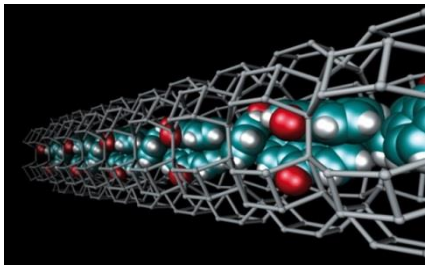
Zeolites and microporous materials

Giovanna Vezzalini, Michelangelo Polisi

Diamond anvil cell for X ray diffraction in-situ at high pressure

European SynchrotronRadiation Facilities,
ESRF, Grenoble

Hybrid material zeolite L/dye Fluorenone: close packed fluorenone molecocules in 12-membered channel of ZTL



CONTACTS

Prof. M.Giovanna Vezzalini
mariagiovanna.vezzalini@unimore.it
Tel. +39 059 205 8471

RESEARCH TOPICS

Zeolites are hydrated microporous materials. They consist of corner-sharing $(Si,Al,P)O_4$ tetrahedra forming an open framework with cages and channels of molecular dimensions. For this reason, zeolites are considered as "nanoporous" materials, in which the “open space” can be filled by suitable guest molecules and cations. Steric hindrances due to the geometry of zeolite voids allow to select the guest systems according to their size and/or shape, so that molecular separation, and therefore their use as molecular sieves, is possible. Zeolites are also being adopted as "nano-reactors" in the field of heterogeneous catalysis; actually, their relevance for the petrochemical industry makes zeolites one of the most exploited and economically relevant nanosystems up to date. The high selectivity and yield of zeolites-catalyzed reactions is due to the fact that shape and size of framework pore systems control the access of reactants and products to/from the catalytically active sites within the voids. Zeolites are also promising framework materials for innovative applications: due to their structural voids, they are being used as a mould for creating regular arrays of semiconductor quantum dots and wires, wires of organic dyes for new luminescent materials. In general, species of different nature (organic or inorganic, neutral or ionic) can be encapsulated in zeolites pores.

Thermic and baric behavior and stability of natural and synthetic zeolites
The knowledge of the stability fields and of the temperature-induced structural modifications of these materials is of prime importance to assure their persistence and effectiveness in technological applications. Also the understanding of the behavior of zeolite materials under pressure is of fundamental importance due to the impact of this thermodynamic parameter on their structures, stability, the accessibility of the zeolite catalytic sites for the molecular species entering the porous material and consequently their applications. For both these topics a combined approach of experimental (Synchrotron X-Ray Powder Diffraction and Rietveld structural refinements) and computational (Molecular Dynamics) methods are used.

Study of the pressure-induced aggregation of molecules in microporous cavities
Aim of this topic is to explore whether and how the morphology of the nanoporous frameworks affects the properties of the guest species encapsulated through compression. The shape-controlled aggregation of hyperconfined nanophases is achieved by using, as pressure transmitting media, liquid solutions containing the molecular species to be segregated inside the zeolitic nanopores.

Hybrid materials zeolite/dye
Incorporation of dye molecules in zeolite channels, allowing for the supramolecular organization of the photoactive species. The ordered distribution of zeolite channels imposes severe space restrictions and geometrical constraints to the inserted guest species, leading to very high concentrations of well oriented dye molecules. These composites can be used as more efficient devices for artificial photosynthesis, water splitting, photovoltaic applications and targeting therapeutic agents. The structural characterization of these materials is carried out with (UV-Vis) spectroscopy, simulations of Molecular Dynamics and X-ray diffraction.

Skills:
The group skills can be summarized as follows:
i) Single crystal X-ray diffraction (SC-XRD)
ii) X-ray powder diffraction (XRPD) at ambient and non-ambient conditions
iii) In-situ X-ray diffraction using synchrotron light
iv) Synthesis of hybrid materials zeolite/dyes

Collaborations:
Prof. Simona Quartieri –Università di Messina
Prof. Rossella Arletti- Università di Torino
Prof. Ettore Fois, DSAT-Università dell’Insubria
Prof. Gloria Tabacchi, DSAT-Università dell’Insubria
Dr. Francesco Di Rienzo, Directeur de recherche Matériaux Avancés pour la Catalyse et la Santé Institut Charles Gerhardt Montpellier, ENSCM
Dr. Joël Patarin, Directeur de Recherche CNRS, Equipe Matériaux à Porosité Contrôlée (MPC), Institut de Science des Matériaux de Mulhouse, Université de Haute-Alsace, Institut J.B. Donnet