IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	Design and characterisation of new electrocatalysts for clean energy conversion	
Project Number	**IMURA0965**	
Monash Main Supervisor (Name, Email Id, Phone)	Dr Cameron Bentley, cameron.bentley@monash.edu	*Full name, Email*
Monash Co-supervisor(s) (Name, Email Id, Phone)		
Monash Head of Dept/Centre (Name,Email)	Prof Phil Andrews, phil.andrews@monash.edu	*Full name, email*
Monash Department:	School of Chemistry, Faculty of Science	
Monash ADGR (Name,Email)	Prof Peter Betts, Peter.Betts@monash.edu	*Full name, email*
IITB Main Supervisor (Name, Email Id, Phone)	Dr. Arindam Sarkar	*Full name, Email*
IITB Co-supervisor(s) (Name, Email Id, Phone)		*Full name, Email*
IITB Head of Dept (Name, Email, Phone)	Prof. Madhu Vinjamur	*Full name, email*
IITB Department:	Department of Chemical Engineering	

Research Clusters: Research Themes:

Highlight which of the Academy's CLUSTERS this project will address? *(Please nominate JUST **one.** For more information, see www.iitbmonash.org)*		**Highlight which of the Academy's Theme(s) this project will address?** *(Feel free to nominate more than one. For more information, see www.iitbmonash.org)*	
1	*Material Science/Engineering (including Nano, Metallurgy)*	***1***	*Advanced computational engineering, simulation and manufacture*
2	*Energy, Green Chem, Chemistry, Catalysis, Reaction Eng*	2	*Infrastructure Engineering*
3	*Math, CFD, Modelling, Manufacturing*	3	*Clean Energy*
4	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*	4	*Water*
5	*Earth Sciences and Civil Engineering (Geo, Water, Climate)*	5	*Nanotechnology*
6	*Bio, Stem Cells, Bio Chem, Pharma, Food*	6	*Biotechnology and Stem Cell Research*
7	*Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng*	7	*Humanities and social sciences*
8	*HSS, Design, Management*	8	Design

The research problem

The sustainable production, storage and utilisation of clean energy from renewable sources constitutes one of the most important scientific challenges facing humankind. Among technologies developed so far, those based on the interconversion of electrical and chemical energy from carbon-free or carbon-neutral fuels (*e.g.*, from the splitting of water and oxidation of hydrogen in electrolysers and fuel cells, respectively) are particularly attractive since they offer excellent scalability for industrial implementation. Commercially feasible technologies require the use of highly stable and active electrodes, known as **electrocatalysts**, to overcome the high energy barrier(s) associated with the pertinent reactions, *e.g.*, fuel oxidation and oxygen reduction taking place at the anode and cathode of fuel cells, respectively. A major obstacle in designing advanced catalysts is the immature understanding of the complex interplay between electrode surface structure and reaction kinetics/mechanisms. Indeed, despite the known (nanoscale) complexity of electrode surfaces, electrochemical measurements still routinely rely on classical macroscopic techniques (e.g., "bulk" voltammetry) that provide activity averaged over a wide range of interacting surface sites, which may obscure the nature of key elementary processes. To fully understand the overall behaviour of complex electrodes, it is essential that structure and activity can be related at the scale of surface heterogeneities (*e.g.*, from single defects or nanoparticles to the individual grains and grain boundaries of a polycrystal). Thus, experimental techniques and approaches that can unambiguously resolve nanoscale structure–activity are much needed in order to identify the structural motifs that constitute an "active" surface, which will ultimately facilitate the rational design of "next-generation" functional materials.

Project aims

To achieve major advances in electrocatalysis and nanoscience, in this joint project, we intend to integrate the state-of-the-art electrochemical imaging capability at Monash University with the materials synthesis and characterisation capabilities of IITB. The project aims are as follows:

1. **Synthesise and characterise "first-generation" of electrocatalysts:** materials/reactions with a large associated body of literature will be initially targeted, *e.g.*, polycrystalline platinum catalysts for oxygen reduction or fuel (*e.g.*, formate) oxidation. This will be later expanded to more complex materials and reactions (see *Aim 4*).
2. **Reactivity mapping at the nanoscale:** scanning electrochemical cell microscopy (SECCM), a recently-established high-resolution electrochemical imaging technique, will be deployed in tandem with complementary microscopy/spectroscopy to explore the role of surface structure and defects in various energy-related electrocatalytic processes.
3. **Rational design and engineering "next-generation" electrocatalysts:** understanding nanoscale structure–activity (*Aim 2*) will guide the development of "next-gen" optimised materials, which will be characterised and screened for increased activity and stability *etc.*
4. **Establish rational analysis/design principles:** coupling the information gained from *Aims 1–3* will establish a set of general analysis/design principles that will be applicable to any class of material/reaction, *e.g.*, structurally/compositionally complex materials (nanomaterials or alloys) and multi-electron fuel-producing reactions (electrochemical CO_2 reduction).

Expected outcomes

In terms of science and academia, the following outcomes are anticipated:

- Discovery and design of advanced catalysts with enhanced functionality (*e.g.*, high activity, selectivity, stability etc.) in order to address a global challenge;
- Establishment of rational design principles that can be generally applied to optimise any class of electrochemical material/reaction;
- Dissemination of results via publications in top scientific journals relating to the fields of electrochemistry, nanoscience, electrocatalysis and (electro)materials science.

More broadly, the project will facilitate the:

- Establishment of a world-class research team that will enhance Australia's and India's reputations for excellence in research;
- Provision of high-quality training for the next generation of scientists in clean energy conversion and nanotechnology to maintain competitive edge in these globally-relevant and interdisciplinary areas;
- Facilitation of networking and collaboration through the two-way transfer of knowledge between Monash (electrochemical imaging) and IITB (materials design/synthesis).

How will the project address the Goals of the above Themes?

Clean Energy (theme #3) lies at the heart of the electrochemical reactions and materials investigated, as well as the new technologies to be developed in this project. The development of commercially feasible electrochemical processes for the production, storage and utilisation of clean energy is essential if we are to shift towards a sustainable, secure and reliable energy supply, as well as mitigate the environmental impact of climate change. Spurred on by this significant global challenge, there is an ongoing search for new functional materials (electrocatalysts) that are Earth-abundant and possess desirable properties such as high activity, selectivity and stability. To meet this demand, this project introduces a new paradigm to characterise, design and synthesise "next-generation" nanomaterials (discussed below) with enhanced function, which will ultimately find application in clean energy technologies such as fuel cells and electrolysers.

Nanotechnology (theme #5) plays a central role in both the characterisation and design/development stages of this project. In terms of characterisation, SECCM will be deployed to understand the nanoscopic structural factors that give rise to desirable properties (*e.g.*, electrocatalytic activity, selectivity or stability). In terms of design/development, this nanoscale "structure–property" information will be used to rationally design new materials through the use of "nanoengineering strategy", which entails the design and synthesis of nanostructured interfaces. Ultimately, after screening and characterisation, these "nanoengineered" electrodes with enhanced function will give rise to "next-generation" clean energy technologies (discussed above).

Potential RPCs from IITB and Monash

Potential RPCs from Monash, all of whom have backgrounds in electrochemistry, materials science and clean energy technologies:

1. Prof Jie Zhang
2. Prof Douglas MacFarlane
3. Dr Alexandr Simonov

Potential RPC from IITB

1. Prof. S. Mahajani
2. Prof. P. C. Ghosh
3. Prof. P. Bhargava

Capabilities and Degrees Required

The student is expected to have some basic idea of electrochemistry and material synthesis (hands on experimental skills not required), and should be comfortable with advanced mathematics such as calculus. It is desired to have students with MTech. in Chemical/materials engineering, MSc. in chemistry/materials science/physics.

Necessary Courses

1. CL 611 (Electrochemical Reaction Engineering)
2. MM 684 (X-Ray Diffraction and Electron Microscopy)
3. CL 605 (Advanced reaction engineering)
4. EN 604 (Fuel cells)

Potential Collaborators

Please visit the IITB website www.iitb.ac.in OR Monash Website www.monash.edu to highlight some potential collaborators that would be best suited for the area of research you are intending to float.

Select up to **(4)** keywords from the Academy's approved keyword list **(available at http://www.iitbmonash.org/becoming-a-research-supervisor/)** relating to this project to make it easier for the students to apply.

Novel functional materials (1), Materials Chemistry/Science (20), Electro Chemistry (22), Novel Batteries and Fuel Cells (23), Catalysis and Reaction Engineering (28)