



Efficient algorithm for the use of classical DFT in porous media

CONTEXT

Understanding the thermodynamic properties and adsorption phenomena of extremely confined fluids has a great interest not solely in terms of knowledge but also for many practical and industrial applications such as, for instance, storage of natural gas and hydrogen, carbon dioxide capture, characterization of porous materials... Hence, for several years, substantial efforts have been dedicated to the development of on the one hand molecular simulations and theoretical models and on the other hand experimental techniques to study the properties of confined fluids.

Among the theoretical developments, density functional theory (DFT) has emerged as one of the most powerful and convenient molecular approach for the description of the thermodynamic properties of inhomogeneous fluids. DFT approaches retain detailed information of the microstructure of heterogeneous fluids but with a much less computational expense than molecular simulations. Until very recently most of the studies involving application of DFTs have used very simple surfaces with substantial symmetry and uniform properties. But, the increasing complexity of systems under consideration (both fluids and solids) leads to the need to consider more efficient and faster algorithms to solve the equilibrium equations of DFTs.

OBJECTIVES

The aim of this Master internship is to implement, test and compare several algorithms recently proposed in the literature for the application of DFTs to fluids confined in porous materials. The specific cases of methane and water confined in activated carbons and silica nanostructures will be specially addressed.

LABORATORY AND INTERNSHIP LOCATION

Laboratory of Complex Fluids and their Reservoirs (LFCR), team G2MP « GeoMechanics and Porous Media », Anglet, Univ. Pau Pays Adour. The candidate will be integrated in the Hub NewPores¹ and will work in close collaboration with the two PhD students already working on the application of DFTs in the project.

DURATION- From March to August 2021 (6 months).

GRANT- 560 € / month.

Supervisors : Christelle Miqueu & David Grégoire.

Contacts :

Christelle Miqueu : christelle.miqueu@univ-pau.fr

David Grégoire : david.gregoire@univ-pau.fr

¹ NewPores is an international hub dedicated to the mechanics and physics of porous materials, which intends to answer to new Energy and Environment challenges. This is a joint effort of the group on Geomechanics and Porous Materials (G2MP) of the Laboratoire des Fluides Complexes et leurs Réservoirs at E2S UPPA (France), the Centre for Sustainable Engineering of Geological and Infrastructure Materials (SEGIM) at Northwestern University (USA), the University of Vigo (Spain), the Technical University of Madrid (Spain) and University of Liège (Belgium).