Open Postdoc Position
Co-adsorption in MOFs materials: Combining Molecular Dynamics & Grand Canonical Monte Carlo simulations"

Position for 1 year. Starting Date: July 2016

Keywords: Molecular Dynamics, Grand Canonical Monte Carlo, Metal Organic Frameworks, liquid and gas phases, CO_2, CH_4, CO, N_2, selectivity, self and transport diffusivities.

Over the past decade, a novel class of inorganic-organic porous materials, nowadays known as MOFs or Metal-Organic Frameworks, emerged as a new domain in solid state research. MOFs are tailor-made nanoporous materials formed by self-assembly of metal ions or clusters, linked together via a variety of bridging ligands. What was initially a scientific curiosity has transformed into a fully qualified field of research. Rapid developments and recent breakthroughs indeed have resulted in the discovery of close to 1000 different MOF structures, even if only a limited number have stable open structures with sufficiently large pores for applications. In order to achieve tailored dimensions of cages and tunnels, and to maximize surface areas, one method is to systematically vary the polyfunctional ligands in MOFs. It is well known that both the adsorption performance of such MOFs are strongly influenced by a combination of competitive adsorption and differences in transport properties.

The present project will focus on innovative classes of MOFs synthesized by the Institut Lavoisier in Versailles. Classical simulations including ***Grand Canonical Monte Carlo (GCMC)*** and ***Molecular Dynamics (MD)*** will be used to fully characterize the selectivity and transport properties of several newly synthesized MOF materials with respect to different gas mixtures. Both, MD and GCMC on small and large MOF systems will be conducted using either rigid or flexible force field we have recently developed. We will look in particular at the gas/vapor applications including CO_2-N_2 ***and*** CO_2-CH_4 ***separations***. Furthermore, our expertise on equilibrium MD simulations will provide additional information on the molecular diffusion mechanisms of the separation processes in gas phase. In a mean time, the ***impact of moisture on the coadsorption process*** will be explored. A special effort will be dedicated to ***implement ab initio forcefield*** in GCMC code to accurately describe the interactions between some guest molecules and the coordinatively unsaturated sites present at the surface of the MOFs.

This work will be performed in strong interactions with groups expert in synthesis of MOF and characterization of their adsorption performances.

The candidate has a strong expertise in Grand Canonical Monte Carlo and Molecular Dynamics simulations.

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