

PhD contract offer

High surface area and high density materials for hydrogen storage

General information

Workplace: Epinal (Lorraine), France

Type of contract: PhD contract funded by the Ministry of Higher Education

Contract period: 36 months

Expected date of employment: 1st October 2022

Proportion of work: Full time

Remuneration: 2135 € gross monthly (1715.89 € net)

Desired level of education: Master's degree in materials science or chemical physics

Experience required: -

Subject description

Hydrogen adsorption is proportional to specific surface area and often capacities are reported per mass of sorbent. In practice, the volume of the tank is decisive, and capacities should be reported per tank volume. The objective of the thesis is to obtain activated carbons (ACs) and MOFs with a high density and a high specific surface area in order to reach high hydrogen release capacities.

- High specific surface areas in ACs are accompanied by supermicropores (0.7-2nm) and mesopores (>2nm) that increase the equilibrium pressure required to reach maximum adsorption capacity, and thus reduce the adsorptive storage capacity in the reservoir [1]. Conventional methods of activating carbons with potassium salts, either by physical mixing or impregnation, do not achieve pore size distributions centered on 0.7 nm. The use of novel mixing methods available in our laboratory allow a homogeneous distribution of the activating agent and to decrease the amount of activating agent to obtain narrower pores while keeping the same final surface around 2600 m²/g.
- MOFs with high specific surface areas often have low bulk densities, so the volume storage capacities are not always in agreement with what would be expected by simple application of Chahine's law [2,3]. We have shown that the incorporation of nanographite during the synthesis of UiO-66 MOF increases the specific surface area, wet stability and gas adsorption capacities [4]. The challenge will be to synthesize hybrid materials from MOFs with very high surface area, > 5000 m²/g, whose adsorption capacities will be enhanced by the addition of different carbonaceous materials.

The candidate will be responsible for the synthesis and characterization of the materials as well as the determination of hydrogen storage capacities from 40 to 300K. An important part of this topic is understanding the adsorption process and predicting the performance of the materials after proper characterization of the textural properties.

Keywords: Hydrogen storage; Adsorption; Activated carbons; MOFs; Porous materials.

References:

- [1] P. Ramirez-Vidal, R.L.S. Canevesi, G. Sdanghi, S. Schaefer, G. Maranzana, A. Celzard, V. Fierro, A Step Forward in Understanding the Hydrogen Adsorption and Compression on Activated Carbons, *ACS Appl. Mater. Interfaces*. 13 (2021) 12562–12574. <https://doi.org/10.1021/acsmi.0c22192>.
- [2] P. Ramirez-Vidal, R.L.S. Canevesi, A. Celzard, V. Fierro, Modeling High-Pressure Hydrogen Uptake by Nanoporous Metal–Organic Frameworks: Implications for Hydrogen Storage and Delivery, *ACS Appl. Nano Mater.* (2022). <https://doi.org/10.1021/acsnm.1c03493>.
- [3] P. Ramirez-Vidal, G. Sdanghi, A. Celzard, V. Fierro, High hydrogen release by cryo-adsorption and compression on porous materials, *Int. J. Hydrog. Energy*. 47 (2022) 8892–8915. <https://doi.org/10.1016/j.ijhydene.2021.12.235>.
- [4] A. Policicchio, M. Florent, A. Celzard, V. Fierro, J. Jagiello, T.J. Bandosz, Enhancing the gas adsorption capacities of UiO-66 by nanographite addition, *Microporous Mesoporous Mater.* 309 (2020) 110571. <https://doi.org/10.1016/j.micromeso.2020.110571>.

Work context

The PhD student will work in a research team specialized in materials science, the "Biosourced Materials" team from the Jean Lamour Institute (IJL, UMR CNRS 7198), housed in the ENSTIB premises, in Epinal, under the supervision of Pr. Vanessa Fierro and Pr. Alain Celzard.

The team enjoys one of the largest experimental platforms of the Greater Region dedicated to porous materials in general, and to biosourced materials in particular and hydrogen adsorption devices able to work from 40 to 300 K and up to 20 MPa.

Skills

The candidate must have followed training in solid-state chemistry or materials science as a priority, but knowledge of adsorption will be particularly appreciated. The candidate must demonstrate great ease with the materials synthesis and characterization tools (hydrothermal synthesis, pyrolysis, gas adsorption, UV-visible spectrometer, DRX and TGA / DSC) on which he/she will be trained to become quickly autonomous. Knowledge in MOF synthesis and MATLAB will be a plus. He/she must be dynamic, curious and persevering to carry out the multiple syntheses, characterisations, tests and interpretations of the results, and demonstrate the ability to work in a team.

Constraints and risks

No major risk.

About Institut Jean Lamour

The Institut Jean Lamour (IJL) is a joint research unit (UMR 7198) of CNRS and Université de Lorraine. The IJL is focused on materials and processes in science and engineering, and covers activities in condensed matter physics, materials, metallurgy, plasmas, surfaces, nanomaterials and electronics. The IJL staff consists of 183 researchers/lecturers, 91 engineers/technicians/ administrative staff, 150 doctoral students and 25 post-doctoral fellows. The IJL has active partnerships with 150 companies and our research groups collaborate with researchers from more than 30 countries throughout the world. The IJL's exceptional instrument platforms are spread over 4 sites; Epinal is one of them.

Application

Applicants are invited to send a CV and a motivation letter, together with diploma copies and/or marks obtained during the Master degree, to the supervisors before 15th May 2022:

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Then, interviews and visits of the labs will be organised.