

An Indian-Australian research partnership

Project Title: Nano-confined multi-component metal hydride systems for hydrogen buffer for stable fuel cell operation

Project Number IMURA0468(a)

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IITB Department:

Electrical Engineering, Energy Science and
Engineering, Chemical Engineering

Research Academy Themes:

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. Advanced computational engineering, simulation and manufacture
2. Infrastructure Engineering
3. **Clean Energy**
4. Water
5. **Nanotechnology**
6. Biotechnology and Stem Cell Research

The research problem

We propose efficient hydrogen storage/buffers for stabilized operation of fuel cells [1]. The hydrogen will be generated from water using photo-electro-chemical process. At present, the problem with the solid state host active phases such as Magnesium (Mg) etc. are high thermodynamic stability and poor kinetics. Nano-confining the active phase in these hydrides can destabilize the active phase by two mechanisms: (i) elastically clamping [2] the latter; (ii) by increasing the interface energy of the active phase [3].

Moreover, the interfacial regions such as grain/phase boundaries act as channels to enhance hydrogen diffusion thus improving kinetics [4]. The destabilization effect can be further enhanced in the multi component systems such as Mg-Li, Mg-Al [5].

Thus the nano-confinement and destabilization strategies can be utilized for the development of hydrogen storage materials.

In the present project Mg-based nano-confined multi-component materials will be developed for hydrogen storage. Various techniques such as electro-deposition, sputter deposition etc. will be used to prepare these materials in powder and thin film form. The thermodynamic and kinetic hydrogen storage properties will be studied using Sievert's type apparatus. The materials will be characterized using techniques such as Hi-Resolution Transmission Electron Microscopy (HRTEM) and X-Ray Diffraction (XRD). The developed materials will be tested in portable fuel cell systems for their performance.

References:

1. B. Sakintuna, F.L.-Darkrim, M. Hirscher, "Metal hydride materials for solid hydrogen storage: A review", *International Journal of Hydrogen Energy*, 32, 1121-1140 (2007)
2. A. Baldi, M. Gonzalez-Silveira, V. Palmisano, B. Dam, R. Griessen, "Destabilization of the Mg-H System through Elastic Constraints," *Physical Review Letters*, 102, 226102 (2009)
3. K.-J. Jeon, H. R. Moon, A. M. Ruminski, B. Jiang, C. Kisielowski, R. Bardhan, J. J. Urban, "High-Capacity Hydrogen Storage in Air-Stable Magnesium Nanocomposites", *Nature Materials*, 10, 286-290 (2011)
4. K. Nogita, X. Q. Tran, T. Yamamoto, E. Tanaka, S. D. McDonald, C. M. Goulay, K. Yasuda, S. Matsumura, "Evidence of the hydrogen release mechanism in bulk MgH₂", *Scientific Reports*, 5, 8450 (2015)
5. J. J. Vajo, S. L. Skeith, F. Mertens, "Reversible storage of hydrogen in destabilized LiBH₄", *Journal of Physical Chemistry B*, 109, 2719-3722 (2005)

Project aims

1. To prepare nano-confined, multi-component materials for hydrogen storage
2. To understand the thermodynamic destabilization and kinetic mechanisms during hydrogen absorption/desorption (sorption)

Expected outcomes

1. Nano-confined multi-component materials exhibiting superior hydrogen storage properties
2. Thermodynamic and kinetic models of hydrogen sorption

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

The above effort is aligned with the parallel (IITB-Monash) proposal for efficient hydrogen generation from water via photo-electro-chemical path (Artificial Leaf). Hydrogen generation, storage and conversion are key green energy technology challenges. In particular, hydrogen storage for vehicular use will be significant in reducing CO₂ emissions.

Capabilities and Degrees Required

- (1) Laboratory experience connected to nanomaterial processing and characterization
- (2) Simulation and modeling experience
- (3) Masters in Engineering and Sciences (MTech)

Potential Collaborators

S Sontakke, Institute of Chemical Technology, Mumbai University

Additional costs and equipment

Total cost INR 3 Lakhs towards purchase of consumables and equipment

Please provide a few key words relating to this project to make it easier for the students to apply.

Nanotechnology, hydrogen storage

Detailed justification - Additional costs and equipment

Please justify why is this level funding is required?

Not Applicable

	INR/\$AUD	
What is the total funding required for the entire project?	INR 1 million	(X)
How much bare minimum seed funding will be required to kick off the collaboration?	INR 0.3 million	(Y)
What are the additional funds that will need to be sourced?	INR 0.7 million	(X-Y)

How will the additional funds (X-Y) be sourced?

There is a proposal in preparation for submission to Indian Government Agencies to provide supplementary funds

What happens if the PIs are unsuccessful in sourcing (X-Y) and we have a student selected?

Explore alternate funding sources internally (IIT Bombay) and from external agencies

Is there any industrial partner that might fund this project that we might approach?

Not required at the Proof of Concept stage

Please also fill up the Project Consumables Budget Excel spreadsheet template(available from The Academy) which is required for any budget request which is in excess of INR 3 lakhs OR \$6000: Not Applicable