Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Smart Mechanochemistry for a Solvent-free MOF Synthesis
Supervisors at Bath: Supervisors at Monash:	Dr Bernardo Castro-Dominguez A/Prof. David Turner
Home Institution (Bath):	Chemical Engineering
Indicative period at Host Institution (Monash):	October 2024-2025

Project Summary (to include a brief description of the relevance to sustainable & circular technologies)

Named by IUPAC as a chemical innovation with potential of changing the world, mechanochemistry (MECS) offers the opportunity to generate a paradigm shift in science and society by unlocking a new realm of chemical possibilities. Chemical reactions today are not only dependent on solvents, but also deeply rely on the use of heat, light or electricity to initiate reactions. However, by delivering extremely high localized heating through mechanical action, MECS enables us to target molecules and materials previously deemed impossible to synthesize and to access these in a solvent-free and therefore highly sustainable manner.

At present, our understanding of MECS is primitive and continues relying on trial-and-error approaches. The literature considers it a "magic box" and that "some mystique guards the rules of MECS". Indeed, this field is in its infancy, akin to organic chemistry in the early 1800s. Therefore, **this PhD project will unveil the mysteries of MECS by implementing a "smart" methodology that allows predicting and understanding the synthesis of metal-organic frameworks (MOFs).**

MOFs are porous materials formed by the coordination bond between a metal and an organic molecule. These materials have enormous surface areas, well-defined pore sizes and structures, all of which can be exploited for carbon capture, hydrogen storage and catalysis. These materials are considered essential to develop a truly sustainable industry. However, their synthesis requires large amounts of solvents, making them highly unsustainable and non-economical. Therefore, to discover new solvent-free method for synthesizing MOFs, we will leverage innovations in scientific experimentation to capture and digitalize MECS's physicochemical phenomena. This encrypted digitalized data will be cracked using advanced machine learning algorithms.

The objectives of this PhD project include:

1. Generate a wide range of MOF structures via high throughput MECS synthesis.
2. Develop a machine learning models to predict and assess mechanochemical reactions for MOFs.
3. Outline the mechanisms that drive MECS MOF synthesis.
4. Demonstrate the reach of the developed model by discovering new, more sustainable synthetic MOF pathways.

Relevant scientific publications:

[1] J. Grols, B. Castro-Dominguez, Mechanochemical co-crystallization: Insights and predictions, Computers & Chemical Engineering 153 (2021) 107416

[2] M. Wilkinson, et al., Predicting pharmaceutical crystal morphology using artificial intelligence, CrystEngComm, 43 (2022) 7545

[3] E. Engel, et al. Green Synthesis of Bio-based Metal–Organic Frameworks, John Wiley & Sons Ltd. (2022)

Features of the programme

- PhD researchers will be registered at both institutions and will be awarded a joint PhD degree.
- PhD researchers will be jointly supervised by academics from both Monash and Bath Universities.
- All PhD researchers in the joint programme will also undertake a bespoke advanced training plan covering a range of topics focusing on sustainability.
- Applicants can apply to either Monash University or the University of Bath as their nominated home institution.
- PhD researchers will undertake a period of no less than 12 months at the partner institution.
- Up to four scholarships/studentships will be offered. Additional and suitably qualified applicants who can access a scholarship/studentship from other sources will be also considered. Evidence of funding must be provided.
- The scholarships/studentships include:
  - a *full tuition fee sponsorship* provided by Monash or Bath for the course duration (up to a maximum 42 months). Note, however, that studentships for Bath-based projects will provide cover for UK/EU tuition fees ONLY.
  - *a living allowance (stipend)* provided by Monash or Bath Universities.

Note: Overseas Student Health Cover (OSHC) must be paid by the student, unless covered by the university.

How to apply

You MUST express interest for three projects in order of preference. Please submit your application at the Home institution of your preferred project ('Home' institution details can be found in the project summary). However, please note that you are applying for a joint PhD programme and applications will be processed as such.

The deadline to submit applications is 30th January 2023

Monash University

Expressions of interest (EoI) can be lodged through https://www.monash.edu/science/bath-monash-program. The EoI should provide the following information:

CV including details of citizenship, your Official Academic Transcripts, key to grades/grading scale of your transcripts, evidence of English language proficiency (IELTS or TOEFL, for full requirements see: https://www.monash.edu/graduate-research/faqs-and-resources/content/chapter-two/2-2), and two referees and contact details (optional). You must provide a link to these documents in Section 8 using Google Drive (Instructions in Section 8).

University of Bath

Please submit your application through the following link: https://www.csct.ac.uk/bath-monash-global-phd-programme/

Please make sure to mention in the "finance" section of your application that you are applying for funding through the joint Bath/Monash PhD programme for your specified projects.

In the "research interests" section of your application, please name the three projects you are interested in and rank them in order of preference. Please also include the names of the Bath lead supervisors.