



PhD position at University Pau & Pays Adour (France)

**Synthesis of nanostructured and hierarchical micro/mesoporous materials
for the study of adsorption-induced deformation in the context of gas storage
and transport
(Newpores project)**

NewPores research project presentation

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).

General context

Following the IUPAC recommendation, the pore space in porous materials is divided into three groups according to the pore size diameters: macropores of widths greater than 50nm, mesopores of widths between 2 and 50nm and micropores of widths less than 2nm. Zeolites, activated carbon, tight rocks, coal rocks, source rocks, clay, cementitious materials and biomaterials are among these materials. In recent years, a major attention has been paid on these microporous materials because the surface-to-volume ratio (i.e., the specific pore surface) increases with decreasing characteristic pore size. Consequently, these materials can trap an important quantity of fluid molecules as an adsorbed phase. This is important for applications in petroleum and oil recovery, gas storage, separation, catalysis or drug delivery.

For these microporous materials, a deviation from standard poromechanics is expected. In nanometer-scale pores, the molecules of fluid are confined. This effect, denoted as molecular packing, induces that fluid-fluid and fluid-solid interactions sum at the pore scale and have significant consequences at the macroscale, such as instantaneous deformation. A lot of natural and synthesised porous media are composed of a double porosity: the microporosity where the fluid is trapped as an adsorbed phase and a meso or a macro porosity required to ensure the transport of fluids to and from the smaller pores. If adsorption in nanopores induces instantaneous deformation at a higher scale, the matrix swelling may close the transport porosity, reducing the global permeability of the porous system or annihilating the functionality of synthesised materials.

Within NewPores, a new enhanced poromechanics framework is proposed allowing the prediction of adsorption-induced deformation in micro and mesoporous materials and the PhD candidate will be in charge of synthesising mono and poly-disperse micro/mesoporous media with controlled characteristics in order to assess the proposed models in simple and controlled configurations.

Partners

- *E2S Newpores project* (an international hub for the mechanics and physics of porous materials).
- *The Institute of Analytical Sciences and Physico-Chemistry for Environment and Materials* (IPREM, UMR 5254) at E2S UPPA.
- *Geomechanics and Porous Materials* research group (G2MP, LFCR UMR5150) at E2S UPPA.

PhD candidate objectives

In a particularly multidisciplinary framework involving skills in both materials physics, modelling, physico-chemistry, chemistry, the main objective of the PhD candidate will be to develop model nanostructured inorganic surfaces using the sol-gel process with hierarchically organized porosities. These materials prepared by dip-coating with precise control of the deposition conditions (relative humidity, temperature, deposition rate, etc.) will be subjected to fine structural but also physical characterizations to evaluate their mechanical behaviour during gas adsorption.

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Methodology

Two approaches are considered in this context.

- A first part will concern the development of mesoporous materials organised in the form of interconnected channels for which it will be a question of evaluating the gas adsorption mechanisms at the connection points (boundary conditions). Sol-gel syntheses using the self-organization of inorganic precursors and surfactants of different sizes will be used.

- A second part will consist in developing microporous materials using the self-organization of block copolymers and inorganic precursors. After heat treatment, the porous structures will be filled in a controlled manner by successive inorganic deposits to obtain the defined microporous surfaces.

Modelling studies in theoretical chemistry of self-organization processes in materials are planned to anticipate the structures obtained at the nanometric scale.

Research team and environment

Joachim Allouche	(E2S UPPA/IPREM)	Micro/mesoporous materials synthesis	- <i>PhD supervisor</i>
David Grégoire	(E2S UPPA/LFCR/G2MP)	Multiphysics coupling in porous media	- <i>PhD supervisor</i>
Antoine Bousquet	(E2S UPPA/IPREM)	Polymer and materials synthesis	- <i>Researcher</i>
Delphine Flahaut	(E2S UPPA/IPREM)	Chemical characterization of materials	<i>Researcher</i>
Germain Vallverdu	(E2S UPPA/IPREM)	Modelling of self-organization processes	- <i>Researcher</i>
Christelle Miqueu	(E2S UPPA/LFCR/G2MP)	Adsorption modelling and porosimetry	- <i>Researcher</i>
Laurent Perrier	(E2S UPPA/LFCR/G2MP)	Experimental measurement of adsorption	- <i>Researcher</i>

Candidate's profile

Physico-chemist, chemist or polymerist by training (MSc degree), the candidate should have solid skills in sol-gel synthesis of hybrid materials and / or polymers. Good knowledge in physics, mechanics of materials and / or theoretical chemistry applied to hybrid materials will be an asset. Proficiency in English is mandatory for both oral and writing communication.

Job details

The successful candidate will be mainly hosted at IPREM lab (UMR 5254) in Pau. Residencies in the G2MP research group in Anglet are envisioned for the physical characterisation of the synthesised materials.

The envisioned starting date is October 1st, 2021, and the maximum duration is 3 years.

The position includes full social security coverage and a gross salary of approx. 1878 € per month. This salary encompasses 32h of teaching hours at E2S UPPA per year.

Evaluation procedure

Candidates will be ranked in a first phase based on their submitted application. In a second phase, an interview will be organized with the selected candidates (possibly via Skype).

Applications should include a cover letter, CV, passport/ID copy, transcripts of diplomas and lists of courses attended (with grades obtained), recommendation letters, and names and contact details of at least two references.

Applications should be submitted **before 01/05/2021** at www.davidgregoire.fr/opening-positions

The interview will take place during the second half of May. Final answer will be provided by the end of May.

Contact

For further information about this position, please contact [joachim.allouche\[at\]univ-pau.fr](mailto:joachim.allouche[at]univ-pau.fr).

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