XLII cycle PhD Course, Academic Year 2026/2027
Ph. D Course "Models and Methods for Material and Environmental Sciences"

Research title:

Structural Characterization of Defects in Zeolites for Tunable Hydrophobicity and VOC Adsorption

PhD student: Irene Pini[1]
First supervisor: Rossella Arletti[1]
Second supervisor: Svetlana Mintova[2]

[1]*Department of Chemical and Geological Sciences, University of Modena E Reggio Emilia, 41125 Modena, Italy;*
[2]*Laboratoire de Catalyse et Spectrochimie, LCS, UMR 6506, ENSICAEN, France.*

Despite stringent environmental regulations, the effective abatement of Volatile Organic Compounds (VOCs) emitted from industrial processes and diffuse sources remains a critical challenge for air quality and public health, making the development of advanced solutions for their selective capture and removal a high priority. Among porous materials, zeolites are prime candidates for the selective capture of VOCs. Zeolites are crystalline tecto-aluminosilicates characterized by a three-dimensional framework of interconnected TO_4 tetrahedra (T = Si,Al) that enclose an open system of pores, channels, and cavities of molecular size. Thanks to their porosity, zeolites act as molecular sieves able to trap gaseous species inside their framework. In environmental applications, the efficiency of VOC adsorption is strongly related to the hydrophobic character of the adsorbent material, which is essential to prevent atmospheric moisture from competing with organic contaminants for access to the pores. Even though research so far has focused on controlling bulk compositional parameters — especially the silica-to-alumina ratio (Si/Al) and the extra-framework cation composition (K^+, Ca^{2+}, Na^+, Zn^{2+}, Cs^+) — the decisive role played by local imperfections and framework defects (such as silanol groups) formed during synthesis, or post-synthesis treatments, is still not fully understood. In fact, these defects can significantly affect hydrophobicity and in turn, surface energy, local chemistry of adsorption sites and transport dynamics within the pores. This PhD research project aims to fill this gap by exploring defect engineering as a key strategy to tune hydrophobicity and affinity toward specific model VOCs: benzene, toluene and hexane. This study focuses on comparing different zeolite topologies such as MFI, MWW, FAU and MER topologies. The experimental work will be based on an analytical and multi-technique approach. The morphology and microstructure of the crystallites will be investigated using scanning electron microscopy (SEM), while the bulk chemical composition will be determined by X-ray fluorescence (XRF) and inductively coupled plasma mass spectrometry (ICP-MS). The channel architecture and the identification of framework defects, both before and after the gas capture process, will be studied in detail by combining Fourier-transform infrared spectroscopy (FT-IR) with X-ray powder diffraction (XRPD) including Rietveld refinement on synchrotron data and neutron diffraction (ND). Finally, VOC adsorption performance, the amount of retained molecules, and the subsequent regenerability of the solid material will be quantified through thermogravimetric and differential thermal analysis (TG/DTA). In this way, the project aims to establish quantitative correlations between defect density, pore topology, hydrophobicity, and adsorption isotherms, paving the way for rational design principles for new-generation zeolitic adsorbents with high efficiency and environmental sustainability.