Project Title:	**Mg-graphene-Ni-Mxene nanocomposites for near-ambient hydrogen storage**	
Project Number	**IMURA1183**	
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IITB Department:	Energy Science and Engineering	

Research Clusters:

Highlight which of the Academy's CLUSTERS this project will address?
(Please nominate JUST ***one.*** *For more information, see www.iitbmonash.org)*

1	***Material Science/Engineering (including Nano**, Metallurgy)*
2	*Energy, Green Chem, Chemistry, Catalysis, Reaction Eng*
3	*Math, CFD, Modelling, Manufacturing*
4	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*
5	*Earth Sciences and Civil Engineering (Geo, Water, Climate)*
6	*Bio, Stem Cells, Bio Chem, Pharma, Food*
7	*Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng*
8	*HSS, Design, Management*

Research 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	*Artificial Intelligence and Advanced Computational Modelling*
2	*Circular Economy*
3	***Clean Energy***
4	*Health Sciences*
5	*Smart Materials*
6	*Sustainable Societies*
7	*Infrastructure*

The research problem

With the depleting fossil fuels and growing demand for renewable energy, hydrogen storage for fuel cell applications is emerging as a promising area of research, particularly in transport sector. Important initiatives and national level e.g. National Green Hydrogen Mission (India) and National Hydrogen Strategy (Australia) are driving research in this area.

Magnesium hydride (MgH_2) offers reversible, single-step hydrogen storage for vehicular applications with 7.6wt% hydrogen capacity. However, it exhibits poor hydrogen sorption (ab/desorption) kinetics at near-ambient conditions. For example, MgH_2 releases hydrogen only at ≥400 °C. Moreover, Mg exhibits incubation periods up to several hours (leading to 1 day), during which it does not absorb any significant hydrogen. Hence, nanosizing and using suitable catalysts is a common practice to improve its kinetics of sorption. Nanosized $Mg(H_2)$ with reduced graphene oxide (rGO) and Ni as catalysts can demonstrate hydrogen release at ~215 °C, as per our reports. However, this is higher than the operation temperature PEM fuel cells (80-120 °C). Hence, it is needed to decrease this temperature further.

MXenes are promising and emerging materials which can act as both hydrogen hosts and catalysts for hydrogen release. However, research in employing MXenes for hydrogen sorption is still in its nascent stages.

In the present project, MXenes (e.g.$Ti_3C_2T_x$, where $T=F^-$, OH^-), rGO and Ni will be used as catalysts to synthesis Mg-rGO-Ni-MXene nanocomposites by ball milling. Hydrogen sorption in these nanocomposites will be studied and also will be attempted at near-ambient conditions of $P_{H2}≤5$ bar and 80-120 °C. X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Electron density maps, X-ray photoelectron spectroscopy (XPS), Raman, FTIR will be used for characterizing these materials. Our earlier research shows that the MgH_2 unit cell shrinks after H-uptake, in the presence of rGO and Ni, favouring H-release at lower temperatures. This was termed as "Structural catalysis", in our work. Such structural catalysis will be explored in the Mg-rGO-Ni-MXene nanocomposites. The reasons for such structural changes and their eventual favourable influence on H-release temperature will be studied. This will be done using thorough microstructural analysis of the active phases (i.e. the phases taking/releasing hydrogen) and those that are in the proximities of these active phases. Possible sets of crystallographic orientation relationships between these phases will be explored. The reasons behind their influence on Hydrogen uptake/release will be understood by corroborating the analyses from microscopy and spectroscopy.

Project aims

Objectives:
1. Synthesis of novel Mg-rGO-Ni-MXene nanocomposites using ball milling
2. Studies on hydrogen uptake/release by these nanocomposites
3. Exploring hydrogen uptake/release by these nanocomposites at near-ambient conditions ($P_{H2}≤5$ bar and 80-120 °C)
4. Thorough spectroscopic and microscopic characterization of these nanocomposites
5. Understanding crystallographic and microstructural features upon hydrogen uptake/release e.g. changes to unit cell dimensions, orientation relationships among various active and supporting phases
6. Corroborating the analyses from spectroscopy and microscopy for understanding their influence on favourable hydrogen uptake/release from these nanocomposites
7. Possible synthesis of novel Mg-rGO-Ni-MXene nanocomposites exhibiting near-ambient hydrogen uptake/release

What is expected of the student when at IITB and when at Monash?

Highlight how the project will gain from the students stay at IITB and at Monash

At IITB the project would gain the following:

1. Expertise in synthesis of novel Mg-rGO-Ni-MXene nanocomposites using ball milling
2. Exploration of hydrogen uptake/release by these nanocomposites and at near-ambient conditions ($P_{H2}≤5$ bar and 80-120 °C)
3. Preliminary spectroscopic and microscopic characterization of these nanocomposites and their correlation

At Monash University the project would gain the following:

1. Thorough microscopic characterization of these nanocomposites
2. Understanding crystallographic and microstructural features upon hydrogen uptake/release e.g. changes to unit cell dimensions, orientation relationships among various active and supporting phases

Together through discussions by the student and both the supervisors:

1. Corroborating the analyses from spectroscopy and microscopy for understanding the reasons behind (possibly) favourable hydrogen uptake/release from these nanocomposites
2. A new direction towards material analysis in hydrogen storage research, in general

Expected outcomes

Highlight the expected outcomes of the project

1. Detailed synthesis strategies for Mg-rGO-Ni-MXene nanocomposites, with minimal sacrifice of their structural features
2. Novel Mg-rGO-Ni-MXene nanocomposites exhibiting hydrogen uptake/release (possibly) at near-ambient conditions ($P_{H2} \leq 5$ bar and 80-120 °C)
3. Methodologies for studying orientation relationships in hydrogen storage materials
4. Strategies to corroborate the spectroscopic analysis (inter-elemental interactions, valence states, Fermi-levels) with crystallographic changes in the materials and orientation relationships among different phases upon hydrogen uptake/release
5. A new direction towards material analysis in hydrogen storage research, in general

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 aims to address the theme of "Clean Energy". If the project is successfully implemented then the novel Mg-rGO-Ni-MXene nanocomposites exhibiting hydrogen uptake/release at near-ambient conditions can be synthesized. Eventually, scale-up efforts can be explored. Scaled-up hydrogen storage reactors containing these materials can be coupled with electrolysers for hydrogen supply on one end. On the other end, fuel cells can be coupled to utilize the hydrogen released from these reactors. Such integrated hydrogen supply and storage systems can inspire the efforts in hydrogen fuelling stations (housing electrolysers) and fuel cell powered automobiles.

Potential RPCs from IITB and Monash

Provide names of the potential research progress committee members (RPCs) and describe why they are most suited for the proposed project

The potential RPC members are (tentative):
From IITB:

1. Prof. Abhijit Chatterjee, Dept. Chemical Engineering – Experienced in hydrogen storage at atomic and molecular level
2. Prof. Chandramouli Volla, Dept. Chemistry – Experienced in Spectroscopic analysis

From Monash:

1. Dr. Sebastian Thomas, Department of Materials Science and Engineering – has expertise in the interaction of hydrogen with materials, eg hydrogen embrittlement of metal alloys.
2. A/Prof. Matthew Weyland, Monash Centre for Electron Microscopy and Department of Materials Science and Engineering – has expertise in the characterisation of materials by transmission electron microscopy.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Feel free to 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.

Degrees Required: B.Sc., B.E., B.Tech., M.E., M.Tech., M.Sc.

Disciplines: Metallurgical Engineering, Materials Science, Chemical Engineering, Mechanical Engineering, Nanotechnology, Energy Science and Engineering, Chemistry, Physics, Nanoscience

Capabilities: Knowledge in electron microscopy, spectroscopy, experience with chemical synthesis, ability to interpret the data constructively

Necessary Courses

Name three tentative courses relevant to the project that the student should complete during his/her coursework at IITB (the student will require to secure 8 point in these courses)

The candidate may choose to study the courses on the following topics: Hydrogen storage, Hydrogen Energy, Introduction to Materials, Analytical Techniques (SEM, TEM, Spectroscopy), Thermodynamics of Materials, Kinetic processes in Materials, Mathematics

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.

The potential collaborators are (tentative):

IIT Bombay:
Prof. Abhijit Chatterjee, Chemical Engineering
Prof. Amartya Mukhopadhyay, Metallurgical Engg. and Materials Sci.
Prof. M.J.N.V. Prasad, Metallurgical Engg. and Materials Sci.

Monash:
Prof. Nikhil Medhekar, Department of Materials Science and Engineering
Prof. Akshat Tanksale, Department of Chemical and Biological Engineering

Keywords relating to this project to make it easier for the students to apply.

hydrogen storage, mxene, max, graphene, magnesium, microscopy, spectroscopy, clean, energy, automobile, transport