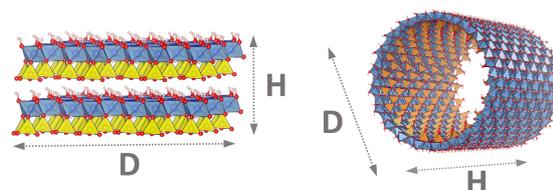


Hydrogen in anisotropic clay mesopores: structural, thermodynamical and dynamical features

Hydrogen is the carbon-free fuel par excellence because its combustion, or its use in fuel cells, emits only water. The recent discovery of high hydrogen contents in clay-rich rocks [1] underlines the potential of clays for hydrogen storage. Considering low-cost and green materials, such as clays, for hydrogen storage at room temperature and at moderate pressure could be an interesting perspective.

One may take advantage of the original properties of hydrogen when confined within small pores. Recently, a transition from a low-temperature, low-density phase to a high temperature, higher density phase was evidenced in graphitic Saran carbon, under moderate pressure [2]. The high-density phase is characterized by a large proportion of ortho- H_2 (with total molecular spin $S = 1$) which is forced to adopt a collective orientation to pack inside sub-nanometric pores. The density of the solid H_2 phase stabilized by the adsorbent interaction reaches a larger value than that of the liquid state, a limit that was thought not possible to cross [3]. It is now important to search for new materials aiming at stabilizing these solid phases. One aspect in this direction is to change the H_2 -adsorbent bonding interactions, by choosing clays with tuneable pore size.

The anisotropy and porosity of clay materials is primarily determined by the anisotropy of the clay particles themselves [4]. An unprecedented range of aspect ratios (ratio R between the height H and diameter D of the clay particle), from 0.1 to 100, will be studied.



Lamellar and tubular clays [5].

A comprehensive set of experimental methods (X-ray scattering, small angle neutron scattering, quasielastic and inelastic neutron scattering and adsorption measurements) will be used, coupled with molecular dynamics simulations. Expected results are the determination of the particle and pore networks and of quantities of adsorbed hydrogen, the understanding of the retention mechanism, of thermodynamic properties in play and the analysis of the diffusion processes for H_2 at the molecular level.

The thesis is a fundamental research thesis in connection with the energy issue. The PhD student should have a **solid background in physics** and **be highly interested by experimental and numerical approaches**.

The thesis is funded by the Agence Nationale de la Recherche. It will be directed by Pascale Launois (Laboratoire de Physique des Solides (LPS), Orsay, France) and co-directed by Laurent Truche (ISTerre, Grenoble, France) and Stéphane Rols (Institut Laue-Langevin, Grenoble). *The PhD student will be based at LPS, Orsay and he/she will have to carry out missions at ISTerre and ILL at Grenoble.*

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Expected date of employment: September or October 1st 2021

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