PHD STUDENT – CALL FOR APPLICATIONS

Position: PhD student in the discipline of physical sciences

Unit of the project realization: Faculty of Science and Technology – University of Silesia in Katowice

The University of Silesia in Katowice is seeking a candidate for a PhD project investigating mechanism of intrusion of liquids into hydrophobic porous materials. The aim of the project is to develop an innovative method of energy storage. The desired candidate would have the ability to think creatively and understand basic physico-chemical principles.

The position is available in cooperation between two teams Thermodynamics in Action Team and Structure and Dynamics of Matter at the University of Silesia, Poland. This innovative project will also involve active international collaboration.

Scope of work in the project:

- Investigation of structural properties of porous materials during water intrusion, under nanoconfinement and characterization of the solid-liquid interface.
- Study of the structural response and change of symmetry upon intrusion-extrusion of different non-wetting liquids (water, heavy water) into crystalline nanoporous materials.

Research will be carried out in the frame of the project „*Molecular springs as a new method of compact thermal energy storage*", financed from National Science Centre (NCN; project number UMO-2018/31/B/ST8/00599).

Duration of the scholarship: 12 months

Scholarship amount: 4500 PLN per month before taxes (about 1000 EUR).

Project description:

A system consisting of a porous material immersed in a non-wetting liquid, also called molecular spring, can be used for energy applications [1-4]. Thus, mechanical [1-4], thermal [2,3] and electrical [2] energy can be stored/restored in the form of solid/ liquid interfacial energy in the reversible cycle of intrusion/extrusion of the nonwetting liquid. Penetration of a nonwetting liquid into lyophobic pores is achieved under application of external pressure and energy must be supplied to the system (charging). Upon the release of pressure, a spontaneous extrusion of the liquid (discharging) takes place and the energy is released. Despite growing interest in the properties of molecular springs, thermal effects of

intrusion-extrusion are poorly explored even though they are essential for practical use and understanding of the operating mechanisms [5].

During her/his work PhD candidate will thoroughly investigate properties of systems comprising nonwetting liquids and porous materials. The candidate will use several experimental techniques foxusing on x-ray and neutron powder diffraction (in-situ and ex-situ), complemented with Molecular Dynamic simulations. Special attention will be given to the reversibility of the intrusion process, e.g. to the hysteresis phenomena in a cycle of a non-wetting liquid “forced intrusion – spontaneous extrusion” into-from nanopores. The project's final goal is to understand the structural mechanisms taking place during intrusion-extrusion and maximize them for the benefit of new generation thermal energy storage applications.

References:

1. Tinti, A., Giacomello, A., Grosu, Y., & Casciola, C. M. (2017). Intrusion and extrusion of water in hydrophobic nanopores. Proceedings of the National Academy of Sciences, 114(48), E10266-E10273.

2. Grosu, Y., Mierzwa, M., Eroshenko, V. A., Pawlus, S., Chorążewski, M., Nedelec, J. M., & Grolier, J. P. E. (2017). Mechanical, Thermal, and Electrical Energy Storage in a Single Working Body: Electrification and Thermal Effects upon Pressure-Induced Water Intrusion–Extrusion in Nanoporous Solids. ACS applied materials & interfaces, 9(8), 7044-7049.

3. Grosu, Y., Li, M., Peng, Y. L., Luo, D., Li, D., Faik, A., ... & Grolier, J. P. (2016). A highly stable nonhysteretic {Cu2 (tebpz) MOF+ water} molecular spring. ChemPhysChem, 17(21), 3359-3364.

4. Amabili, M., Grosu, Y., Giacomello, A., Meloni, S., Zaki, A., Bonilla, F., ... & Casciola, C. M. (2019). Pore Morphology Determines Spontaneous Liquid Extrusion from Nanopores. ACS nano, 13(2), 1728-1738.

5. E. Amayuelas, M. Tortora, L. Bartolomé, J. D. Littlefair, G. Paulo, A. Le Donne, B. Trump, A. A. Yakovenko, M. A. Chorazewski, A. Giacomello, P. Zajdel, S. Meloni, Y. Grosu Mechanism of Water Intrusion into Flexible ZIF-8: Liquid Is Not Vapor, Nano Letters 23(12) (2023) 5430-5436, http://dx.doi.org/10.1021/acs.nanolett.3c00235

Job responsibilities:

- Perform quality research within the scope of the project.
- Publish the obtained results in high-impact journals.
- Present the obtained results at international conferences.
- Develop the project as seen fit with others.

Essential Qualification:

- Masters of Science or qualified equivalent in the chemistry or physical science or applied sciences.
- Strong academic record.
- History of participation in research projects.
- Strong verbal and written communication skills in English, with a desire to improve.

Desired Qualifications:

- A team player who can collaborate with other groups, technical centers, and industries.
- Basic knowledge in computation and programming (Python) will be considered an asset.
- Self-motivation and ability to work independently.

Required Documents:

1. Resume with information about previous studies/employment,

2. Copy of the M.A. degree

3. List of publications and conference presentations

4. Opinion of previous supervisors

5. Copies of other documents proving possession of required qualifications

Documents should be submitted by October 1st 2023 to an e-mail: miroslaw.chorazewski@us.edu.pl

If you have any questions, please contact the project manager at the above e-mail address before formally submitting your application.

The documentation submitted by the candidates will be evaluated by a committee chaired by the project manager. Recruitment will be conducted in accordance with the appropriate NCN regulations. Recruitment can be conducted in Polish or in English. The interview will take place on-line. The decision of the committee will be presented to candidates via e-mail.