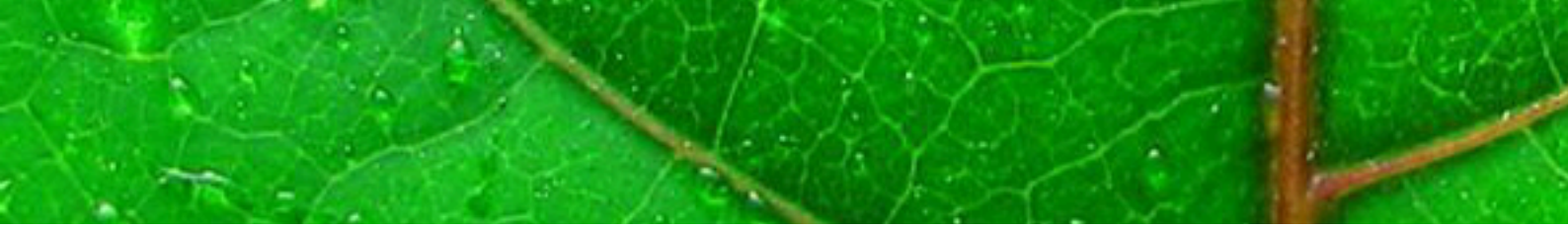


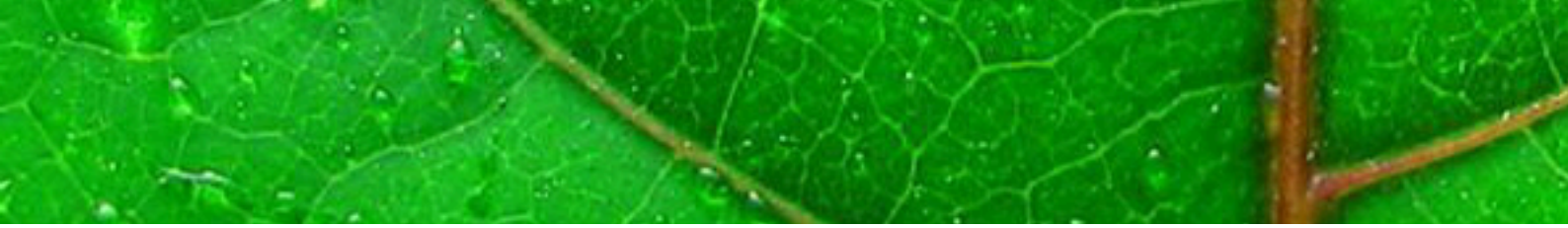
MolecularSimulation Chair

Atomistic and multi-scale simulations of coupled transport of confined fluids in nanoporous media

The chair "Atomistic and multi-scale simulations of coupled transport of confined fluids in nanoporous media" aims at providing fundamental insights and practical bottom-up simulation strategies for the transport processes of confined fluids (CO2, hydrocarbon mixtures, contaminants) in porous materials that are of great interest for numerous applications involving geo-resources exploitation or artificial membranes (microporous carbons, gas hydrates, cement).

Recently, solutions for energy and environment (CO2 sequestration, enhanced oil recovery, radioactive waste management) increasingly involves extremely confined fluids.

In such cases where solid-fluid interactions prevail, Amaël proposes to use and develop molecular simulations to elucidate transport and adsorption properties as well as their links with the mechanical and structural properties of the solids, and to upscale them at the engineering scales with lattice based methods..



Amaël Obliger : 2014, PhD at Université Pierre et Marie Curie. Electrokinetic transport in charged porous media.

2014-2017, postdoc at MIT. Transport properties of source rocks' organic matter.

2017-2018, postdoc at UC, Berkeley. Ionic diffusion and charge carriers dynamics in semiconducting perovskites