PhD PROJECT PROPOSAL

## **PhD Project Title**

## Metal-Organic Framework Topology in Nanofluids for Energy-Related Applications

## **PhD Supervisory Team**

Principal Supervisors: Dr Yueting Sun, y.sun.9@bham.ac.uk, Birmingham Centre for Energy Storage, School of Engineering

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## **Project Abstract**

## The high-pressure water adsorption of hydrophobic nanoporous structures offers a great potential in energy related applications, including energy absorption, storage, conversion, and heat decarbonisation. Our recent work found that the nanopore geometry plays an important role on the water mobility and nanofluidic energy phenomena inside the porous metal-organic frameworks (MOFs). The project aims to understand how the framework topology of MOFs or colloidal topology of MOF nanoparticles affects the liquid transport process and how we can design such materials at different length scales for innovative energy technologies.

## **Detailed Project Description**

**Research background, intended outcomes and methodology**

A new energy absorption mechanism has recently been developed (Figure 1), which works by mechanically squeezing liquid into extremely small spaces; these spaces are made so small that liquid water must split into water molecules to be able to enter and flow inside and therefore a substantial amount of energy can be absorbed. A sponge-like material called Metal-Organic Frameworks (MOFs) are used to provide such pores at the nanoscale, one-billionth of a metre, comparable to the size of water molecules. It's found that such a high-pressure water adsorption process can not only enable remarkably effective and reusable energy absorption1, but also has great potential in various energy related applications, including energy storage, conversion, and heat decarbonisation.

Our recent work found that the nanopore geometry plays an important role on the confined water transport inside MOFs, and the spatial arrangement of MOF nanoparticles in liquid can also be an important factor. Therefore, this project aims to bring the concept of topological design into this emerging research field and understand how the framework topology of MOFs or the colloidal topology of MOF nanoparticles affects the water molecule transport and thermophysical properties of the material system. Such knowledge can then be used to design materials at different length scales to enable innovative energy technologies.

Pioneering experimental techniques have been developed in our group. The student will have the access to the state-of-the-art in-house facilities and central synchrotron facilities to design and characterise the chemical and physical properties of the material system and gain fantastic support from collaborators in this research area.

The student can start by experimenting a group of zeolitic imidazolate frameworks (ZIFs) of different topologies identified in a recent work1 to gain a basic understanding of the relationship between material structures and properties. Topological analysis of ZIFs will be conducted to understand how the connectivity and topology affect the porosity, pore structure, and stability. Alternatively, the student can also choose to focus on the topological analysis at the particle level for colloidal ZIFs. Experimental results and topological designs can then be synthesised to create new understandings on material optimisations with new structures and recipes to be proposed. The diversity of the building blocks of MOFs with respect to their pore size, shape, and crystal morphology offers the feasibility of the project.



Figure 1. Water intrusion into ZIF-8 for energy absorption2

**Training and skills to be developed over the PhD**

The student will gain skills in multiple disciplines from a diverse supervision team and collaborations, which may include MOF chemistry, topological design, thermodynamics, and nanofluidic physics. The student will be encouraged to attend external schools and conferences to broaden their horizon and develop skills in communication and collaborations. It is expected that the student will become an independent cross-disciplinary expert by the end of the project capable of bridging different fields.

**Explanation of why the project is suitable for the CDT in Topological Design**

This project takes a topological approach to understand and design framework materials for their liquid intrusion and extrusion behaviours. Currently, there is a significant knowledge gap on the topological effect on confined liquid transport especially when the length scale is down to the molecular level. The stability of MOFs is also affected by the connectivity of secondary building units (SBUs) and ligands3. The project is highly multi-disciplinary complementing existing research at the CDT in topological design.

**Links with research in the research groups of the supervising team**

This project builds on the latest research of Dr Yueting Sun on nanofluidic energy absorption1, Dr Hamish Yeung’s expertise in MOF synthesise and characterisation4, and Prof Yulong Ding’s research on nanofluids and energy applications5. The research groups host outstanding facilities for material synthesis, characterisation, and testing, with an excellent environment for the student to fulfill their full potential in this exciting area.

**Links with research strategies, possibly including UoB, EPSRC, partner organisations**

The research addresses the EPSRC prosperity outcome of resilient nation and aligns with priority areas such as materials engineering, chemical structure, continuum mechanics, energy storage, surface science, and topology. The student will benefit from interacting with the community of MOF research at UoB and contribute to cross-school collaborations and knowledge exchange.

**An ideal/acceptable undergraduate background and interests**

The student should have an interest in pursuing interdisciplinary research that can be across engineering, material science, chemistry, and physics. The student can have an education background from one of these disciplines and expand their expertise through the training provided during the PhD programme.

**References**

1. Sun, Y., et al., *High-rate nanofluidic energy absorption in porous zeolitic frameworks.* Nature Materials, 2021. **20**(7): p. 1015-1023.

2. Sun, Y., et al., *Framework flexibility of ZIF-8 under liquid intrusion: discovering time-dependent mechanical response and structural relaxation.* Physical Chemistry Chemical Physics, 2018. **20**(15): p. 10108-10113.

3. Wang, H., et al., *Topologically guided tuning of Zr-MOF pore structures for highly selective separation of C6 alkane isomers.* Nature Communications, 2018. **9**(1): p. 1745.

4. Orr, K.W.P., et al., *Single-step synthesis and interface tuning of core–shell metal–organic framework nanoparticles.* Chemical Science, 2021. **12**(12): p. 4494-4502.

5. Wen, D., et al., *Experimental investigation into convective heat transfer of nanofluids at the entrance region under laminar flow conditions.* International Journal of Heat and Mass Transfer, 2004. **47**(24): p. 5181-5188.