Ph.D. position at the University of Bourgogne Franche-Comté (UBFC) in Dijon France

At the physical chemistry department INTERFACE, Laboratory ICB associated to CNRS (UMR 6303).

Graduate school EIPHI-BFC, école doctorale "Carnot-Pasteur".

Project title:

Molecular simulation of small molecules in interaction with porous materials and ice at cryogenic temperature.

Background:

It is well known that nanoporous materials (zeolite, graphite, clay, clathrates, etc.) and ice can act as host matrixes for the storage and separation by physisorption of small gaseous molecules (H_2, N_2, NO_x, SO_x, CO, CO_2, CH_4, C_2H_4, O_2, etc.). According to their adsorption affinity with the solids and the temperature the composition of the gas phase can change. These properties are used for example in the industry for separating isomers or isotopes, clean atmospheres, or again to store energy or molecules.

Their consequences are also visible in nature and in particular in the context of astronomy where the observed atmosphere of planets and planetoids are partially explained by these selective storage properties at low temperature. This aspect of the thesis is part of a larger project in collaboration with the lab. UTINAM in Besançon (group SPACE astrochemistry).

The PhD thesis will be done in the group "Adsorption on porous Solids" of the ICB laboratory, specialized on the adsorption of small molecules in porous systems by using experiments and molecular simulation.

Ph.D. project:

The aim of the project is to simulate the trapping properties of small molecules (H_2, N_2, CO, CH_4, C_2H_4, O_2, CO_2) from gas mixtures on different type of zeolites (MFI, FAU, LTA), clathrate hydrates, Metal Organic Framework (MOF) using molecular dynamics simulations. The candidate will use molecular dynamics and Monte-Carlo codes and should be able to modify them and develop the necessary analysis tools. From simulations equilibrium properties like adsorption isotherm, adsorption heat and transport properties (e.g.,diffusion) will be computed inside the pores and at the external surface. The external surface is a relevant issue to better understand the kinetics of adsorption or exchange between different types of gas. In parallel, experiments will be performed to compare with simulations. Thermodynamic and kinetic models will be proposed to model the adsorption phenomena. A focus will be put on the extension of nanothermodynamics to adsorption.

Expected skills of the candidate:

Masters degree in physics, physical chemistry or related field. Good knowledge of thermodynamics. Basics in statistical mechanics. Experience in programming and / or numerical simulations is an advantage. Great motivation for scientific research and good writing skills.

Supervisor and Research institutes at the University of Bourgogne-Franche Comté, France:

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