Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Big data and machine learning for sustainable synthesis
Supervisors at Bath: Supervisors at Monash:	Dr Matthew Grayson (lead) Prof David Lupton
Home Institution:	University of Bath
Indicative period at Host Institution:	2 years at Bath; 12 months at Monash

Project Summary

The synthesis of bespoke molecules is essential in meeting the global demand for new agrochemicals, consumer products, materials and pharmaceutical drugs. Experimental trial-and-error has historically dominated reaction discovery but more cost effective, rapid and sustainable alternatives are becoming increasingly sought after. Density functional theory (DFT) calculations have been widely used post-experiment to explain observed reactivity and selectivity which enables the rational design of new reactions and helps to reduce the need for trial-and-error in reaction discovery. However, the computational design of new reactions pre-experiment is regarded as one of the "Holy Grails" of computational chemistry as high-accuracy DFT calculations are much slower than experimental screening methods; a typical computational mechanistic study can take 2-6 months. Faster computational methods can be used to study catalytic transformations but lack the accuracy needed to design reactions.

Big data and machine learning offer new opportunities for the computational design of reactions. Machine learning models, once trained, can make predictions for previously unseen molecules in seconds. This study will train machine learning models that can predict the outcomes of organocatalytic reactions important in pharmaceutical and polymer chemistry in a fraction of the time it would take to calculate them with DFT. Our work will provide the foundations for a new high-throughput *in silico* approach to designing and optimising reactions.

Use of these models for selected important enantioselective transformations will lead to a reduction in experimental trial-and-error and thus a more sustainable approach to reaction discovery. Furthermore, these models could be used to optimise atom economy which aligns with the second principle of circular chemistry (maximize atom circulation, *Nat. Chem.* 2019, *11*, 190).

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 23rd February 2020

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.