PhD position

Title : Molecular simulation of gas adsorption and transport in flexible porous carbons : coupling chemistry, mechanics, adsorption and transport

Affiliation : Institute for Molecular Sciences, Theoretical Chemistry Group, University of Bordeaux (https://www.ism.u-bordeaux.fr/spip.php?rubrique9)

Supervisor: Dr Jean-Marc Leyssale (https://www.ism.u-bordeaux.fr/spip.php?auteur624&lang=en)

Project description: Gas adsorption/desorption in/from porous carbons occurs in many natural (hydrocarbon expulsion) or industrial (gas separation and storage, batteries, etc...) processes. However, the couplings existing between the chemical nature of the carbons, their elasticity and their adsorption and transport properties remain unclear. Molecular simulation techniques (molecular dynamics (MD) and Monte Carlo (MC)) are powerful tools to investigate adsorption and diffusion in nanoporous media, yet they require having at hand (i) realistic atomistic models of the considered carbon adsorbents, and (ii) being able to account for the adsorbent deformation due to adsorption.

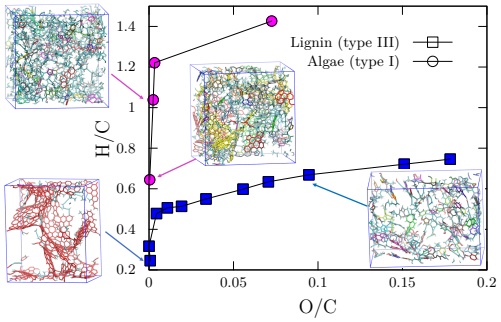

Fig. 1: Evolution of porous carbon upon geological burial of Lignin and Algae (REMD simulations).

In recent work we have shown (Fig. 1) that it is possible to generate accurate models of natural porous carbons by simulating their geological genesis and evolution using the replica exchange molecular dynamics method (REMD)[1,2], an accelerated MD technique. Also, combining Monte Carlo simulation in the Grand Canonical ensemble (GCMC) and isothermal-isobaric (NPT) MD, we have been able to account for adsorption-induced deformation in model porous carbons [3].

In this PhD we propose to build a detailed structure-property relationship allowing to relate adsorption and transport properties to the chemical nature, structure and porosity of the carbons and to their elasticity. In that aim, REMD simulations will be performed to identity and complete a data-base of structural models. Structural, elastic, adsorption and transport properties will then be investigated using MD and GCMC simulations. An applicative objective will be the quest for optimal performance in enhanced natural gas recovery via CO_2 adsorption, a promising clean energy (positive carbon balance) process aiming at long-term CO_2 sequestration in geological layers.

References: [1] Atmani L., Bichara C., Pellenq R.J.-M., Van Damme H., van Duin A. C. T., Raza Z., Truflandier L. A., Obliger A., Kralert P. G., Ulm F. J., Leyssale J.-M., *Chem. Sci.* **8** (2017) 8325; [2] Atmani L., Valdenaire P.-L., Pellenq J.-M., Bichara C.,Van Damme H., van Duin A. C. T., Ulm F. J., Leyssale J.-M. *Energy & Fuels* **34** (2020) 1537; [3] Obliger A., Valdenaire P.-L., Capit N., Ulm F.-J., Pellenq R. J.-M., Leyssale J.-M. *Langmuir* **34** (2018) 13766; [4] Obliger A., Valdenaire P.-L., Ulm F.-J., Pellenq R. J.-M., Leyssale J.-M. *J. Phys. Chem. B* **123** (2019) 5635.

Applicant profile: Applicants should (or be about to) hold a Master in Physical chemistry or Physics with a solid background in condensed matter and statistical mechanics. Experience with molecular simulations and good computer skills (Linux, programming in python/Fortran/C, etc...) would be a plus.

Funding: The secured 3 years PhD grant (net salary of about €1400/month) is offered by the French Ministry of Higher Education, Research and Innovation. Selection of the candidate will involve a 10' interview in front of a scientific committee selected by the Doctoral College of Chemical Sciences (https://ed-chimie.u-bordeaux.fr/). The selected applicant is supposed to start on September-October 2019.

Application: Please send an application letter together with a detailed CV and the names of at least two references to Jean-Marc Leyssale (jean-marc.leyssale@u-bordeaux.fr) by May 22.