Centre for **Sustainable** **& Circular** Technologies

MONASH University

UNIVERSITY OF BATH

Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Atomic Layer Deposited Heterojunctions for Light-Driven Water Splitting in Tandem Cells
Supervisors at Bath: Supervisors at Monash:	Andrew Johnson (lead); Frank Marken; Chris Bowen Jie Zhang
Home Institution:	University of Bath
Indicative period at Host Institution:	2.5 years at Bath; 1 year at Monash with exact dates to be confirmed

Project Summary

Light driven chemical processes will be of growing interest and processes like sunlight-powered sea water splitting to give hydrogen could be of key importance in future energy supply infrastructure. The efficiency of light-driven reactions is strongly dependent on the design of semiconductor interfaces to (i) effectively harvest light, (ii) convert the light to charge carriers, (iii) separate the charge carriers, and (iv) deliver chemical products without energy losses.

Atomic layer deposition (ALD) relies on alternated, self-limiting reactions between gaseous reactants and an exposed solid surface to deposit highly conformal coatings with a thickness controlled at the sub-monolayer level. These advantages have rendered ALD a mainstream technique in microelectronics and have triggered growing interest in ALD for a variety of nanotechnology applications, including energy technologies. Often, the choice for ALD is related to the need for a conformal coating on a 3D nanostructured surface, making the conformality of ALD processes a key factor in actual applications.

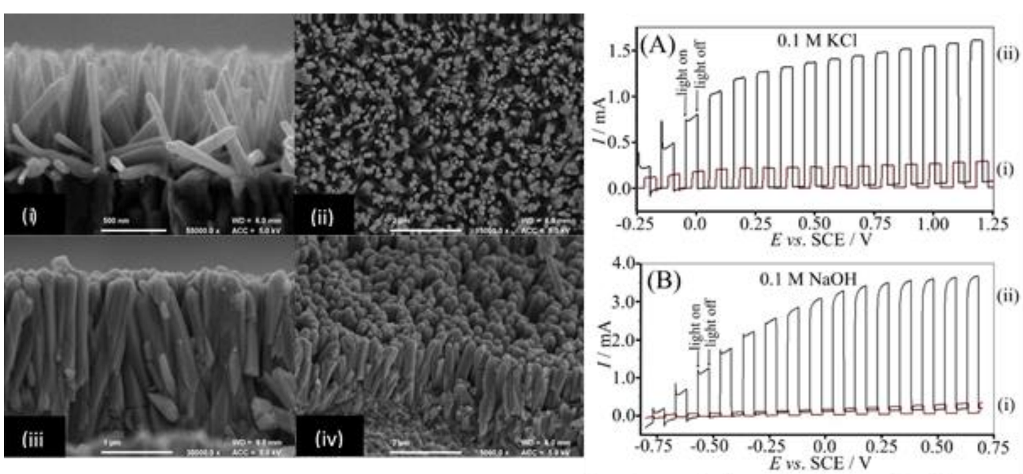

Figure 1. FE-SEM images of TiO_2 nanorods. **i** and **ii** show the TiO_2 nanorods and **iii** and **iv** show the nanorods after coating with 20 nm of NiO. (A) Photocurrents (scan rate 0.01 V/s) in 385 nm pulsed light (5 s on 5 s off) for TiO_2 and TiO_2 with NiO coating in 100 mM KCl solution. (B) Photocurrents in 385 nm pulsed light for TiO_2 and TiO_2 with NiO coating in 100 mM NaOH solution.

In proof-of-concept experiments we have tested coating of nano-crystalline n-type titania needles (grown on a ceramic substrate) with p-type NiO using the ALD. Initial results (see Fig. 1) show enhanced (by an order of magnitude) photocurrents for water splitting. However, many aspects of the mechanism and the tuning of the performance remain unresolved. A wider range of materials could be employed.

In this project, we want to follow up this proof-of-concept experiment. The student will engage in ALD techniques and coating technologies. Hydrothermal reactions will be employed to create the nano-crystalline semiconductor substrates. The resulting coated nano-structured "heterojunction interfaces" will be characterized and systematically tested and improved. The type of p-type coating, the thickness and distribution over the nano-crystal needles will be investigated. Complementary theory will be developed and photo-electrochemical measurements will be performed aiming at sea water splitting. The nano-crystal morphology has unique features based on "through-crystal" harvesting of electrons and the possible tuning of both nanocrystal length and doping. Components for both oxygen evolution and hydrogen evolution will be developed and paired. The mechanism of photo-electrochemical processes will be carefully studied.

The project is divided into (A) a materials production part in order to master hydrothermal synthesis, growth of ALD layer coatings, changing thickness and nano-crystal size, exploring different p-type materials, introducing vacuum annealing to control defect densities, (B) electrochemical characterization with photo-electrochemical methods in Bath, and (C) photocatalysis and electrocatalysis studies with advanced methods at Monash. There is a strong materials component and a wide range of materials characterization methods will be employed (electron microscopy, spectroscopy, electrochemical spectroscopy, etc.). There is also an engineering component in the development of 3D-printed reactors.

The relevance of this project **to sustainable and circular technologies** is based on the use of light for the production of products such as hydrogen. The initial aim of the work will be directed towards hydrogen production from sea water (in a clean photo-driven process). In later stages of the work additional targets such as carbon dioxide reduction in sea water are possible, as well as reactor and prototype development based on 3D-printed components. The project will allow us to start new collaborations across the Monash-Bath institutional partnership, and to develop new contacts to industry, e.g. the marine industry such as ECO Marine Power or EC-OG in Scotland.

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.