

**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**

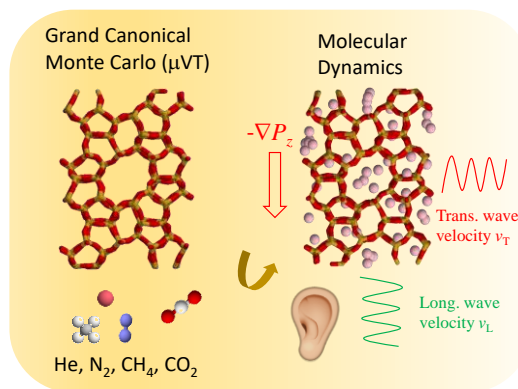
Benoit Coasne's Research Group (<https://benoitcoasne.github.io/>)

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<sub>4</sub>, CO<sub>2</sub>) 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.**).

**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-grenoble-alpes.fr](mailto:benoit.coasne@univ-grenoble-alpes.fr)



**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,  $\nabla P$ ). For different adsorption and transport conditions, the acoustic response of the system will be determined.

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