Open PhD Position
"Computational exploration of the performances of mechanically constrained MOFs for gas separation"

Position for 3 years; Starting Date: Flexible

Keywords: Grand Canonical Monte Carlo, Molecular Dynamics, Flexible Metal Organic Frameworks, mechanical behavior, gas separation.

One fascinating property of many porous Metal-Organic Frameworks (MOFs) is their stimulus-induced flexibility, a unique feature in the field of nanoporous adsorbents with respect to other reference materials such as active carbons and zeolites. Guest-induced pore size/shape modulation of this class of porous solids (breathing, ligand flip, pore gating…) has revealed unexpected adsorption/separation phenomena pointing towards new horizons for adsorption-based technologies. Such structural changes have been also tuned by a mechanical stimulus. In this context, this project aims to seize opportunities via the mechanical fine-tuning of the pore architectures of flexible MOFs to modulate their gas and/or vapor adsorption properties. This synergistic combination of pore architecture and adsorption properties will be a unique opportunity to develop **new concepts to optimize current separation-based processes with controlled molecular sieving, gate opening and entropy-driven phenomena**. A joint theoretical/experimental approach will be taken where new tools will be designed to tackle this address this challenging project. The joint PhD position between the Institut de Physique de Rennes (Université Rennes 1, France) and the Institut Charles Gerhardt Montpellier (Université Montpellier, France) will aim to apply **force field based-Molecular Dynamics simulations** on a series of **flexible MOFs** to predict the amplitude, the reversibility/irreversibility and the energetics of the pressure-induced structural changes of the guest-loaded MOFs as a function of the magnitude of the applied pressure and to capture the physical insights into the structural transition. The PhD will further apply **Hybrid Osmotic Monte Carlo** (HOMC) approach to **predict the single and binary mixture component adsorption isotherms and enthalpies** for the diverse mechanically constrained MOF/guest systems that will be directly compared to the experimental data collected by our collaborators and (ii) to gain microscopic insight into the synergistic interplay between the dynamics of the MOFs framework and the confinement of the guest molecules at the origin of the adsorption/separation processes.

This project is supported by a French Collaborative Project ANR assembling complementary groups working in MOF synthesis/structure (Institut des Matériaux Poreux de Paris-IMAP-C. Serre, Paris), experimental adsorption (MADIREL-P.L. Llewellyn, Marseille) and molecular simulation (ICGM and IPR) It will offer a great opportunity for the fellow to build strong collaboration with both experimental and theoretical partners.

Potential candidate should have a background in theory for forcefield-based simulations including Grand Canonical Monte Carlo or/and Molecular Dynamics.

Contact : CVs should be sent to Dr. Aziz Ghoufi, Institut de Physique de Rennes UMR 6251, Université de Rennes 1, email : aziz.ghoufi@univ-rennes1.fr, tel +33 2 23 23 69 93 & to Prof. G. Maurin, Institut Charles Gerhardt UMR CNRS 5253, Université Montpellier, France, email : guillaume.maurin@univ-montp2.fr, tel +33 4 67 14 33 07.