

PhD Thesis proposal

What? Synthesis of Hybride functionalized and catalyzed MOFs for the storage of Hydrogen – HyMOFHy

Where? Institut Jean Lamour (University of Lorraine and CNRS) – Team [ESPRITS](#) (reactive plasmas and surface processing)

When? Starting date: September 2018

Application deadline: 30 March 2018

Subject description:

The PhD thesis HyMOFHy addresses the hydrogen storage challenge. It promotes the use of dry plasma processes to achieve in-situ both the functionalization and the hybridization by metal hydrides of catalyzed Metal-Organic Frameworks (MOFs). The objective is therefore to study the elaboration and functionalization of such porous structures by cold plasmas in order to get a wide range of functionalized ecological MOFs, at low cost. The selected materials will be crucial since they will permit the formation of innovative, flexible and safe hybrid materials by integrating ultimately both chimisorption and physisorption properties. The synthesis of these hybrid MOFs will be the result of a detailed parametric study focused on the capabilities to improve the hydrogen evolution reaction (HER).

Hydrogen storage is one of the main challenges to tackle for the use of hydrogen as a new energy vector. Current technologies involve the compressing or liquefying the gas. However, these methods are limited because they need additional control and refrigeration system which are, energy costly for the mobile applications (e.g. automotive sector). The capability of solids (e.g. metal hydrides) to store hydrogen gas has therefore been raised and is now the research topic of many research groups. Nevertheless, the inelastic deformations of the solid matrices generated by the repeated process of storage and release of hydrogen are still a concern.

Among the various H₂ storage possibilities under study, porous matrices appear to offer significant capacity of storage with interesting elasticity and flexibility of the solid structures, such as the MOF-type absorbents. Moreover, materials forming metal hydrides such as Mg/MgH₂ enable storing up to 7.6% of their mass in H₂. Therefore, the combination of physisorption and chimisorption properties seems to be a promising way to design such hybrid storage materials in order to get large storage capacities on flexible but resistant media and with an improved chemical kinetics.

The desired physicochemical properties of functionalized MOFs will have to be accessible over temperature and pressure ranges close to those of our environmental conditions. By considering the purpose of storage and release of hydrogen systems, the synthesis of these hybrid MOFs will be the

result of a detailed parametric study focused on the capabilities to improve the hydrogen evolution reaction (HER).

Research work will consist of 4 aspects that will be studied consistently:

- Plasma functionalization of MOFs organic ligands
- MOFs plasma hybridization by metal hydride
- Elaboration of catalysed MOFs by plasma coatings to promote the chemical dissociation of H₂.
- Testing of the capacity MOFs regarding H₂ storage.

This ambitious and multidisciplinary PhD work represents a major scientific breakthrough for the deployment of the era of hydrogen as a vector of energy. With hydrogen as an energy vector, this doctoral project aims to bring out a radical change in our methods of production and of consumption of energy.

Requirements

- Master Degree (or equivalent) with a major relevant to plasma physics or to material science & engineering; excellent study record
- Knowledge of surface processing by plasmas is an advantage
- Good ability to formulate research questions, design experiments and critically interpret their results
- Ability in team working
- Skills in scientific communication and writing
- Languages: English; French is considered a significant advantage.

Contacts

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Documents to provide

- CV
- Motivation letter
- Transcripts and ranking Master degree (those already available if master is still ongoing)
- Copy of identity document (passport, ID card)

Letter (s) of recommendation will be appreciated