

Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Molecular Understanding of the role of Surface Functionality on the properties of cellulose films and surfaces
Supervisors at Bath:	Steve Parker (lead); Janet Scott
Supervisors at Monash:	Warren Batchelor
Home Institution:	University of Bath
Indicative period at Host:	2.5 years at Bath; 12 months at Monash with exact dates to be confirmed

Project Summary

Cellulose is the most abundant and bio-mass derived polymeric material that has potential to be the major sustainable feedstock for many applications, from absorbents and gels to protective films. Cellulose will play a critical role in the transition away from using the fossil-fuel derived polymers that are difficult to recycle and are environmentally persistent. Despite the abundance of cellulose, it is often challenging to characterise experimentally, not least because of considerable flexibility of the chains which leads to marked differences in solubility and aggregation. In addition, the presence of ions and small molecules can also alter the behaviour at the interfaces, which then gives rise to a considerable variation in the functional properties.

The building block of these films is the individual cellulose nanofibres, assembled into a nonwoven structure, together with the pores between them. The cellulose nanofibers have a structure built up of crystalline cellulose domains of 4 nm diameter combined into larger 20-50 nm diameter structures with amorphous cellulose. The performance of these materials as barriers is controlled by transport of oxygen and water molecules through the pores, their interaction with the cellulose surfaces and transport around the surface of the crystalline cellulose domains.

We will aim to obtain a quantitative understanding of the behaviour of these interfaces by developing and applying molecular simulation approaches, coupled with targeted experiments. We will begin by investigating the interfacial properties of cellulose nanomaterial-based films, and how the presence of small molecules and ions affect the structure, dynamics and transport. The next stage would be to study the role of surface functionalisation, and thus by comparing experiment and simulation we will evaluate a range of properties, such as water vapour and oxygen permeability, needed for improved barrier packaging materials. Furthermore, by being able scan through different surface groups and the composition of intermediate layers we will be able to identify how best to modify the surfaces to drive performance. Once we have shown that such properties can be reliably calculated, we will have the tools to use these molecular level insights to make predictions on how to tune the material properties for improved performance.

Steve Parker will lead the computational work as he has considerable experience in atomistic modelling of materials, particularly on the role of surfaces, which range from cellulose dissolution to electronic properties of energy materials. The complementary experimental component will be led by Warren Batchelor who has expertise in the development and application of cellulose nanofibres for new sustainable materials. His group has developed new feedstocks from agricultural processing waste, new methods of applying barrier layers and has access to a full suite of instruments to quantify material performance. Janet Scott is internationally leading on the use of renewable raw materials, particularly cellulose and will be able to give guidance and help set priorities.

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.