PhD PROJECT PROPOSAL

## **PhD Project Title**

Framework topology in nanofluidic energy absorption and storage

## **PhD Supervisory Team**

Principal Supervisor: Dr Yueting Sun, y.sun.9@bham.ac.uk, School of Engineering

Co-Supervisor/s: Dr Hamish Yeung, h.yeung@bham.ac.uk, School of Chemistry

Associated Academics: Professor Yulong Ding, y.ding@bham.ac.uk, School of Chemical Engineering

## **Project Abstract**

Recently, a new process has been discovered to enable highly efficient and reusable energy absorption systems. It is based on the pressurised water intrusion into hydrophobic nanoporous structures such as zeolites and metal-organic frameworks (MOFs). It's found that the pore structure plays an important role on the water transport in hydrophobic frameworks: nanocages are more effective than nanochannels when used as shock absorbers. Therefore, this project aims to systematically examine the role of framework topology on nanofluidic energy absorption and storage and generate a design rule to propose new materials for emerging technologies.

## **Detailed Project Description**

**Research background, intended outcomes and methodology**

Mechanical energy absorption is important for protections from impact, vibration, and explosion. Current state-of-the-art energy absorption materials rely on processes such as extensive plastic deformation, cell buckling, and viscoelastic dissipation, and it has been challenging to create materials that can provide both high energy absorption density and reusability to withstand multiple impacts. To address these challenges, a new energy absorption mechanism has recently been developed (Figure 1). It 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 liquid intrusion process can enable remarkably effective energy absorbers at realistic high rate loading condition and it is reusable due to the spontaneous extrusion of water molecules from the framework1. Importantly, such nanoscale transport process also provides opportunities to develop innovative energy storage and conversion technologies as well.

The PhD project aims to understand how the framework topology of MOFs affects the confined liquid transport process, including its energy absorption and storage phenomenon and thermal effect, and then use this knowledge to formulate material design rules for applications. Pioneering experimental techniques have already been developed, e.g., the setup to generate and measure sudden shocks onto the sample that replicate those experienced in practical conditions. The student will carry out such experiments in-house as well as synchrotron experiments at central facilities guided by the topological analysis and design of framework materials. These works will be supported by simulations and other complementary work from collaborators.

The student will 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 materials structures and performances. Topological analysis of ZIFs will be conducted to understand how the connectivity and topology affect the porosity, pore structure, and stability, also including the influence of ligand size and geometry (aspect ratio) on the connectivity and resulting framework structure. Then experimental results and topological designs are synthesised to create new understandings on material optimisation for this application, with new structures to be proposed and demonstrated of optimised performance and stability. The vast diversity of the building blocks and tunability of MOFs with respect to their pore size, shape, and surface functionality offers the flexibility and feasibility of this part of the project.



Figure 1. Water intrusion into ZIF-8 for mechanical 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 dynamic mechanics, 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 absorption materials1, Dr Hamish Yeung’s expertise in MOF synthesise and characterisation4, and Prof Yulong Ding’s research on energy storage and conversion. The research groups host outstanding facilities for material synthesis, characterisation, and testing, with an excellent environment for the student to release 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.