PhD Position Available
Lab. Interdisciplinaire Physique (LIPHY)
Grenoble, France

Available Sep/Oct 2022

Acoustic Response of Fluid Adsorption and Transport in Nanoporous Materials: Molecular Simulation and Theory

Benoit Coasne's Research Group (https://benoitcoasne.github.io/)

Fluids within nanoporous materials are the topic of intense research to unravel the impact of nanoconfinement and surface forces on fluid thermodynamics and dynamics. From a practical viewpoint, such nanconfined fluids are at the heart of efficient technologies impacting our economy/ecology: energy storage/conversion, environment protection, health/human welfare, agribusiness/food science, etc. In particular, adsorption and separation in nanoporous solids are expected to address increasingly complex problems such as bio/agropollutants removal, greenhouse gas mitigation, drinkable water production, etc.

In this PhD thesis, we will employ classical molecular modeling and theoretical approaches – from the atomic to the macro scales – to unravel the acoustic signature of adsorption/transport in nanoporous materials. At each scale, we will probe spontaneous acoustic emission by the fluid/solid system and its response to acoustic wave stimulation. Comparison with experiments done in our group and in the context of a national research project will be performed at each scale. Fluids with different interactions (He, CH_4, CO_2) will be studied in nanoporous materials to probe pore size/interaction effects. By varying, statically or dynamically, the pressure gradient inducing flow and the mean pressure/temperature, the role of transport type (Knudsen, diffusion, viscous flow) and adsorption type (partially and entirely filled pores) will be probed (**Fig.**).

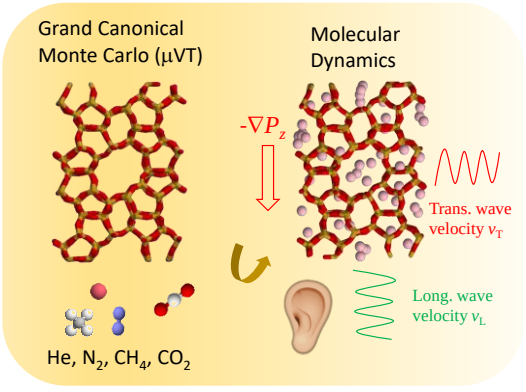

Fig. Acoustic response. Adsorption for different gases will be considered using Monte Carlo simulations. Transport will be also simulated using non-equilibrium molecular dynamics by imposing a transport gradient (here, ∇P). For different adsorption and transport conditions, the acoustic response of the system will be determined.

Candidates. Applicants should have a master in physics, chemistry or materials science with strong background in physics, physical chemistry, chemical physics.

Practical aspects. The position is available starting Sep. 2022 and lasts for 36 months. The net take home salary is about ~1400 euros/month. Applicants should provide a CV, a letter of motivation, and the names and e-mail addresses of 2 or 3 references to: **Benoit Coasne**, benoit.coasne@univ-montp2.fr

More information: https://benoitcoasne.github.io/ (research group website)

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