Open PhD Position CIFRE Total Energies/ICGM Montpellier
Numerical exploration of hybrid porous materials & their composites for H_2/CH_4 separation

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Position for 3 years; Starting Date: October 1 2023

Keywords: force field Monte Carlo, Molecular Dynamics, Metal Organic Frameworks, shaping, gas separation.

MOF (Metal-Organic Framework) materials are one of the most recent classes of porous materials made of metal oxide nodes connected by organic ligands. These materials present an unprecedented versatility in terms of pore sizes/shapes (from the micro- to the meso-sizes usually spanning from 0.3 nm to >2-3 nm) and chemical functionalities that decorate their pore walls. They have attracted interests for a wide range of applications in the fields of energy and environment. Although a large series of computational and/or experimental studies have been able to identify a myriad of promising MOF candidates for diverse gas adsorption/separation applications, while so far only a few MOFs have been proposed/tested as sorbents for the highly challenging separation of CH_4 from H_2. They can potentially offer alternative selective porous materials to the traditional adsorbents such as zeolites and activated carbons for further implementation in Pressure Swing Adsorption processes.
In this PhD, our first objective is to deploy advanced Monte Carlo and Molecular Dynamics simulations to computationally screen the separation performance of a large series of MOFs in order to identify the best candidates for recovering H_2 via different possible physisorption-based separation-mechanisms. As a further step, the impact of the shaping on the separation performances of the best selected MOFs will be assessed computationally. This overall set of numerical predictions will guide the experimental effort towards the selection of the most promising MOF sorbents for H_2 recovery and the fabrication of the optimum shaped MOFs for further testing.
This CIFRE PhD project is funded by TotalEnergies and will imply the collaboration with experts in synthesis of MOFs and adsorption testing. It will offer a great opportunity for the fellow to build strong collaboration between experimental/theoretical/industrial partners.

Potential candidate should have a background in theoretical physical chemistry/chemical physics, statistical physics and in forcefield-based simulations including Monte Carlo or/and Molecular Dynamics applied to porous materials and eventually composites.

Salary: 1650 euros/month for 3 years

Contacts: CV and letter of motivation should be sent to Prof. G. Maurin, Institut Charles Gerhardt UMR CNRS 5253, Université Montpellier, France, email: Guillaume.maurin1@umontpellier.fr, and to Dr. Yann Magnin, TotalEnergies, email: yann.magnin@totalenergies.com