Project Title:	Machine learning for sustainable catalyst design: A combined computational and experimental approach
Supervisors at Bath:	Dr Matthew Grayson
Supervisors at Monash:	Prof David Lupton
Home Institution:	2 years
Indicative period at Host Institution (Monash):	12 months

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

We have an exciting opportunity to undertake a PhD in machine learning (ML) and synthesis in the Grayson (Bath, UK) and Lupton (Monash, Australia) groups. You will work on building and experimentally testing ML models for catalytic reaction design.

The synthesis of enantiopure molecules is of fundamental importance in the preparation of agricultural chemicals, flavours, fragrances, materials and pharmaceutical drugs. However, the discovery of new reactions needed to synthesise these chiral molecules has traditionally relied upon experimental trial-and-error. Accurate and fast computational approaches to designing catalytic reactions are therefore needed to provide cost-effective alternatives to this trial-and-error. This project will use state-of-the-art ML methodologies coupled with synthesis to probe the conditions necessary to undertake efficient asymmetric catalysis for challenging C–C bond-forming reactions.

After extracting reaction data from the catalysis literature, ML models will be trained on this dataset that can rapidly predict reaction outcomes (yield and enantioselectivity). Predictions of yield and enantioselectivity will then be made for novel substrate, catalyst, solvent and temperature combinations using the ML models. During the year in Australia, you will test these experimental predictions in the Lupton lab to validate the ML models and to generate more data on which the models can be trained. Use of these ML models will lead to a reduction in experimental trial-and-error and thus a more sustainable approach to the design of catalytic reactions. Furthermore, these models could be used to optimise atom economy which aligns with the second principle of circular chemistry (maximise atom circulation, *Nat. Chem.* **2019**, *11*, 190).

This project involves a diverse mix of synthetic organic chemistry, catalysis and state-of-the-art ML techniques and will leave you well-rounded in synthesis and theory with a diverse and highly desirable skillset.

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 <u>30th January 2023</u>

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.