

An Indian-Australian research partnership

Project Title: **Generation of dihydrogen from sea water: design of robust and efficient electrocatalysts**

Project Number **IMURA0902**

Monash Main Supervisor
(Name, Email, Phone)

Dr Alexandr N. Simonov
alexandr.simonov@monash.edu

Full name, Email

Monash Co-supervisor(s)
(Name, Email, Phone)

Prof Douglas R. MacFarlane
douglas.macfarlane@monash.edu

Monash Head of Dept/Centre (Name, Email)

Prof Philip C. Andrews
phil.andrews@monash.edu

Full name, email

Monash Department:

Chemistry / Science

Monash ADGR
(Name, Email)

Prof Peter Betts
Peter.Betts@monash.edu

Full name, email

IITB Main Supervisor
(Name, Email, Phone)

Prof Aswani Yella
aswani.yella@iitb.ac.in

Full name, Email

IITB Co-supervisor(s)
(Name, Email, Phone)

Full name, Email

IITB Head of Dept
(Name, Email, Phone)

Prof. K Narasimhan

Full name, email

IITB Department:

Metallurgical Engineering and Materials Science

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

Define the problem

Global transition towards renewables as our major energy source requires robust and efficient technologies for storage of the intermittent renewable electricity, as recognised by both academia and industry. At current stage of technological development, batteries are not an economically viable solution to this problem, which is in contrast to green chemical fuels like hydrogen gas and ammonia that can be synthesised from water and air *via* renewables-powered electrochemical processes. For the gigawatt scale of green H₂ (and NH₃) production, very significant amounts of water are required rendering sea water the only feasible substrate for this purpose. However, the majority of existing low-temperature electrolyser devices cannot use sea water directly, which introduces additional costs associated with purification *via* multiple filtration and reverse osmosis steps. While the cathode half-reaction of the water splitting process, the hydrogen evolution reaction ($2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2$), is not significantly affected by salts present in sea water (except for the scaling problem during long term operation), the anode presents a much more significant challenge. In the latter case, the oxygen evolution reaction ($2\text{H}_2\text{O} \rightarrow \text{O}_2 + 4\text{H}^+ + 4\text{e}^-$) has to compete with the kinetically more facile and undesirable in this context chlorine evolution reaction ($2\text{Cl}^- \rightarrow \text{Cl}_2 + 2\text{e}^-$). Therefore, further development of the water splitting technology requires electrocatalysts that operate efficiently in the presence of the significant amounts of NaCl and other inorganic salts that are abundant in sea water. The development and detailed characterisation of such catalysts is the key focus of the present PhD project.

Project aims

Define the aims of the project

The ultimate aim of the project is the invention of novel efficient and robust electrocatalysts for the electrooxidation of sea water. Specific focus will be on:

- Identification of the strategies for the efficient suppression of the CER and facilitating the OER, including surface layer modification and doping of benchmark electrocatalysts, as well as creation of novel compositions;
- Detailed investigation of the effects of the operating conditions (pH, temperature, flow rate, potential) on the selectivity of the kinetics of the OER and CER for the best performing catalysts, and modelling of the reaction kinetics;
- In-depth physical characterisation of materials, including by *in situ* spectroelectrochemical methods, to understand the mechanisms of operation and predict strategies for further improvements.

Expected outcomes

Highlight the expected outcomes of the project including likelihood of patents

Key outcomes of the project will be as follows:

1. Top-quality training in high-end techniques relevant to the very rapidly emerging field of renewable energy technologies;
2. Expert knowledge in physical chemistry and materials science;
3. Publications in top-tier journals;
4. Links to our existing industrial partners in Australia and India;
5. Possibility for patenting materials developed for the very rapidly developing technology.

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

Describe how the project will address the goals of one or more of the 6 Themes listed above.

The project will directly address the goals of theme **Clean Energy** by developing novel materials for the critical technology for the storage of renewable energy.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Be as specific or as general as you like. These capabilities will be input into the online application form and students who opt for this project will be required to show that they can demonstrate these capabilities.

The prerequisite skills critical for this project are knowledge of physical chemistry and well-developed experimentalist skills. Extended knowledge of physics and mathematics is also highly desirable. Practical skills in electrochemistry are not critically required, as those will be acquired by a suitable candidate

during the very initial period of training.

Candidates with the following degrees are desirable:

1. M.Sc. in Chemistry (Physical Chemistry or Analytical Chemistry with Mathematics at the B.Sc. level)
2. B.Tech./M.Tech. in Chemical Engineering, Materials Engineering
3. M.Sc. in Physics (with strong interest in chemistry)

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.

Energy, Energy Storage, Energy Materials

Novel Functional Materials

Electro Chemistry

Green Chemistry and Renewable Energy