Offer for a Thesis Allowance

Subject: HYdrogen storaGe in Innovative hybrid matErials

From August 26, 2019 to October 31, 2019

Storage by absorption of hydrogen in a solid, which enables to obtain sufficient storage capacities at ambient temperature, consists of the formation of reversible metal or complex hydrides. The advantage of this storage mode is that the pressures involved are moderate (of the order of ten bars). However, these materials have two major disadvantages: the hydride formation and dehydriding kinetics are slow and the dehydration temperatures are high. In order to overcome these limitations, the use of nanoporous materials to confine hydrides is a solution. In parallel, recent work shows a possible alternative storage by considering the trapping of hydrogen within solid organic molecular crystals called clathrates. In that case, the reaction involves relatively low energies in addition to extremely fast capture/release kinetics (a few seconds). But the major drawback of this storage is that it requires too high pressures to be considered in the state.

Missions

Objectives

The objective of this project is to propose, characterize and test in in situ conditions, two innovative hybrid materials for the storage of hydrogen, each containing a phase-change material (complex metal hydride or organic molecular crystal) confined within a porous matrix (carbon xerogel) having a double porosity. The phase change materials will be inserted into the nanoporosity (storage porosity) so that they can capture hydrogen under acceptable temperature and pressure conditions by shifting the thermodynamic equilibria: lower formation pressures in the case of organic crystals, lower dehydrogenation temperatures in the case of hydrides. Indeed, when the bulk pressure is of the order of several tens of bars, the pressure of a gas confined within pores of a few nanometers can be several hundred times greater than this one because of the interactions between the adsorbed and the solid molecules.

The transport of hydrogen to the storage porosity will be ensured by the transport porosity, which will promote the kinetics of capture/release. Moreover, the confinement of these materials into fine particles should also allow:

* to increase the storage capacities because of the large accessible surfaces in a restricted volume and the combination (or synergy) of two storage modes for hydrogen: entrapment in hydride or crystal and adsorption on accessible surfaces of the porous matrix;
* to reduce the sorption/desorption enthalpies, which will reduce the energy cost during the recovery of hydrogen in these materials.
The project would allow to obtain a low-cost hybrid material allowing the rapid and reversible storage of hydrogen at room temperature and moderate pressure with storage capacities, reaction kinetics and very favorable energies for industrial application on a large scale. The innovative challenge is twofold:

* there is currently no study on the storage/deformation coupling of complex hydrides, whereas this latter has a major influence on the storage capacities after several capture/release cycles as well as on the kinetics of reaction;
* the use of organic crystals for hydrogen storage is totally innovative, in complete break with existing storage techniques.

The originality of this project is based on a multidisciplinary approach, combining experimentation and modeling, which allows to consider these new materials from their synthesis to tests in tanks conditions, through the characterization of their structural properties, their storage capacity, the capture/release kinetics and associated energy and mechanical phenomena. It is part of the HYGIE (HYdrogen StoraGe of Innovative hybrid matErials) project funded by the Région Nouvelle Aquitaine, in which several teams are involved: LFCR, Anglet (syntheses, characterizations, storage/deformation experiments, modeling); Univ. Liège, Belgique (synthesis of xerogels); ICMCB, Bordeaux (metal hydrides); LGC and LCC, Toulouse (tests in tank conditions and analyses); Bertin Technology (industrial partner). It is also part of the New-Pores HUB funded by E2S (https://e2s-uppa.eu/)

**Work plan**

Development of an experimental device for the simultaneous measurement of H2 storage capacities and induced deformations.

Modeling with a coupled thermodynamic/poromechanics model.

Hydrogenation / dehydrogenation of hybrid materials in *in-situ* conditions

**Hosting laboratories:** Laboratory of Complex Fluids and their Reservoirs (LFCR), UMR 5150

**Localisation address:**

LFCR, Geomechanics and Porous Media team, Anglet, FRANCE

**Secondary location:** LGC, Toulouse, FRANCE

**PhD supervisor:** Christelle Miqueu (Associate professor HDR, LFCR, UPPA)

**PhD co-supervisor:** Laurent Perrier (Associate professor, LFCR, UPPA)

**In Collaboration with:** Jean-Philippe Torre (CNRS Researcher, LGC, Toulouse)
Starting date: January 2020

Length: 3 years

Employer: Université de Pau et des Pays de l’Adour (UPPA)

Funding: E2S UPPA

Gross monthly salary: 1878 €

(UPPA doctoral contract, according to E2S UPPA project, including 96h of teaching during the three years)

Required skills and competences - Who can apply?

The candidate should hold a Master degree in Physics, Mechanics, Materials, Chemical Engineering or a similar field.

Previous experience with experimental developments is an asset.

The candidate should have a strong interest in performing experimental development and in working with partners of various profiles (chemists, physicists, chemical engineers...).

Proficiency in English is mandatory.

Interest in teaching is required: PhD contract includes a teaching charge of 32h/year, preferentially at the undergraduate level (in French language) or in the master (in English language).

Autonomy, dynamism, creativity, good communication skills are recommended.

Application - Evaluation criteria

Selection process:

* Establishment of the selection committee
* Evaluation of the applicants’ file
* Interview with the selected candidates and ranking

Application files will be evaluated based on the following criteria:
* Candidate's motivation, scientific maturity and curiosity
* Candidate's knowledge in physics, mechanics, thermodynamics, chemical engineering
* Grades and ranking during your Master degree, steadiness in your academic background
* English language proficiency
* French proficiency for teaching in Bachelor's degree
* Oral and written communication skills
* Candidate's ability to present her/his work and results
* Professional experience (e.g. internships in laboratory, previous research works, publications ...)

**Application file composition and submission deadline**

Application will include (in a single pdf file):
* CV
* Cover letter detailing the candidate's motivations and interest in the scientific aspect of the PhD
* Candidate's Master grade transcripts and ranking
* Reference letters
* Contact details of at least two people (academic or industrial referees) who can be contacted for further reference

Applications must be sent with the title “Doctoral application” to the following addresses:

christelle.miqueu@univ-pau.fr
laurent.perrier@univ-pau.fr


 Submission deadline : October 31st, 2019