving towards a circular economy. Mechanical recycling alone is not adequate for addressing this global challenge. Chemical recycling via heterogeneous catalytic conversion has the potential to take PSW and convert it into usable monomers, fuels, synthesis gas, and adsorbents under more sustainable conditions than thermal degradation.

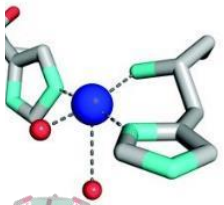
Objectives: developing new catalysts for degrading polyolefins to olefins and understanding their working principles.

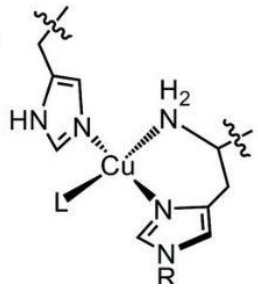
Approaches: Synthesis and characterization of porous materials with acidic functions. Exploration of their behaviour in the catalytic degradation of polyolefins to gaseous products and in particular olefins.

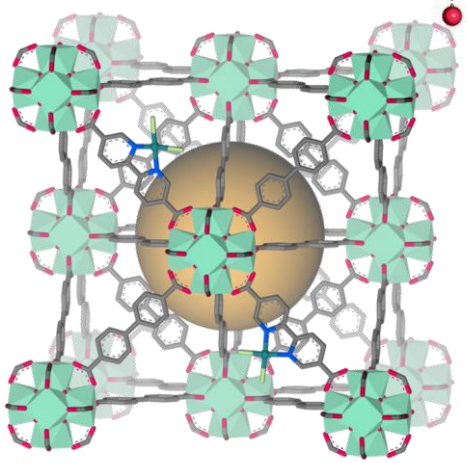
UNRAVELLING THE SECRETS OF CU-BASED CATALYST FOR C-H ACTIVATION (CUBE)

Supervisors: S.Bordiga, M. Signorile **In collaboration with**: Oslo; Max Plank and NMBU
Number of available positions: 2
When: from September 2021
Where: Chemistry Department (Via Quarello 15)

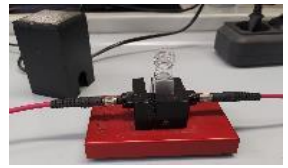
Horizon 2020
European Union Funding
for Research & Innovation







Description: 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. For this purpose, metal-organic frameworks (MOFs), based on Cu-functionalized ligands, have been suggested. In this work line, starting from a set of ligands made and characterized widely, some mixed ligand Cu-MOFs will be made and tested.



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.

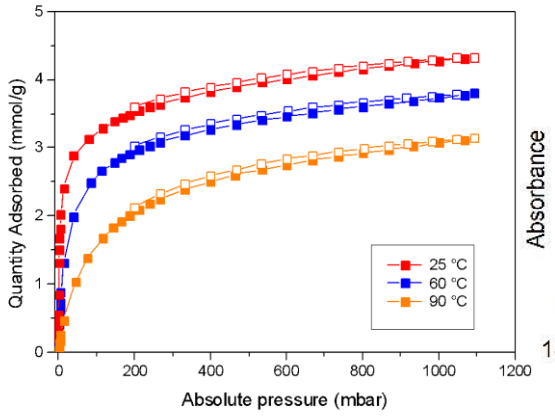
Approaches: *Use of in situ and operando spectroscopies on Cu-complexes (UV-Vis; IR; Raman) and Cu-MOFS combined with GC analysis to follow the target reaction. Possibility to combine molecular modelling activities.*

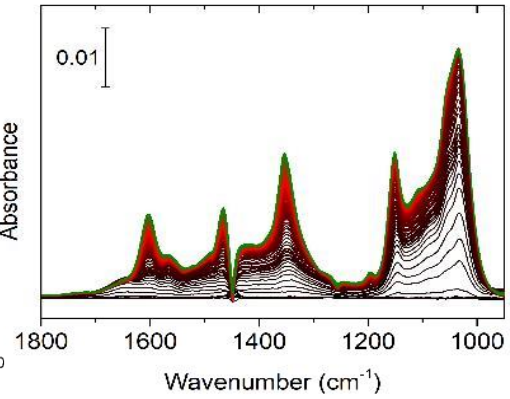
FUNCTIONAL MATERIALS FOR CARBON DIOXIDE CAPTURE AND UTILIZATION

Supervisors: F. Bonino, S. Bordiga, V. Crocellà, M. Signorile

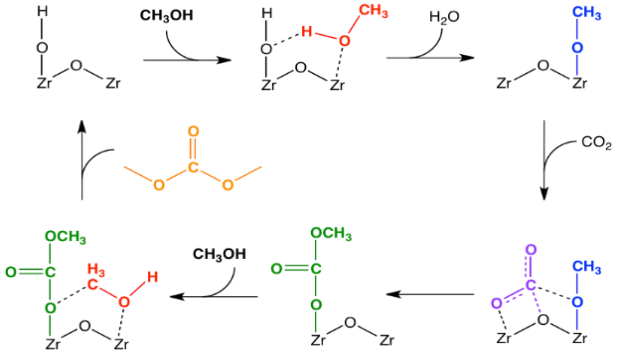
Number of available positions: 3
When: from September 2021
Where: Chemistry Department (Via Quarello 15)
In collaboration with: PoliTO, Istituto Italiano di Tecnologia

Description: The presence of a large amount of carbon dioxide in atmosphere is one of the most important environmental problem for our generation. Indeed, CO_2 is a greenhouse gasses and its presence causes an increase in the earth average temperature with serious consequences for life. In order to reduce its emissions in atmosphere, carbon capture storage (CCS) and carbon capture and utilization (CCU) have been proposed as solutions.





Objectives: Synthesis, functionalization, modification and advanced characterization of materials (zeolites, ordered mesoporous silica, Metal-organic-frameworks, composites, oxides, mixed oxides and bio-based ionic liquids) for CO_2 capture and conversion.



Approaches: multi-technique advanced characterization to study the materials, their capture capacity and their reactivity towards CO_2, mainly employing *in situ* and *operando* IR spectroscopy, volumetric approaches and microcalorimetric experiments.

CO2MOS
4AirCRAFT
Commissione europea
SATURNO

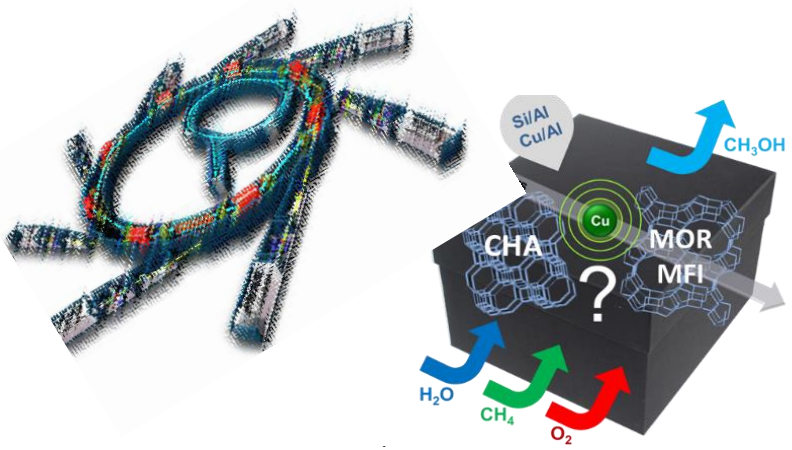
REDOX CHEMISTRY IN CU-ZEOLITES AND CU-MOFS INVESTIGATED BY ADVANCED X-RAY SPECTROSCOPY METHODS

Supervisor: E. Borfecchia
Number of available positions: 1
When: from September 2021
Where: Chemistry Department (Via Giuria 7)

Horizon 2020
European Union Funding
for Research & Innovation

In collaboration with: ESRF

DESCRIPTION Cu-exchanged zeolites today represent promising platforms for high-impact selective redox reactions, such as the direct oxidation of methane to methanol (DMTM), a potentially game-changing process in the environment and energy sector.



In situ/operando X-ray spectroscopy combined with innovative data analysis protocols provides unprecedent information on Cu-speciation under reaction conditions, helping to identify active sites and reaction mechanisms.

OBJECTIVES: To progress in the understanding of DMTM conversion over Cu-ZEO and Cu-MOFs, revealing structure/speciation ↔ activity relationships, while contributing to the development of innovative X-ray spectroscopy methods.

Approaches: *Depending on beamtime allocation @ ESRF and on student inclinations: operando XAS during CH_4-TPR analysed with statistical/multivariate approaches; in situ X-ray Raman Scattering, development of codes for treatment & analysis of time-resolved XAS datasets.*

ZEOLITES FOR CATALYSIS: TAILORING NEW HIERARCHICAL STRUCTURE AND ACTIVE SITES

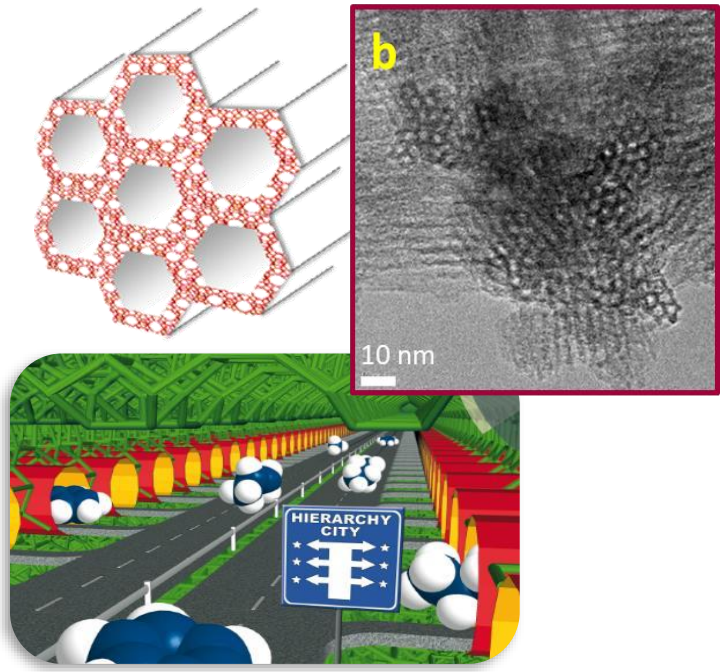
Supervisors: F.Bonino, V. Crocellà, M. Signorile

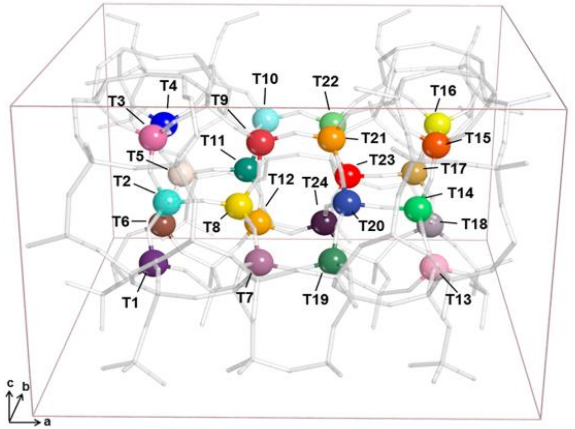
Number of available positions: 2
When: from September 2021
Where: Chemistry Department (Via Quarello 15)

Description: A promising field in heterogeneous catalysis is represented by the production of hierarchical zeolites, able to overcome the major drawbacks related to the dimensions of the zeolitic micropores. Ti-doped zeolites are extensively utilized as catalysts in industrially important oxidation reactions in the presence of H_2O_2 as oxidizing agent. The employment of hierarchical Ti-zeolite materials would help to catalyse oxidation reactions with bulky reactants, by overcoming the rate of intracrystalline diffusion for reactants and products.

Objectives: Synthesis of hierarchical Ti-zeolites. Advanced characterization to achieve a deep knowledge of the structural arrangement and how the zeolitic lattice is disposed in the multi-level porous system. Evaluation of the effect of the synthetic route on the Ti insertion into the framework and spectroscopic characterization of Ti species.

Approaches: Synthesis and multi-technique advanced characterization, in situ and operando approaches.





IMPROVING THE PERFORMANCE OF CATALYSTS FOR THE DENOX NH_3 SELECTIVE CATALYTIC REDUCTION

Supervisors: G. Berlier, S. Bordiga

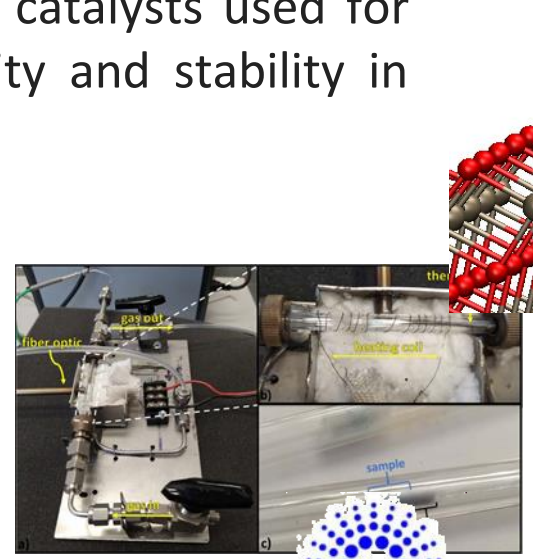
Number of available positions: 2
When: from September 2021
Where: Chemistry Department
In collaboration with: UMICORE and ESRF

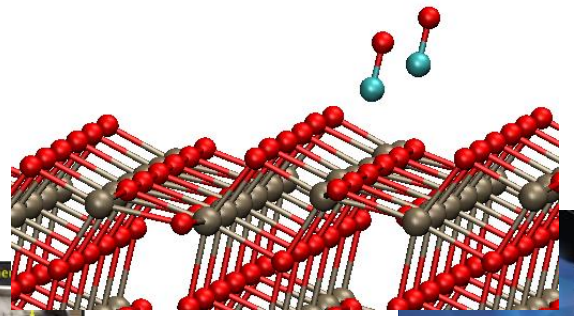
DESCRIPTION: The selective catalytic reduction of NO_x to N_2 by ammonia (NH_3-SCR) plays an important role in the abatement of NOx emissions in the exhausts of diesel engines and power plants since the 1970's. **Cu-CHA zeolite** and **VO_x-TiO_2** are the main catalysts used for the reaction, thanks to the good activity, selectivity and stability in different temperature ranges

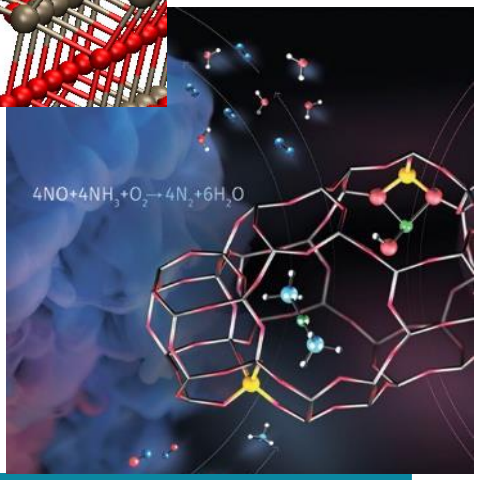
OBJECTIVES:

- Understand the deactivation process occurring in presence of SO_2 on Cu-zeolite catalyst.
- Understand the role of the support and of promoters on the dispersion, reducibility and catalytic activity of VO_x on TiO_2

Approaches: combined use of in situ and operando spectroscopies on industrial materials (DR-UV-Vis; IR; Raman). EPR to study reducibility and Raman for VOx dispersion.







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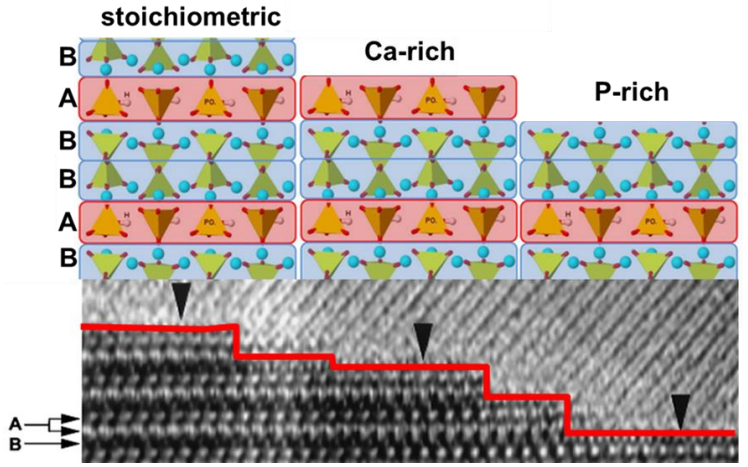
umicore
Automotive Catalysts

$$4\,NH_3 + 4NO + O_2 \rightarrow 4\,N_2 + 6\,H_2O$$

$$2\,NH_3 + NO_2 + NO \rightarrow 2\,N_2 + 3\,H_2O$$

FUNCTIONALIZED SYNTHETIC NANOHYDROXYAPATITES FOR CATALYTIC AND BIOMEDICAL APPLICATIONS

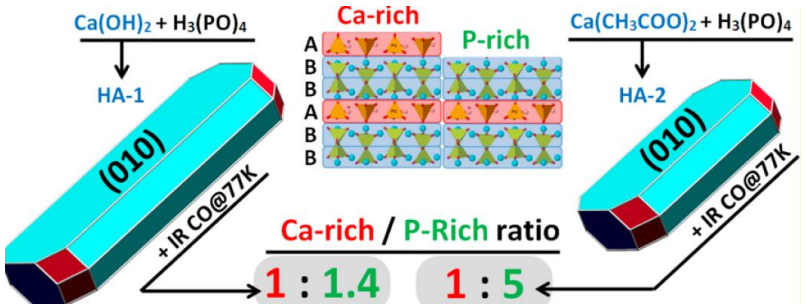
Supervisor: L. Mino
Number of available positions : 1
When: from September 2021
Where: Chemistry Department (Via Giuria 7)
In collaboration with: CNR-ISTEC – Faenza



Description: nanohydroxyapatites (nHA) are intrinsically biomimetic nanomaterials with engineerable shape, size and composition, comparable to the apatite particles in the bone mineral phase. They can be employed in catalytic and biomedical applications (anticancer, antifungal and antibacterial). Their performance can be improved by metal functionalization.

Objectives: nHA synthesis and determination of structure/activity relationships.

Approaches: synthesis of nHA and functionalization by exchange or «one-pot» methods; multitechnique characterization by FT-IR, UV-Vis, BET, electron microscopy, XRD.



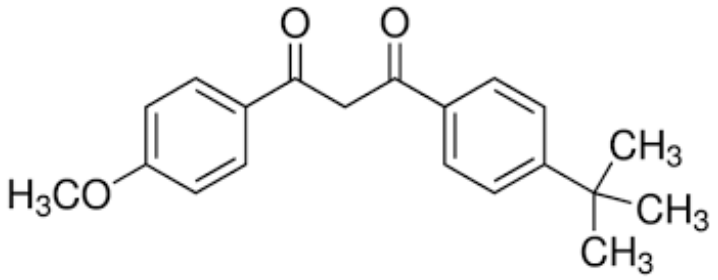
istec
National Research Council of Italy
Institute of Science and Technology for Ceramics

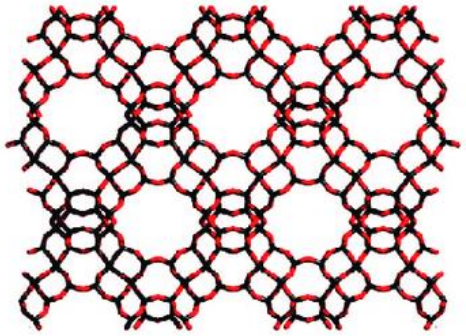
HYBRID ORGANIC-INORGANIC MATERIALS AS INNOVATIVE SUNSCREENS

Supervisor: L. Mino
Number of available positions : 1
When: from September 2021
Where: Chemistry Department (Via Giuria 7)
In collaboration with: Unimore (Patent pending)

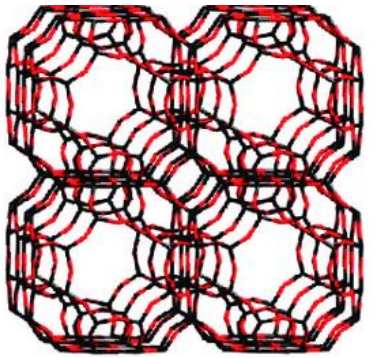
Description: encapsulation of UV filters in inorganic matrices (zeolites) can increase the organic filters stability while preventing their percutaneous intake and release into the environment.
Objectives: testing photostability under UV exposure, determination of the optimal UV filter loading, assessment of encapsulation stability in a simulated marine environment.
Approaches: loading of the UV filter in the zeolites; multitechnique characterization by FT-IR (with *in situ* UV irradiation) and UV-Vis spectroscopies, TGA, BET and XRD.

Avobenzone (organic UV filter)





Faujasite



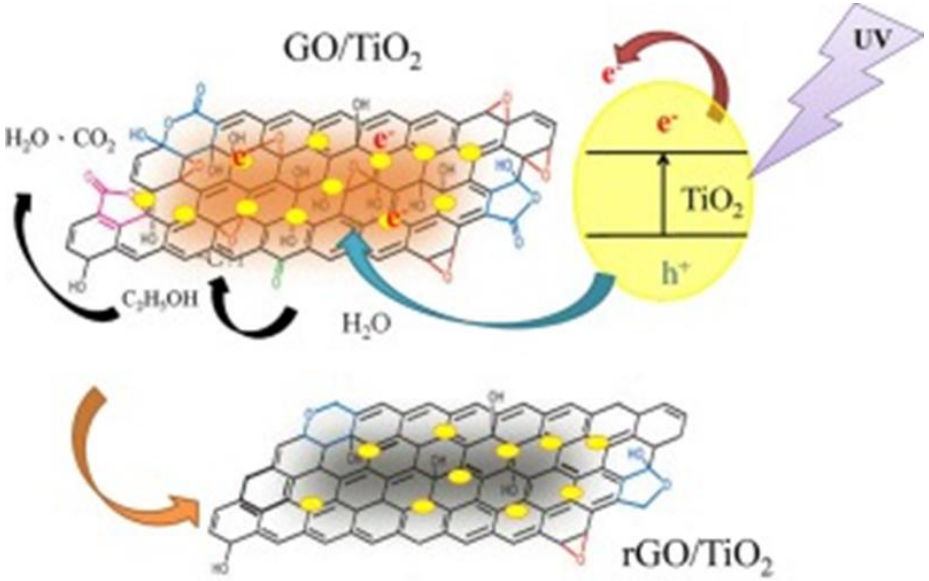
Zeolite A

UNIVERSITAS STUDIORUM MUTINENSIS ET REGIENSIS 1175

UNIMORE
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

OXIDE-BASED NANOCOMPOSITES FOR PHOTOTOCATALYTIC APPLICATIONS

Supervisor: L. Mino
Number of available positions : 1
When: from September 2021
Where: Chemistry Department (Via Giuria 7)
In collaboration with: INRiM



Description: Semiconductor oxide nanoparticles (e.g. TiO_2, ZnO) under irradiation can generate electron-hole pairs which can be exploited in photocatalytic reactions (pollutants abatement, H_2 photoproduction, bacteria photokilling). The functionalization with metal nanoparticles or low-dimensional carbon structures (e.g. graphene) can considerably improve their performance.

Objectives: investigation at the molecular level of the surface processes occurring during the target photocatalytic reactions; determination of structure/activity relationship to improve the photocatalyst performance.

Approaches: synthesis of the nanocomposites; Raman, *operando* FT-IR (under *in situ* UV irradiation), UV-Vis, TGA, BET, electron microscopy, XRD; photocatalytic activity tests; antibacterial activity tests.

INRiM ISTITUTO NAZIONALE DI RICERCA METROLOGICA

SURFACE INTERACTIONS IN GLASS FOR PHARMACEUTICAL PACKAGING

Supervisor: G. Ricchiardi (in collaboration with M. Pazzi)
Number of available positions : 1
When: from September 2021
Where: Chemistry Department (Via Giuria 7-9 and Via Quarello 15)

SOFFIERIA BERTOLINI S.p.A.

Description: Contrary to a common belief, glass is definitely not an inert material! When used for the **packaging of drugs**, the interactions between the drug and the glass container surfaces need to be understood and minimized. This work, in collaboration with a leading industry in the field, explores glass surface corrosion and surface treatments from an industrial production perspective.

Objectives: developing glass pharmaceutical packaging with improved safety and reliability.

Approaches: The main techniques adopted are electron microscopy, advanced chemical analysis, ellipsometry. A stage in the industry can be coupled with this thesis.