# Sujet de stage de Master 2 (2024) proposé par l'équipe PMMD du LMGC

## Fluid-solid coupling simulations in nanoporous materials

Nanoporous materials have pores smaller than hundred nanometers in diameter, have a large specific surface area, and are therefore significantly affected by adsorption-induced deformations. Recent developments of new materials such as metal-organic frameworks have recently attracted renewed interest. Nevertheless, adsorption-induced deformation has been observed in numerous engineering and natural processes, such as natural gas recovery, drying of cement, CO2 sequestration, crack formation after drying in aqueous electrodes of Li-ion batteries, soil erodibility and water actuation of plant seeds.

This project aims to study the *deformations of the microstructure of porous materials due to the adsorption of fluids* by molecular dynamics. The starting point of this work are recent simulation studies [1,2], proposing a framework for coupling fluid-solid interactions. We will develop and use codes to analyze water adsorption in porous materials with simple and complex microstructure and understand the adsorption induced deformations at different length scales.

References:


1. T. Zhou, K. Ioannidou, F. Ulm, M. Bazant, R. Pellenq, "Multiscale poromechanics of wet cement paste", Proceedings of the National Academy of Sciences (2019)
2. T. Zhou, K. Ioannidou, E. Masoero, M. Mirzadeh, R. Pellenq, M. Bazant, "Capillary stress and structural relaxation in moist granular materials", Langmuir (2019)


### Methodology

The study of adsorption in porous materials will be based on Density Functional theory simulations with in-house codes. The mechanical deformation will be studied with Molecular Dynamics simulations using the LAMMPS code in the cluster of University of Montpellier.

### Host laboratory

This Master internship will take place at the Laboratoire de Mécanique et Génie Civil (LMGC) in Montpellier. It can be followed by a PhD thesis.

### Contact


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### Research profile

Master of physics, applied mathematics or mechanics, and strong interest in numerical simulations. The successful candidate for this project must have knowledge in Statistical Physics of Condensed Matter and familiar with related numerical methods (Molecular Dynamics, Density Functional Theory or Discrete Element methods). Ability in coding will be strong advantage and a sufficient command of English will be a plus.