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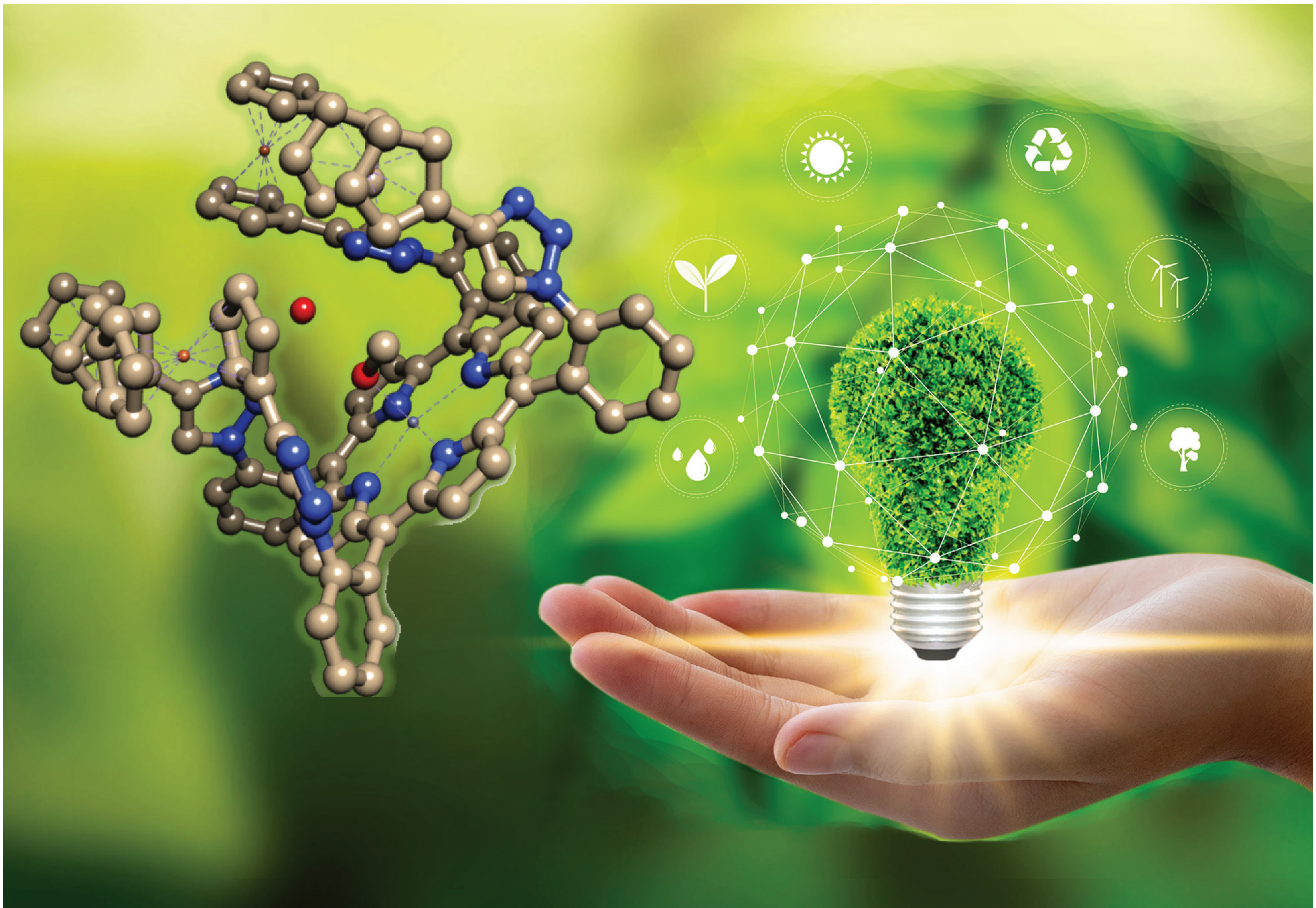

# Compendium on Hydrogen and Fuel Cell

# 2018

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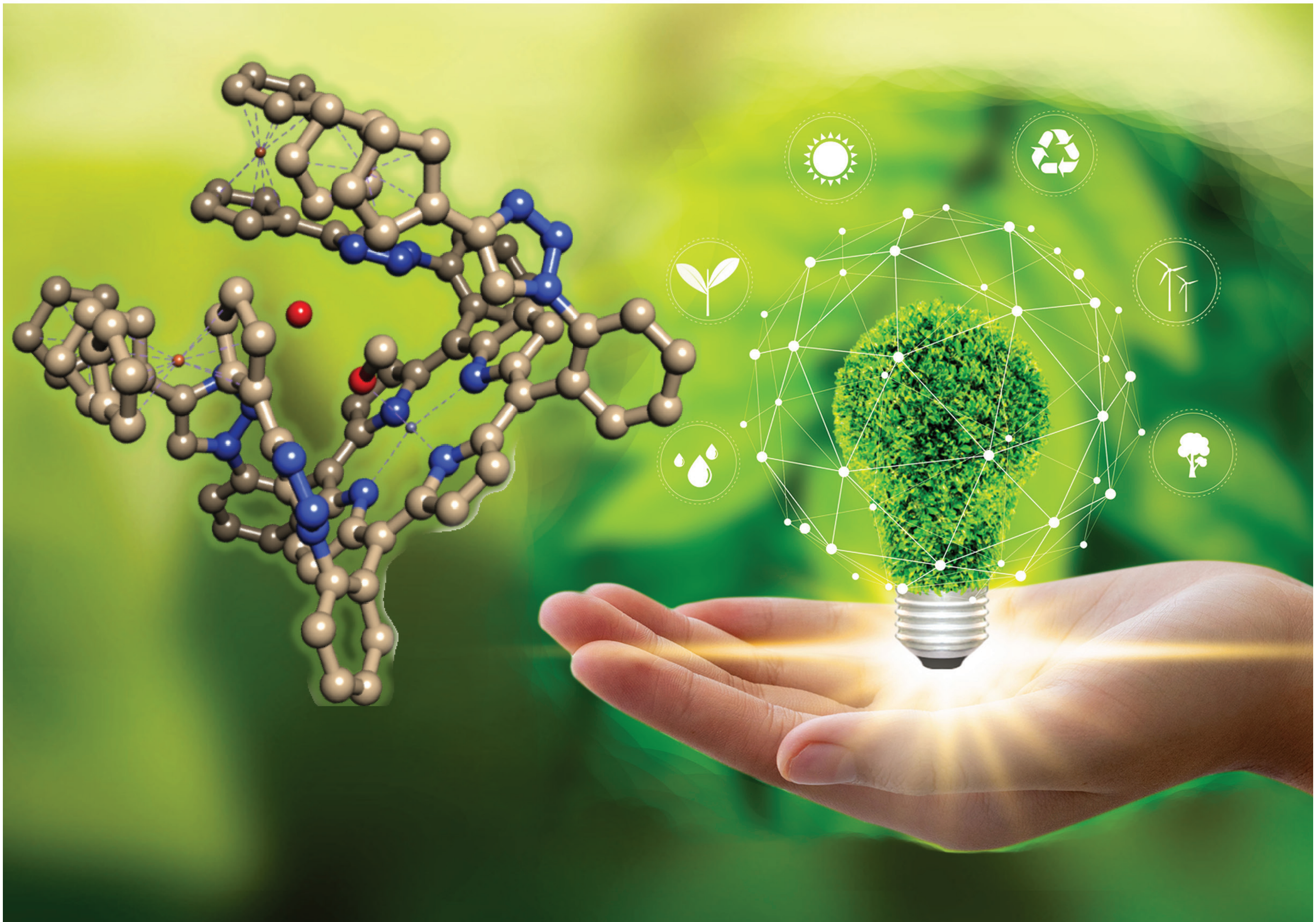

# Compendium on Hydrogen and Fuel Cell

# 2018

## Dr. Ranjith Krishna Pai

**Director / Scientist 'E'**
**Technology Mission Division**
**(Energy & Water), DST,**
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Dr. Ranjith Krishna Pai received the Ph.D. degree in Natural Sciences, from Dr.Othmar Marti's Group, Ulm University, Germany, in 2005. He is currently Scientist 'E' / Director of Technology Mission Division of Department of Science and Technology responsible for research, development and innovation activities in Clean Energy domain. He has represented India in numerous multi lateral event and has articulated national and international endeavors in energy domains.

From 2006 to 2007, he was a Postdoctoral Researcher at University of Chile, Santiago, aworking on Genetic engineering of a novel protein-nanoparticle hybrid system with great potential for bio sensing applications. 2007 to 2009, he spent two years as a Post-Doctoral Scientist at Stockholm University, Stockholm, Sweden, working on synthesis of nanostructured hybrid materials and Characterization of nonlinear optical nanomaterial. From 2009 to 2011, he was a Research Scientist at CFN, Brookhaven National Laboratory, New York, USA, working on photo fabrication of donor- acceptor antenna system for solar energy harvesting, development of bio sensing platforms based on bio-inorganic scaffolds with single molecule/particle sensitivity, fabrication of transparent organic thin-film for use in organic photovoltaic cells. After spending 2 years 5 months at BNL, New York, USA, he spent another 2 years 4 months (2011-2013) as a Research Scientist at INL - International Iberian Nanotechnology Laboratory, Braga, Portugal. His research at INL involved development of transparent conjugated polymer films for capturing solar energy, organic thin-film solar cells based on conjugated polymers and fullerene derivative, hybrid organic/inorganic nanomaterial and synthesis and fundamental study of conjugated polymers, solar device fabrication and electrical and photochemical device measurements.From 2013 to 2015, he was an Associate Professor and Group leader at Nanostructured Hybrid Functional Materials & Devices, Jain University, Bangalore, India.

He published several high impact scientific papers, and author of three book chapters.15 invited lectures at international conferences. Previously served as an Associate Editor of a Journal "Nano tools & Nano machines" and a Guest Editor of International Journal of Polymer Science. His research interest includes energy conversion technologies, including low cost photovoltaic (Organic, and hybrid solar cells) and electrical energy storage (batteries and supercapacitors), synthesis of semiconducting polymers and polymer nanostructures and their application to organic transistors, solar cells, light emitting diodes and other photonic applications, synthesis, characterizations and applications of carbon and inorganic nanotubes, Modeling of the electronic properties of nanostructured semiconductors.

## Dr. Rajiv K. Tayal

**Advisor / Scientist 'G'**
**Head, Technology Mission Division**
**(Energy & Water), DST**
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Dr Rajiv Tayal has been working as an Advisor in the Department of Science & Technology (DST), and is currently heading the Technology Mission Division which is concerned with major R&D initiatives in the areas of Clean Energy and Water, including international programs with several other countries.

He presided over two of the most prestigious institutions in the Indian S&T ecosystem in the immediate past; as Executive Director of the bi-national Indo-US Science & Technology Forum (IUSSTF) and Secretary of the Science & Engineering Research Board (SERB).

His extensive professional experience in Science, Technology and Innovation space, spans across Industry, Government and a large number of academic institutions, research laboratories and industry. He is a Fellow of the Indian National Academy of Engineering, FNAE and The Institution of Engineers (India), FIE.

प्रो. आशुतोष शर्मा
Prof. Ashutosh Sharma

सचिव
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विज्ञान एवं प्रौद्योगिकी विभाग
Secretary
Government of India
Ministry of Science and Technology
Department of Science and Technology

27.04.2021

## Foreword

Greater utilization of renewables in our energy mix is our policy objective to achieve decarbonisation. While there are several pathways for decarbonisation varying in time frames, Hydrogen produced from renewables is considered as the cleanest energy source. Hydrogen has high energy content per unit mass, which is three times higher than gasoline. Hydrogen is being used for energy applications with suitable fuel cells. However, in order to make renewable Hydrogen a viable option, several key challenges related to materials including new material development, electrolytes, storage, safety and standards need to be addressed. Considering the importance of Hydrogen in the emerging landscape of clean energy, Department of Science & Technology (DST) had already incubated a small R&D program few years ago to act as a pilot that can be scaled up according to national needs and priorities in future. A set of twenty-nine projects have been supported under this program till so far, across three important areas related to Hydrogen economy, namely, Production, Storage and Utilization. All these projects are currently in different stages of implementation. The report presents portfolio of R&D projects taken up in this initiative with the participation of several scientists, industries, utilities and other stakeholders from R&D laboratories, academia and industries related to Hydrogen and Fuel Cell. I hope that this compendium will enable researchers and stakeholders connect and collectively contribute to Hydrogen and Fuel Cell research, development, demonstration and deployment.

(Ashutosh Sharma)

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# INTRODUCTION

Considering the importance of Hydrogen in the emerging landscape of clean energy, Department of Science & Technology (DST) had already incubated a small R&D program few years ago to act as a pilot that can be scaled up according to national needs and priorities in future. A set of twenty-nine projects have been supported under this program till so far, across three important areas related to Hydrogen economy, namely, Production, Storage and Utilization. All these projects are currently in different stages of implementation. The program can now be fine-tuned and closely aligned to fulfill the specific R&D needs and priorities of the National Hydrogen Mission, with corresponding scaling up. We have already started the process to assess the potential of past initiatives in terms of their impact and scaling up. The position is being reviewed at the highest level to identify R&D priorities in the current context, conceptualize a roadmap to realize them and launch new initiatives tailormade to address specific R&Drequirement.

# TABLE OF CONTENTS

# 1 Design, Development, Testing And Evaluation Of A Lean Premixed Swirl-Stabilized Gas Turbine Combustor For Stationary Power Generation Using High-Hydrogen-Content Fuel

## Aim

We aim to develop lean premixed (LP) combustion system for stationary gas turbines for standalone power generation. In LP combustion, the combustion zone is operated with excess air in order to reduce the flame temperature (< 1800 K), and therefore the amount of post-combustion dilution air is reduced. Further, the lean operation of the combustion zone (typical equivalence ratio of 0.4–0.6) ensures: (a) lower production of thermal NOx due to lower flame temperature; (b) lower production of prompt NOx due to fuel-lean operation. The flame stability, emission are affected by the fuel composition change. Also, flame instabilities might arise due to change in fuel composition. The influence of fuel composition on the flame is described in Fig. 1. We aim to investigate the combustion characteristics of HHC fuels in a gas turbine combustor operating in a lean-premixed combustion regime, and based on the results, an LP combustor for 100 kWe will be developed.

## Objectives

The objectives of the proposed work are summarized below:

- Design and realization of a 15 kWth laboratory-scale swirl-stabilized LP combustor with optical access
- Study of lean blowout limit for HHC fuel (different blends of hydrogen and CNG) using laser-induced fluorescence imaging of OH and CH radicals at high repetition rate (5-10 kHz)

- Modeling and simulation of LP combustor at different operating conditions using CFD solver
- Conceptual design, realization, and integration of an LP combustor of a 100 kWe MGT unit

## Methodology

A lab-scale 15 kW LP combustor will be designed, and simultaneous PIV-PLIF studies will be conducted to study the lean blow-off and flashback phenomena under various operating conditions. The lab-scale combustor will have a modular design with various geometrical modifications possible, such as change of degree of swirl by changing different axial swirlers, change in the fuel injection locations to study the premixing effects, change/removal of different bluff body shapes to help in flame stabilization. Numerical simulations will be carried out and validated against the experimental data. Finally, an LP combustor will be designed, developed, integrated and tested with 100 kWe MGT in collaboration with the Industrial Partner (TurboTech Precision Engineering Pvt. Ltd., Bangalore).

### Expected Outcome & Deliverables

- A laboratory-scale working prototype of 15 kWth lean premixed combustor
- Experimental analysis of lean blowout limit
- Simultaneous PIV/PLIF imaging of LP combustion at high-repetition rates
- Conceptual design, realization and integration of a LP combustor for 100 kWe MGT unit

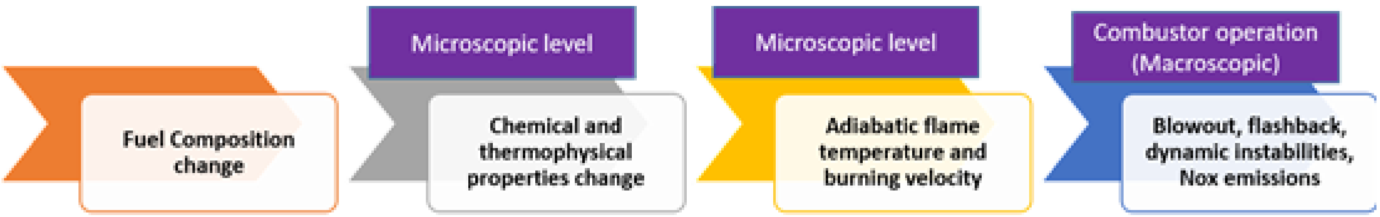


Fig. 1: Effect of fuel composition on flame operability

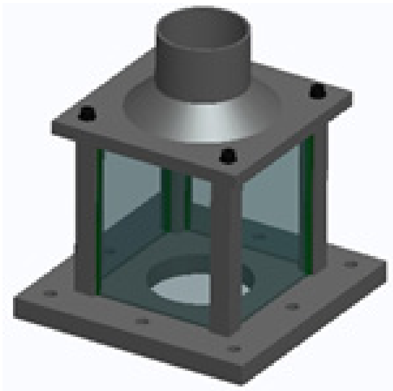

Fig. 2: CAD of optically accessible 25 kWth lab scale combustor

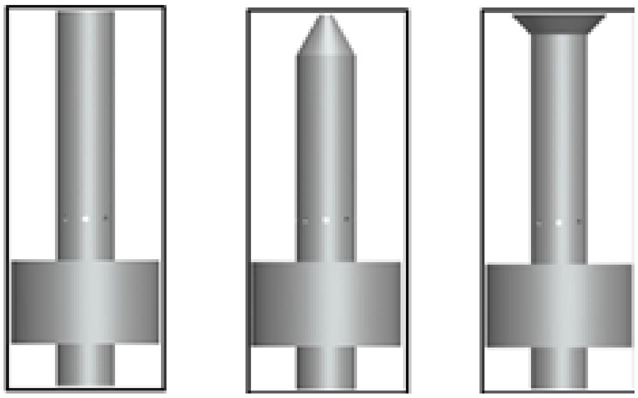

Fig.3: Bluff bodies with different areas for flame stabilization

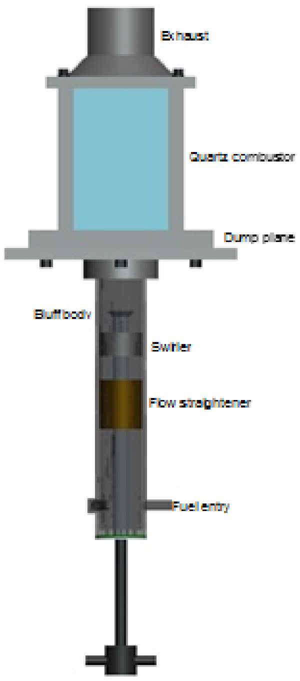


Fig. 4: CAD of Lab combustor test rig

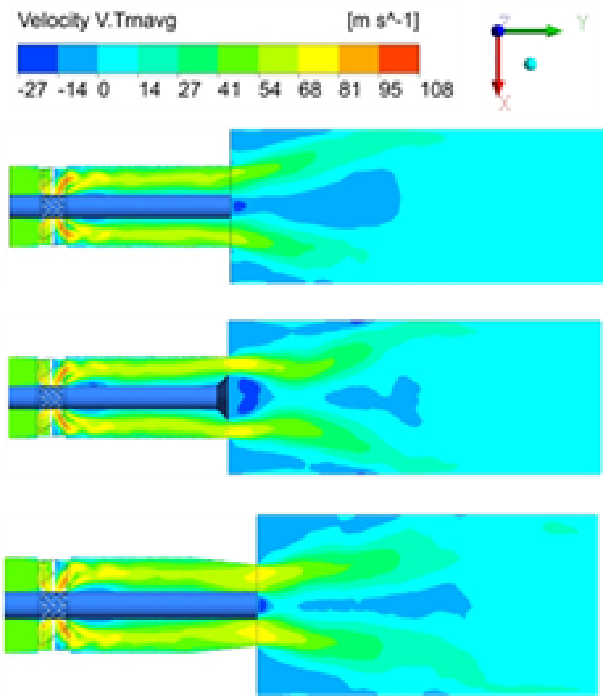


Fig 5: Effect of swirler design on velocity contours

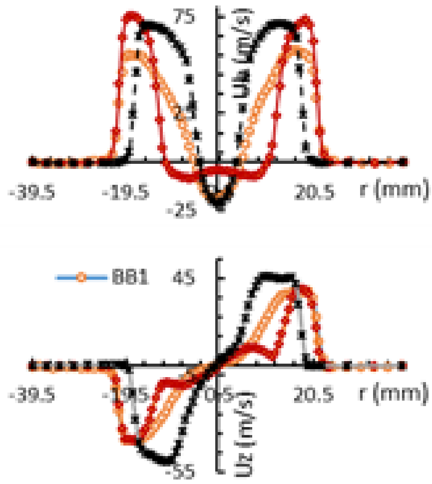


**Fig. 6: Axial (top) and azimuthal (bottom) velocity profiles for isothermal case.**

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Dr. Santanu De leads Combustion and Energy Conversion Systems research group at IITK. He received a Ph.D. in Aerospace Engineering from the Indian Institute of Science, Bangalore in 2012. Prior to his joining at IIT Kanpur, he served as a postdoctoral research scholar at the Michigan Technological University and the Institute of Combustion Technology, University of Stuttgart. His areas of research are numerical and experimental investigation of combustion, gas turbine combustion, turbulent spray atomization and combustion, coal gasification and combustion.

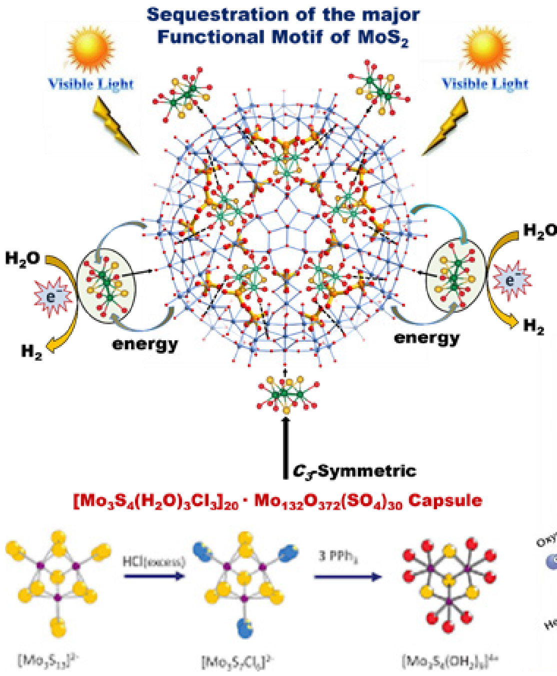
# 2 Boosting the $H_2$ Economy by Harnessing the Beauty of Encapsulation Chemistry: Augmented Kinetics for Water Splitting Reaction under ConfinementErium ad inum mene

## Aim

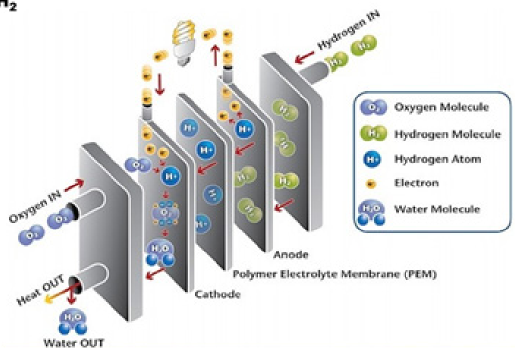
The energy sustainable applications of Polyoxometalate Chemistry will be bencmarked especially for the fascinating Keplerate clusters using of the “Nanoscopic Compartmentalization” strategy. This research will be pioneering to set a bridge between the enormously emerging energy mimetic research and the omnipotent encapsulation chemistry behavior under confinement of the nano-container.

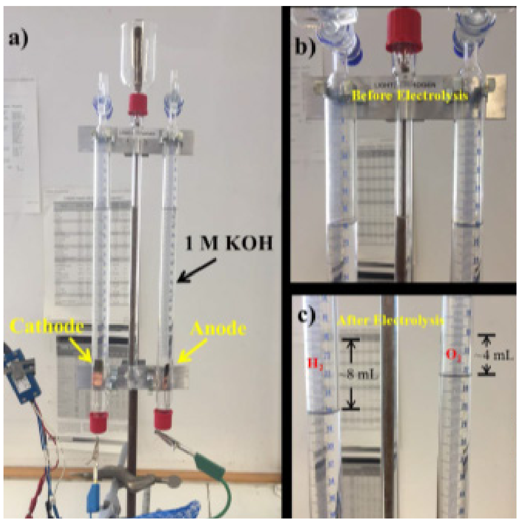
## Methodology

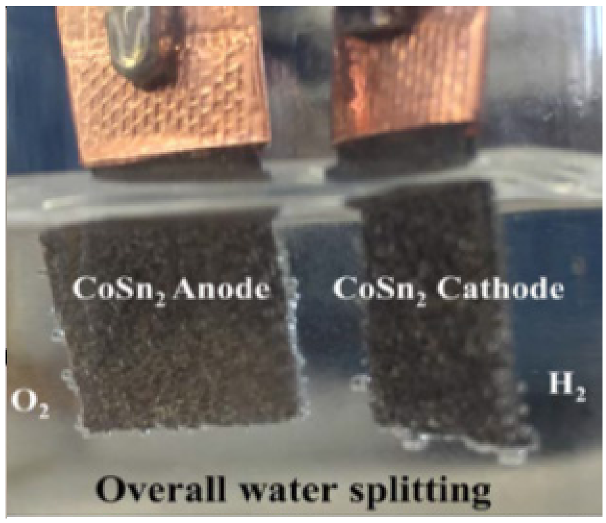
Highly water soluble $Mo_{132}$ nano-Keplerate contain 20 $C_3$-symmetric $\{Mo_9O_9\}$-“metallo-crown” pores grafted on its surface which are in general capable of uptaking a number of cations and can even separate a mixture of cations. This cation receptor ability of the $\{Mo_9O_9\}$-metallo-crown pores may provide a suitably symmetric and appropriate sized platform for hosting the same $C_3$-symmetric $\{Mo_3S_4\}^{4+}$ nanocluster as depicted below. The coordination of the Mo=O spikes with the 3 vacant coordination sites (upon replacement of aqua ligands) and thereby endorsing faster coordination exchange for the sake of higher turnover rates. The capsule being a very strong absorber of visible light at 450 nm, can provide the requisite energy to overcome the corresponding kinetic energy barrier for the Hydrogen Evolution Reaction (HER) from aqueous solution.


Sequestration of the major Functional Motif of $MoS_2$
Visible Light
Visible Light
$H_2O$
$H_2O$
e
e
$H_2$
$H_2$
energy
energy
$C_3$-Symmetric
$[Mo_3S_4(H_2O)_3Cl_3]_{20} \cdot Mo_{132}O_{372}(SO_4)_{30}$ Capsule
HCl(excess)
3 $PPh_3$


Hyundai Fuel Cell Electr
HYUNDAI
$H_2$energy


Hydrogen IN
Oxygen IN
Heat OUT
Water OUT
Anode
Polymer Electrolyte Membrane (PEM)
Cathode
Oxygen Molecule
Hydrogen Molecule
Hydrogen Atom
Electron
Water Molecule


a)
b)
c)
1 M KOH
Cathode
Anode
Before Electrolysis
After Electrolysis
$H_2$
$O_2$
~8 mL
~4 mL


$CoSn_2$ Anode
$CoSn_2$ Cathode
$O_2$
$H_2$
Overall water splitting


H2 NEWS
UPDATE

## Expected Outcome & Deliverables

- To re-evaluate protocol for synthesis of efficient photo and electro-catalyst and its relation with exhibited activity.
- To evaluate sensitivity of pH on catalyst stability, activity and catalytic sites maximize the quantum yield. Identification of feasible mechanism of the catalysis thereby to access the overpotential causing effects for the sake of optimization.
- Final objective is to design suitable technology for production of $H_2$ by solar irradiation which should be suitable running a e-vehicle running on $H_2$-fuel cells.

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Dr. S. Garai received M.Sc. (2010) from IIT Kanpur and PhD (2015) from Universität Bielefeld under the supervision of Prof. Achim Müller on the synthetic strategy developments for the Encapsulation Chemistry inside the novel Mo132-Nano-Keplerate type POM clusters. After two postdoctoral research assignments on Electro & Photo-catalysis (2016-2017) in TU Berlin and Weizmann Institute of Science, Israel, he joined NIT Trichy in 2018 as an Assistant Professor in Chemistry. His current research includes the use of molecular precursors for nano-cavity internal high throughput water splitting & CO2 reduction, detoxification of industrial wastewater etc.

# 3 Development Of Efficient And Robust Working Electrodes/ Photocatalysts For Solar Energy Conversion To Hydrogen Via Photoelectrochemical/Photocatalytic Splitting Of Water: Next Level Up-Scaling Of Laboratory Experience.

## Aim

Research plan involves focused work on pre-screened semiconductor materials for next-level up-scaling of the electrode fabrication process. Extensive R & D explorations would be undertaken to identify and optimize the most suitable and low-cost synthesis protocol for thin films of larger surface area, wherein the continuity, homogeneity and stability/adherence of film with substrate would be essential quality-criteria. The materials chosen for study would be low-cost, electrochemically stable and previously studied by investigators at small-scale level. Expensive and exotic semiconductor materials have been purposefully excluded from the scope of work for want of enough evidence on their stability and reproducibility. Nonetheless, plan of work at any stage would also be responsive to any new and significant development occurring internationally on the selection of appropriate material for above application.

## Methodology

In most studies on hydrogen generation via PEC splitting of water, carried out world over so far, observations are recorded with small geometrical surface area (~1 $cm^2$) semiconductor-electrodes. The up-scalability of these electrodes is still an uphill task and practically unexplored. To fill the gap in knowledge, this project would be directed towards the fabrication of up-scaled electrodes, with surface area raised (~ up to 100 $cm^2$), and their performance evaluation for solar-hydrogen generation via PEC splitting of water. Semiconductors chosen for the study are few among $\alpha$-$Fe_2O_3$,

$Cu_2O$, $Cu_2O$, $BiVO_4$ and $BaTiO_3$, each of which are inexpensive and have exhibited previously high photo-response in laboratory-scale studies. To that extent even other material-candidates emerging with promising results would also be included under the scope of investigations in this project. While developing protocols for material synthesis main thrust would be on economy and easy up-scalability of the process. In order to gain on efficiency of energy conversion, newly emerging concepts/ strategies of material-modification, viz. doping, layering, surface plasmonic effect etc. might also be investigated. Further, transition metal carbide based materials would be explored for photocatalytic water splitting reactions. Synthetic methods such as gel combustion, sol-gel, hydrothermal, microwave-hydrothermal or sonochemical method would be adopted for preparing phase-pure fine powders of photocatalysts having nanoparticles. The X-ray diffraction and absorption (XRD, XANES), X-ray photoelectron spectroscopy (XPS), FT-Infrared Spectroscopy (FTIR), Raman, $N_2$ BET, SEM and HR-TEM, techniques would be employed for bulk and surface characterization of samples. Band gap would be estimated by diffuse reflectance spectroscopy. (DRS). The performance of catalyst samples and their stability towards water splitting reactions would be evaluated.

## Expected Outcome & Deliverables

- New and emerging concepts of material synthesis will be integrated to synthesize better and upgraded photoelectrodes/photocatalysts, exhibiting greater stability and higher efficiency of energy conversion/hydrogen generation. Earth-abundant metal oxide semiconductors, which are low-cost, time-tested and most promising till date for above application, would be of primary interest in the project. However, included under the scope of the project would also be other emerging materials that show greater promise. A photocatalyst system that would decompose simulated sea water under direct sunlight in presence of inexpensive sacrificial agents with targeted SFE > 2% would also be developed.

- Next-level up-scaling of the laboratory systems/modules of PEC/PC hydrogen generation has been proposed under the project. To this effect, up-scaling of the synthesis process to evolve semiconductor thin films of larger area (~ up to 100 $cm^2$) would be attempted. Likewise, the existing laboratory modules of photocatalytic hydrogen generation would also be up-scaled by an order of 10-15 and their performance evaluated

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Rohit Shrivastav is Professor in the Department of Chemistry, Dayalbagh Educational Institute (Deemed University), Dayalbagh, Agra 282 005, India. He has experience of more than 33 years of teaching to undergraduate and postgraduate classes. He is an active researcher in the domain of chemical sciences for more than 36 years, having supervised successfully 11 Ph.D. and 7 M.Phil. students. His current research interests are in the areas of Solar – Hydrogen generation by photoelectrochemical and photocatalytic splitting of water. With total citations of 3045 and h- Index 31, he has published 116 papers in peer-reviewed journals. He has successfully undertaken/completed several research projects funded by different Governmental Agencies, including two Indo-US collaborative research projects; one funded jointly by DST - India and NSF – USA and the other by UGC.

# 4

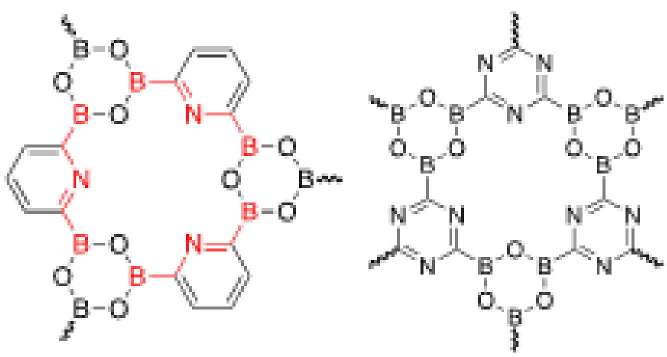
## Exploring The Active Sites Of Nitrogen And Boron Containing / Doped Materials: N-C-B And N2-C-B Type Active Sites For Electrocatalytic 4-Electron Oxygen Reduction Reaction

## Aim

The oxygen reduction reaction (ORR) on the boron and nitrogen containing carbon materials (not as in the form of conventional materials) which has B-C-N bondin nature. The synergistic effect of nitrogen and boron for ORR will be much more concentrated to improve the 4-electron reduction of oxygen by promoting the dual active sites for ORR.

## Methodology

Application of the boron organic framework (BOF) for the oxygen reduction reaction in PEM fuel cells is the first time due to the synergistically improved the BOF by nitrogen and boron. The challenges in the synthetic aspects of BOF having N-C-B and N2-C-B bonding features are addressed elaborately. The precursors for the N-C-B and $N_2$-C-B active sites can be synthesized using the borylation of the following N-hetrocyclic halides. The self-condensation of the above di and triboronic acids leads to the products of corresponding BOF as shown below



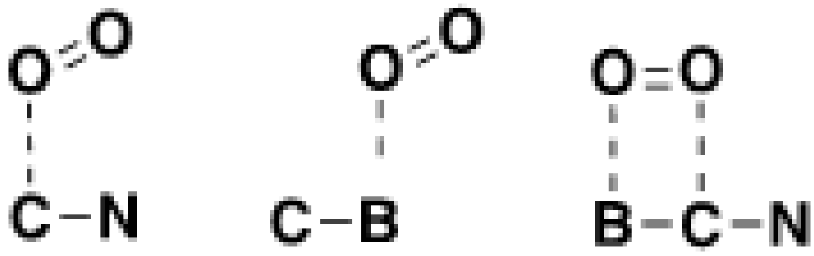
The BOF is used as a metal free electrocatalyst for the ORR. The mechanism of the ORR was completely studied using the mathematical analysis of the electrochemical data. The heat treatment of this BOF also used to prepare the N-C-B and $N_2$-C-B rich active sites for the ORR. The detailed methodology is given in the methodology section

## Expected Outcome & Deliverables

New and emerging concepts of material synthesis will be integrated to synthesize better and upgraded photoelectrodes/photocatalysts, exhibiting greater stability and higher efficiency of energy conversion/hydrogen generation. Earth-abundant metal oxide semiconductors, which are low-cost, time-tested and most promising till date for above application, would be of primary interest in the project. However, included under the scope of the project would also be other emerging materials that show greater promise.

The expected outcomes by using the above-mentioned materials as ORR catalysts are as follows;

1. The boron and nitrogen containing COP are giving larger surface area for the better mass transport.
2. Particularly making B-C-N type sites for the ORR electrocatalysts, will be acting as the dual active site where the molecular oxygen can bind as the bridge cis mode. The importance of bride cis conformation of $O_2$ binding leads to the rupture of O-O bond and promote the 4-electron reduction of molecular oxygen to water.




This work presents a new class of materials enriched with the particular active sites to promote the ORR for 4-electron pathway.

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Dr.A.Muthukrishnan joined as an assistant professor in the school of chemistry, Indian Institute of Science and Education research Thiruvananthapuram on June-2017. He received his M.Sc degree from Indian Institute of Technology Madras and later he joined in the same department and received his PhD in July-2010. Later, He worked as a prost doctoral researcher at Prof. Takeo Ohsaka group, Tokyo Institute of Technology, Japan on developing active and durable carbon alloy catalysts for the fuel cell cathodes. The work includes the identification of active sites of non-platinum group metal nitrogen-doped carbon catalysts by exploring the mechanism of the oxygen reduction reaction. In Jan-2017, he joined as assistant professor at School of Chemistry, University of Hyderabad. After a short period in Hyderabad, he become an assistant professor at IISER Thiruvananthapuram. Currently, he is working in the area of designing non-platinum group metal and metal-free fuel cell electrocatalysts to understand the active site information using fundamental concepts and developing the new materials using the kinetic and mechanistic insights.

5

## Lonogel Electrolyte Membrane Fuel Cell (IEMFCL) with Plasma Electrolytic Nitrided (PEN) Metallic Bipolar Plate and Effective Flow Field Design

### Aim

This proposal is aimed at developing an alternative moderate temperature fuel cell with improved materials: ionogel membrane/acid matrix, durable catalyst and nitrided bipolar plate with improved flow design. This fuel cell would be able to generate a power density of 100 mWcm$^{-2}$ with synthetic air as oxidant.

To develop an alternative membrane based on ionogel/acid matrix to the conventional proton exchange membrane (Nafion) in order to enhance operating temperature upto 120$^{o}$C, which is expected to enhance the oxygen reduction reaction kinetics, tolerance to the CO poison and low humidity operation.

To develop engineered graphene based support for platinum electrocatalyst to enhance the durability.

To develop an effective flow field design with bypass openings to decrease the pressure drop and maintain uniform temperature distribution throughout bipolar plate.

To identify and explore a novel nitriding method (plasma electrolytic nitriding, PEN) to enhance the corrosion resistance of stainless steel (316L) bipolar plate material, while maintaining the same electrical conductivity.

### Methodology

Novelty of this proposal lies in its moderate temperature operation (>120$^{o}$C). Enhancing the operating temperature > 120$^{o}$C requires a suitable ionic conductor (membrane) capable of working at low-humidity condition and corrosion resistance bipolar plate. Hence, ionic liquid incorporated polymer is suggested for low humidity operation at high temperature and electronically conducting nitrided metallic bipolar plate obtained by plasma electrolytic technique.

Further, flow field design suitable for the high temperature operation with minimal pressure drop (optimised computationally) would be tried. Due to operation at high temperature, water would be present in gas phase, which would require only a simple flow field design compared to that used in PEMFC operating at temperatures < 80$^{o}$C. In addition, the platinum loading at the cathode could be reduced significantly from the present level of 0.25 mg $cm^{-2}$, as the high temperature operation would enhance the oxygen reduction reaction kinetics and the CO tolerance of the catalytic layer.

Engineered graphene support with chemical synthesis employing microwave will used for electrocatalyst preparation. The engineered support and the electrocatalyst prepared will be characterized by all the available physical and electrochemical characterisation techniques.

## Expected Outcome & Deliverable

- A 100 $cm^2$ fuel cell with the said components capable of operating at temperatures > 120$^{o}$C.
- Ionogel/acid matrix membrane with conductivities > $10^{-3}$ $Scm^{-1}$.
- Nitrided Bipolar plates with improved corrosion resistance in comparison to its metal based counterpart (~10 $\mu Acm^{-2}$ at 0.6 V to 1 V).
- Engineered grapheme supported Pt catalysts capable of operating at > 90% of initial performance at 0.6 V for 1000 h.

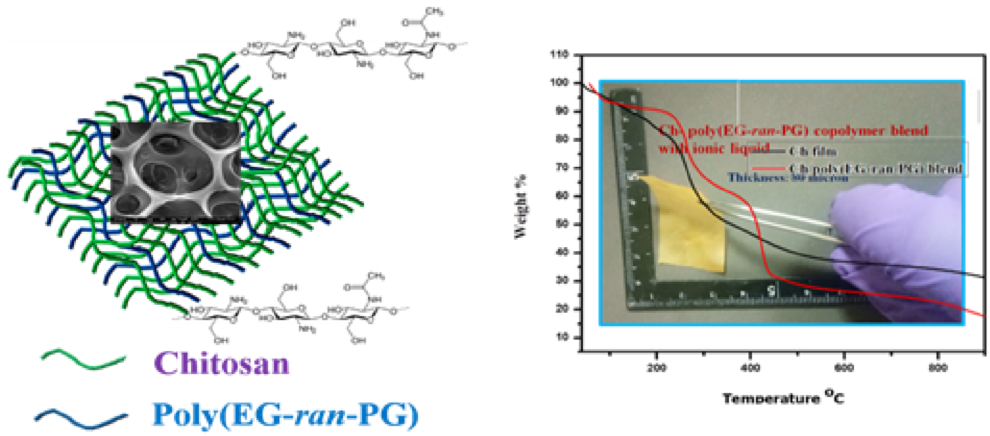


**Fig.2 Ionogel based membrane for IEMFC**

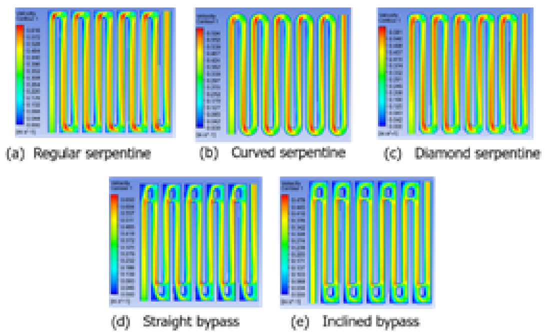


**Fig.3 Coolant plate configurations**

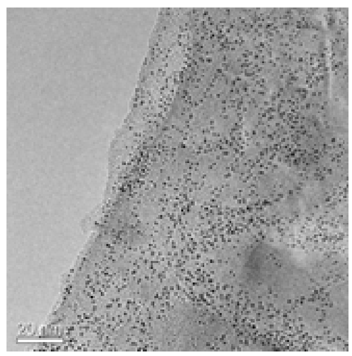

**Fig.1 Pt catalyst produced by microwave synthesis**


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Dr. Lakshman Neelakantan is an Associate Professor, Head of the 'Corrosion Engineering and Materials Electrochemistry' Laboratory in the Department of Metallurgical and Materials Engineering at IIT Madras. LN was a post-doctoral fellow at Ruhr University Bochum (RUB) and Max-Planck Institute for Iron Research(MPIE), Duesseldorf, Germany. He did his Ph.D.at MPIE & RUB during the years 2004-2008.

# 6

## Development of hybrid nanostructured materials for solid state hydrogen storage application

## Aim

Fabrication of nanostructured materials by physical and chemical methods. Study the effect of the particle size in improving the hydrogen storage properties of materials. Synthesis and characterization of hybrid nanostructured materials and optimization of their hydrogen storage characteristics.

## Methodology

Present project is focused on designing and development of lightweight nano-structured materials which can absorb and desorb hydrogen under ambient conditions. In order to achieve this goal nanocluster films (single and multilayer) of various metals will be synthesized by changing the nanocluster size. Characterization of $H_2$ storage mechanism and surface morphology will be done.

### Expected Outcome & Deliverables

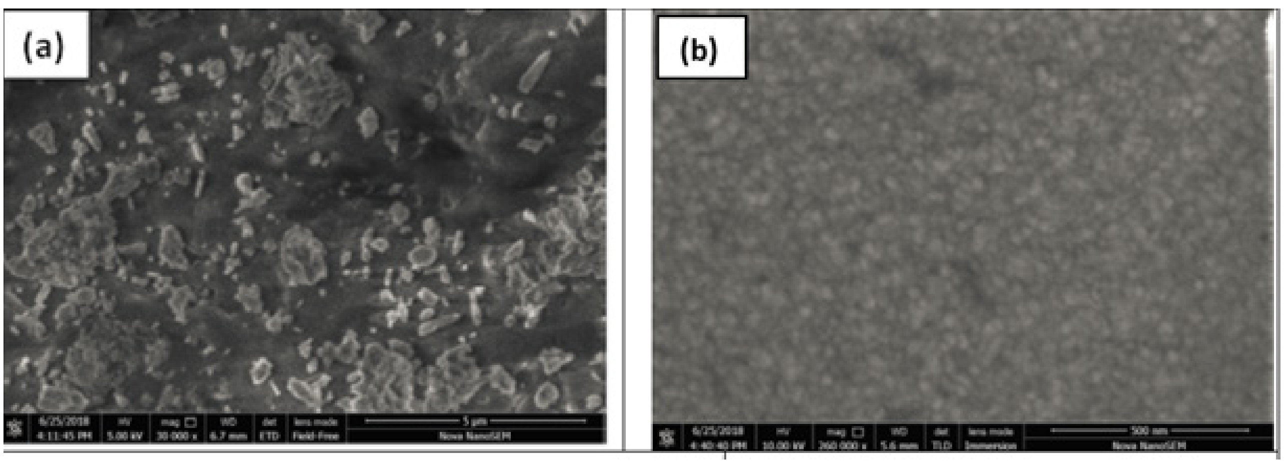
- Development of the hydrogen storage material which can absorb 3.5 wt% of hydrogen at temperature-pressure range near ambient conditions (below 150°C and near 1 atm pressure).
- Information of the effect of particle size reduction in improving the kinetics, and thermodynamic parameter of the material.
- Introduction of the synthesis method of single and multilayer nanocluster

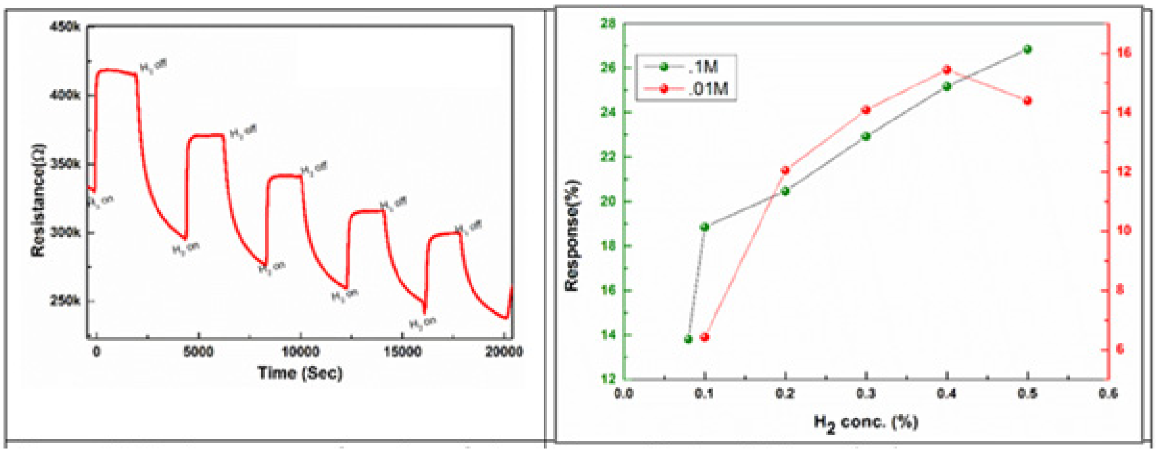
films.

- Improvement in the hydrogen storage capacity by synthesizing the hybrid nanocluster films.
- Reinforcement of the visibility of IISER Thiruvanthapuram and India on the global stage of prestigious academic research institute.


Car enthusiast and Shell scientist Wolfgang Warnecke road tests a hydrogen-powered Mercedes-Benz


A staff member refuels a hydrogen vehicle at a public hydrogen refuelling station in Vancouver, Canada, June 15, 2018. In what it said was a Canadian first, Vancouver launched the hydrogen fuel cell vehicle refuelling station on Friday, kicking off the rollout to a six-station network being established in the Metro Vancouver and Victoria region. (Xinhua/Liang Sen)






**Dr. Deepshikha Jaiswal Nagar**
**Assistant Professor**
**Indian Institute of Science Education and Research, Thiruvananthapuram**
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Dr. Deepshikha received her M.Sc degree in Physics from Banaras Hindu University. She completed her Ph.D. from Tata Institute of Fundamental Research, Mumbai, India, 2007 (Physics). After her Ph.D. she joined Seoul National University as a Postdoc Fellow and worked on hexaferrite single crystals to study multiferroicity using dielectric constant and electric polarisation measurements. She did her second Post-doc from Goethe Universitaet, Frankfurt-am-Main, Germany and worked towards setting up magnetoca-loric experiments to study quantum phase transition in quasi-one-dimensional organic insulators. From 2011 to 2012 she worked as a DST Fellow in University of Hyderabad, Hyderabad. In June 2012 she joined IISER TVM as an Assistant professor. Her area of interest is material designing for energy storage & gas sensing, thin films, superconductivity and magnetization.

# 7 Thermoresistant Polymer - Derived Microporous Ceramic Membranes for Separation of Hydrogen and Carbon Monoxide/ Carbon Dioxide in Hydrogen Production

## Aim

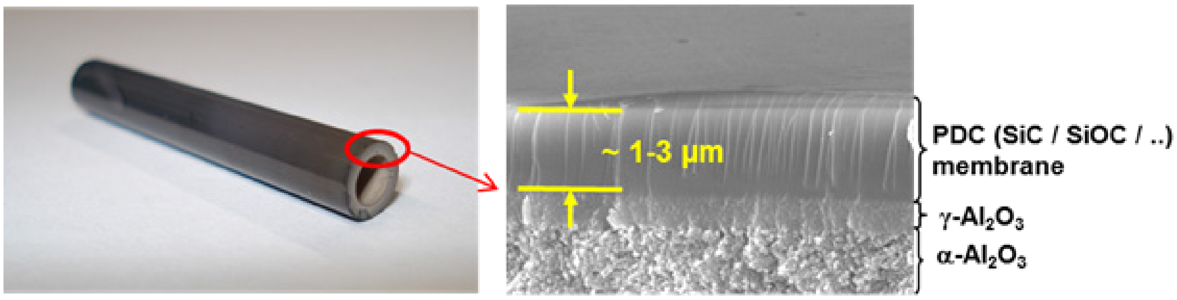
Separation of hydrogen and carbon monoxide/carbon dioxide for production of pure hydrogen for fuel-cell applications using novel polymer-derived microporous ceramic membranes.

## Methodology

- Two types of ceramic membranes will be applied: (i) microporous, and (ii) microporous membranes with a catalyst.
- Novel top hydrogen separation layer – amorphous microporous unmodified (SiC / SiCN / SiOC / $Si_3N_4$) and chemically modified ceramic membranes – will be synthesized through polymer-derived ceramic routes for $H_2/CO_2$ and $H_2/CO$ separation; If $H_2$ can be selectively extracted from the product side during hydrogen production in membrane reactors, then it would be possible to achieve complete CO conversion in a single-step under the thermodynamically un-favourable but kinetically favourable high temperature conditions.

### Expected Outcome & Deliverables

- Development of novel thermally and chemically stable microporous ceramic membranes (SiC / SiCN / SiOC / $Si_3N_4$)
- Development of a novel membrane reactor material using polymer-derived ceramics for simultaneous hydrogen production and purification in steam-methane reforming process





**Dr. Ravi Mohan Prasad**
**Assistant Professor**
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Dr. Ravi Mohan Prasad has obtained his PhD from Technische Universitaet Darmstadt, Germany in the area of ceramic membranes for gas purification and sensing applications. Currently, he is working as Assistant Professor at IIT Ropar. His research focus is in the area of "Materials for Energy and Environmental Applications" and particulary in ceramic membranes for hydrogen purification and sensing applications. Other areas in which his research group is working are hydrogen storage, ceramic coatings for corrosion and high temperature oxidation resistance, metal-matrix composites and lithium-ion batteries.

# 8 Development of Compressed Hydrogen-Fuel Cell Integrated System Suitable for Light Duty Vehicles

## Aim

Development of compressed hydrogen storage-based fuel cell system suitable for light duty vehicles (~20 kW)

Specific objectives:

- Development of high pressure (type IV) tank (37 L; 1.5 kg $H_2$ @700 bar)
- Development of Fuel Cell Stack of capacity ~20 kW
- Development of balance of plant (BOP) suitable for 20 kW system
- Integration of BOP fuel cell stack and high pressure hydrogen tank

Study the performances of the complete system for different drive cycles

## Methodology

A fuel cell is one of the major contenders to replace existing fossil fuels dependency. In fuel cell vehicles, electric traction system coupled to a single speed drive powered with Li-Ion Battery/supercapacitor and PEM based Fuel Cell power system are employed instead of the IC engine. A typical fuel cell power train is as presented in the Fig. 1. For fuel cell vehicles, on-board hydrogen storage in the highly compressed state (up to 700 bar) is considered globally using Type III & Type IV cylinders. While Type III cylinder consists of a metallic liner, Type IV cylinder has a non-metallic (plastic) liner wrapped by high strength polymer-fibre-composite, as shown in Fig. 2.

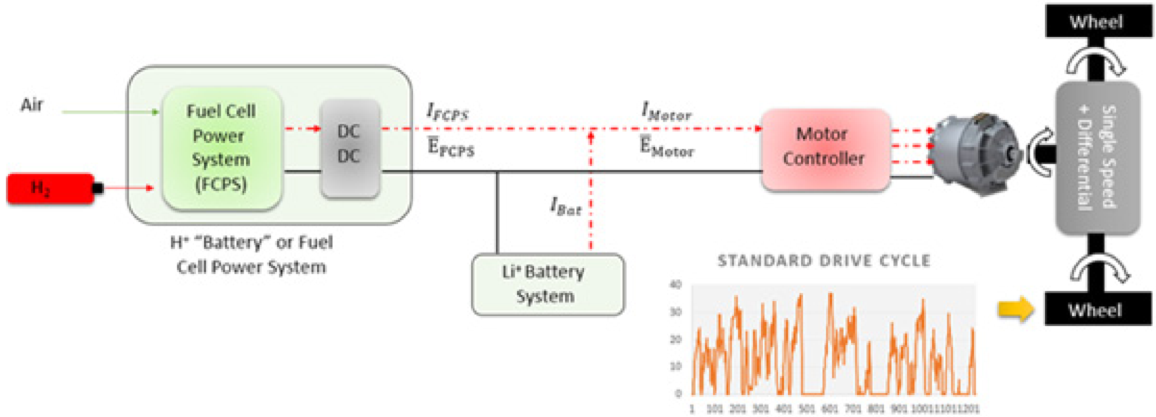


**Fig. 1: Schematic representation of a typical fuel cell based electric power train**

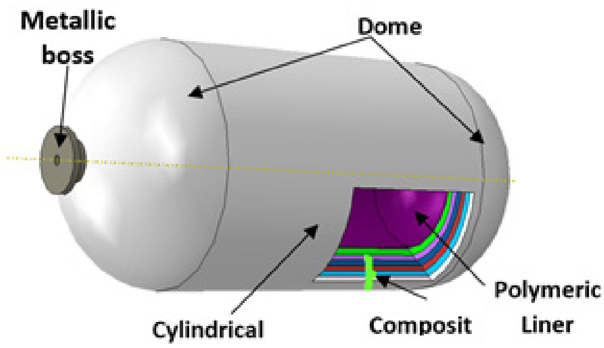


**Fig. 2: An illustration of a typical Type IV hydrogen cylinder with cylinder wall showing the polymer liner core over-wrapped with fibre-reinforced-polymer composite. The dome section host a metallic boss for fitting an in-tank valve that take care of hydrogen filling and low pressure release of hydrogen for fuel cell.**

The prime objective of the present work is to develop an electric drive train suitable for light-duty vehicles based on compressed hydrogen storage and fuel cells. An electric powertrain requires energy system with high volumetric and gravimetric energy and power density.

To achieve this, in this present work, a type IV tank (700 bar) will be developed for hydrogen storage system. For the fuel cells, the conventional graphite plate has a limitation to attain below certain thickness due to the mechanical stability and also gas permeability. Hence, in present work lightweight gas distribution system will be explored to achieve desired gravimetric and volumetric power density. Flow field design is also crucial for the performance and optimum flow field will be designed to minimize water flooding and to improve the current density distribution.

Fig. 3: Schematic representation of typical fuel cell based electric power train

The proposed proposal is divided into four different work (Fig. 3) packages as given below:

- Development of Fuel Cell Stack (FCS) with high volumetric and gravimetric power density [IITB]
- Development of high pressure (700 bar) Type IV Compressed Hydrogen Storage system (CHS) [IITR]
- Development of Balance of Plant (BoP) [TML]
- System Integration and Demonstration (SID) [IITB; IITR; TML]

## Expected Outcome & Deliverables

- Fuel cell stack Protype1 of 600 W
- Fuel cell stack Protype2 of 5 kW
- Fuel cell stack Protype3 of 20 kW
- 37 L Type IV Hydrogen Tank with nominal working pressure of 700 bar
- Integrated system comprises of Type IV hydrogen tank and fuel cell stack

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Dr.-Ing Prakash C Ghosh is a Professor in the Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Mumbai, India. Dr. Ghosh received his doctoral degree in Mechanical Engineering from RWTH Aachen, Germany. He is the recipient of BOYSCAST fellowship from DST, Govt. of India and ERASMUS MUNDUS fellowship from European Union. Dr. Ghosh has worked as a guest scientist in Forschungszentrum Juelich, Germany from 2002 to 2004. He worked in National Chemical Laboratory, Pune, India as a scientist from 2004 to 2006. Dr. Ghosh's research interests include low temperature fuel cells which include designing, modelling, fabrication and characterization of PEFC, HT-PEFC stacks and flow battery. In addition, he is also involved in solar hydrogen energy research. Dr. Ghosh has more than fifty International Journal papers in the field of solar energy, fuel cells and hydrogen energy. He has also five awarded international patent and four filed patents in his name. He has participated in several National as well as International projects with several countries such as the United Kingdom, Canada, Australia and USA in the capacity of Principal Investigator and Co-Principal Investigator. Dr Ghosh has secured funding (>35 crore) as PI and Co-PI.

# 9 Design And Development Of 3D Nanostructured Materials For Electrochemical Energy Conversion And Storage Devices

## Aim

The primary objective of our research activities involves the development of cost-efficient, electrochemically active, and stable nanoarchitectures to accelerate the large-scale application of green energy devices including fuel cells, batteries and solar cells to meet the world's energy demand with an environmental concern.

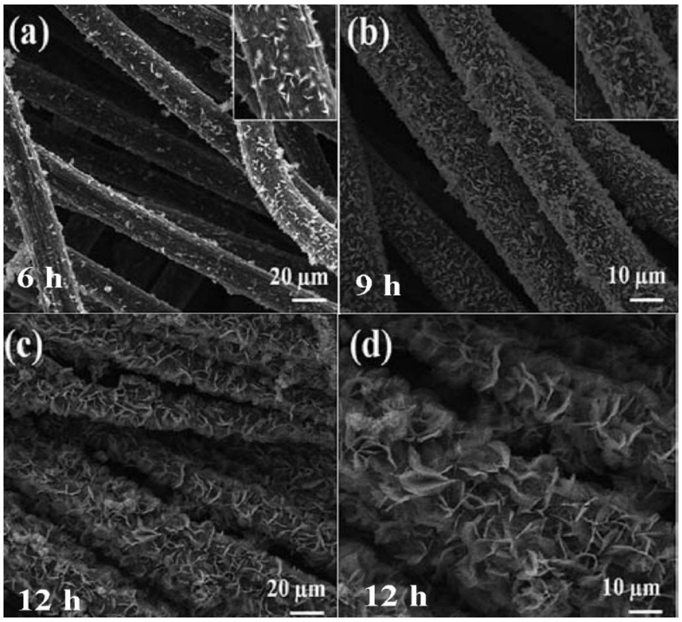
## Methodology

Our research is intended to envision the fundamental approach on understanding the chemical structure-morphology-electrochemical performance relationships of nano-structured materials and improve their applicability in various electrochemical devices.

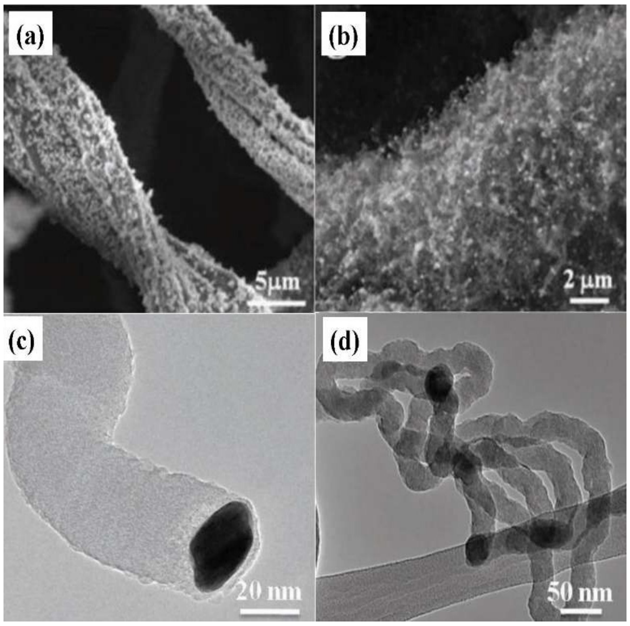
### Expected Outcome & Deliverables

- Develop a portfolio of catalytically active 3D nanostructures and hydrocarbon nanocomposite membranes with environmentally benign characteristics and affordable cost.
- Perform computational modeling to modulate the surface engineering of 3D nanostructures with unique properties
- Electrochemically evaluate and improve the electrochemical reaction kinetics of prepared catalysts and membranes.
- Fabricate the catalysts coated membranes (CCM) and construct the fuel cell single cells and stacks with the developed CCMs.

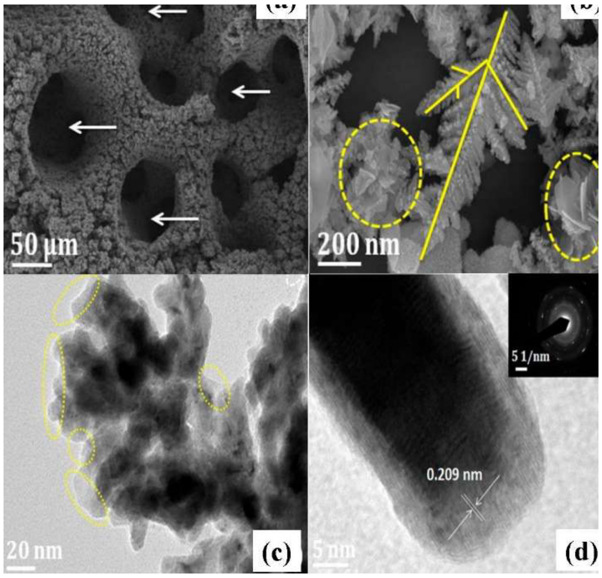
- Evaluation of dynamic and static electrochemical measurements of fabricated Li-sulfur/air/ion battery assemblies.
- Develop the portable electronic devices with the fabricated 3D nano-architectures and validate their applicability against commercial systems.



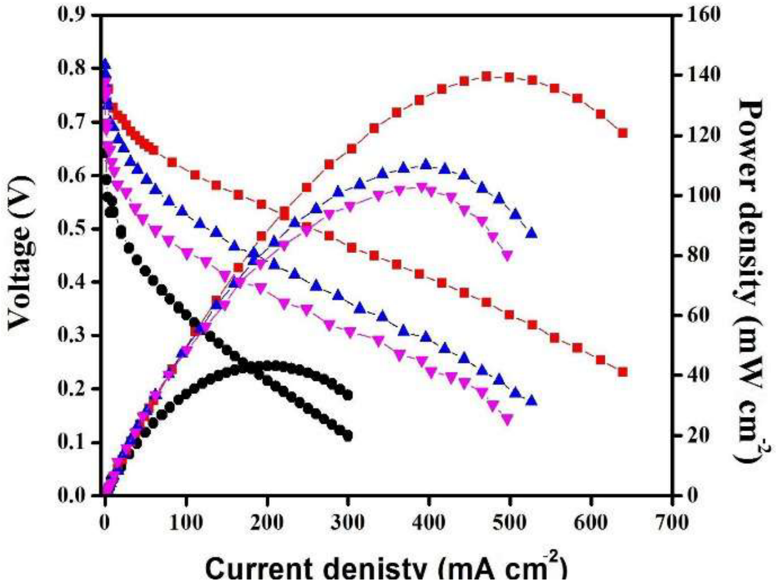

NiCo2O4/Carbon Cloth




Pd52-Ni48/NCNT/Carbon Aerogel




Cu-Co/rGO/Pencil Graphite Electrode





**Dr. G. Gnana Kumar**
**Assistant Professor**
**Madurai Kamaraj University Madurai, Tamilnadu.**
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Dr. G. Gnana Kumar (GG) received his M.Sc., degree in Chemistry at St. Jospeh's College, Trichy, India. He earned his Ph.D., degree at Chonbuk National University, Jeonju, Republic of Korea, focused on the development of polymer nanocomposite proton conducing membranes applicable for Proton Exchange Membrane and Direct Methanol Fuel Cells. After the completion of Ph.D., he was awarded with a Post-doctoral fellowship, centralizing to generate green electricity from Microbial Fuel Cells and waste water treatment. He also gathered good experiences in irradiation grafting polymer, synthesis of nanoparticles via bio analytical method, and large scale fuel cell application techniques.This was the starting point for him to embark on a progressive academic career in the fields of fuel cell, polymer and nanotechnology through publications in peer-reviewed journals, leading to the Assistant Professorship in Department of Physical Chemistry, Madurai Kamaraj University, Madurai.

# 10 Development of Mesoporous Tin@Nitrogen-Doped Carbon Nanostructured support Materials with Less-Pt Electrocatalysts for Durable And Low-Cost PEM Fuel Cells

## Aim

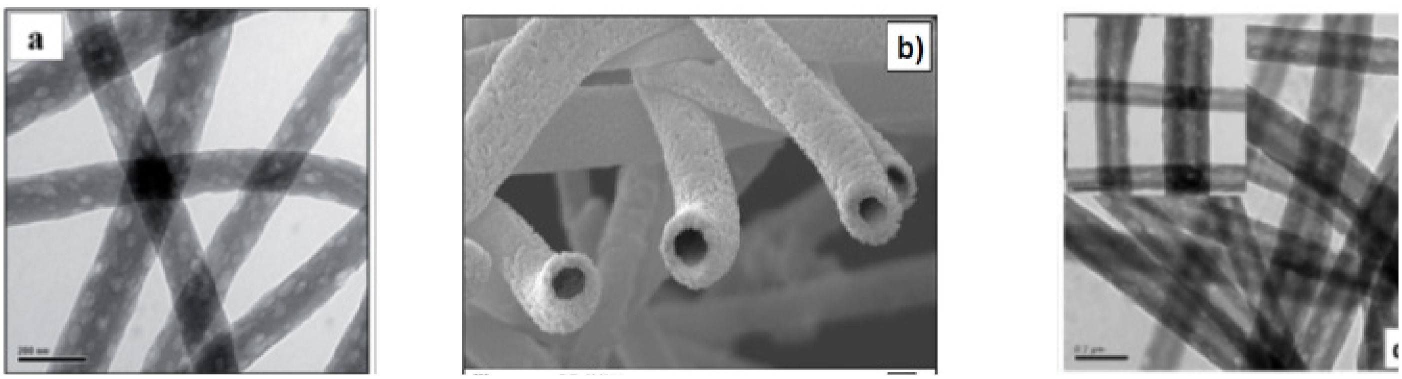
Development durable N-doped mesoporous carbon support materials grafted with less-Pt (bimetallic) electrocatalysts for enhancing the triple phase boundaries in high performance, low-cost PEM fuel cells. Reducing carbon corrosion to improve the durability of electrocatalyst support materials using corrosion resistant transition metal nitride coatings. Evaluation of performance of PEM fuel cells using CFD simulations and analysis. Fabrication of PEMFC stack based on the developed electrocatalyst support materials.

## Methodology

The proposed research plan encompasses fundamental research followed by application aspects of mesoporous carbon nanostructured materials (*m*-CNFs, Hollow carbon nanofibers, 3D Graphene) in PEM Fuel Cells. The developed N-doped (g-$C_3N_4$) carbon nanostructures will be subjected to thin layer deposition of transition metal nitride (TiN, ZrN etc.) to address the durability issues. Morphological and structural characterization of the electrocatalyst support materials will be carried out along with electrochemical performance analysis. A three dimensional, steady state, two phase model will be developed using Computational Fluid Dynamics (CFD) studies for understanding the behavior of the PEM fuel cell under various design and operating conditions with the new catalyst support materials and the developed model will be experimentally validated. After single cell PEMFC fabrication and testing, fuel cell stack will be developed with new electrocatalyst support materials.

## Expected Outcome & Deliverables

- The investigation will lead to significant contributions to fuel cell technology in terms of new experimental approaches and standardization of electrocatalyst membrane assembly to develop high performance PEM fuel cell devices.
- The investigation will also lead to development of products based on PEMFCs stack devices, especially for automobile applications.
- The unique technologies developed during the execution of the project will lead to generation of patents.
- Automobile industry will be benefited with the development of durable and low cost PEM fuel cells.




Mesoporous carbon nanofibers and Hollow carbon nanofibers developed at PSG Institute of Advanced Studies, Coimbatore

Representation of transition metal LDHs as catalyst for efficient hydrogen production via water splitting in three different ways

**Skai's Hydrogen Fuel Cell Rotocraft**


**First Toyota fuel cell bus in Tokyo**


**Mid-size hydrogen fuel cell car -Toyota**

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Dr. P. Biji received her M.Sc. (2003) from Cochin University of Science and Technology and Ph.D. (2009) in Chemistry from IIT Madras. She joined PSG Institute of Advanced Studies, Coimbatore from 2009 onwards and currently she is working as Associate Professor in Nanotechnology. Her major research areas focus on Sensors and Clean Energy Materials. She has completed 6 sponsored projects from SERB, ONGC, DST-SERI, NPMASS etc. Currently, she is leading 3 major projects in sensors and energy funded by DST and ONGC. She is actively leading a strong research group of 6 PhD students and 4 JRFs. 6 PhD students and 2 M.Phil students have completed their degree under her supervision. She has guided more than 25 M.Sc./M.Tech./B.Tech projects. She has published more than 50 journal articles in reputed journals and she has one patent and 2 book chapters in her credit. Her research interests are PEM Fuel Cells, Gas sensors and Ion-selective sensors, Nano-patterning and Self-cleaning coatings.

# 11 Design and Development of Graphene Reinforced Carbon Fiber/Epoxy Composite Based Light Weight Pressure Hydrogen Storage Cylinder for Vehicular Application

## Aim

Design and development of gaseous $H_2$ storage tank is proposed using surface modified graphene incorporated high density polyethylene liner and carbon fiber/ epoxy composites. The presence of graphene is expected to reduce the diffusion of $H_2$ gas, micro delamination and also could resist the embrittlement of the material.

## Methodology

This project proposes to design and develop a graphene based high- performance and lightweight compressed hydrogen storage tank demonstrator for vehicular applciations. The research methodology to develop the graphene-based hydrogen storage system is divided into three work packages: WP1 (Composite Materials development and characterization), WP2 (Hydrogen storage tank design and analysis), WP3 (Development of composite overwrapped hydrogen storage pressure vessel). WP1 mainly focuses on the development of surface modified graphene, characterization of graphene, dispersion of surface modified graphene in the HDPE and epoxy resin, characterization of the graphene/polymer composites, evaluation of diefferent physicochemical properties of the graphene/polymer composites etc. WP2 will be focusing on the numerical analysis of the tank considering different parametrs like service pressure, temperature, amount of recoverable hydrogen etc. A basic design activity will be carried out to estimate the aspect ratio of the pressure vessel depending on the required hydrogen storage. The design and analysis shall take into account the service pressure, external loads like mechanical impacts and service life and safety coefficients for both the static and dynamic conditions. In WP3, inner liner will be developed through injection molding technique. The CF/epoxy will be wrapped onto the HDPE liner through fillament winding technique.

## Expected Outcome & Deliverables

- High strength and low weight composite material.
- Composite material with low-permeability and damage tolerance under static burst fatigue and impact loading conditions.
- Finite element model of hybrid composite structure using higher order shear deformation theory
- Experimental prototype of light weight hydrogen storage tank with approx. dimensions of 100-150 mm diameter and 300-400 mm length which is capable of storing hydrogen at 700 bar pressure.

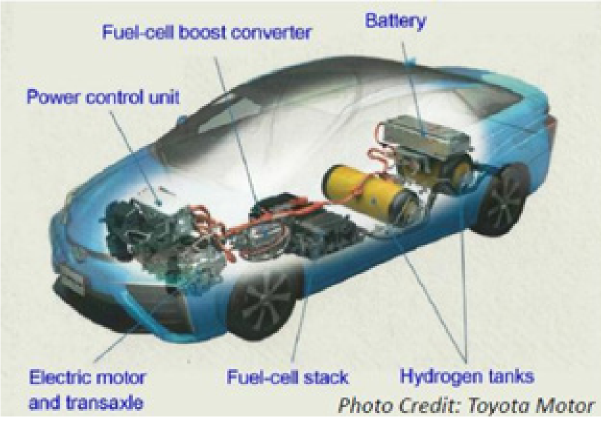


**Fig1: Toyota Mirai**

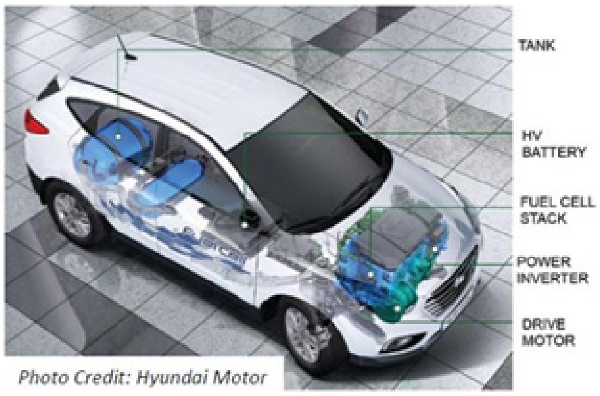


**Fig 2:Hyundai Tucson Fuel cell**

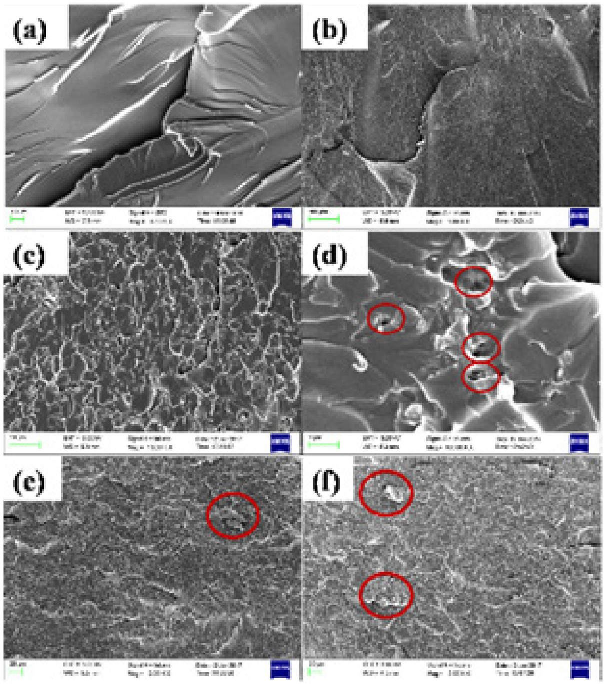


Fig 3: (a) The characteristic mirror-smooth fracture surface of a pure epoxy, (b) coarse, multi-plane surface texture of a 0.1 wt% TZG loaded composites, (c&d) high magnification micrograph of 0.1 wt% TZG loaded composites, and (e&f) 0.2 and 1 wt% TZG/ epoxy composites (ref: Kuila et.al. J. ApplPolymerSci, 2018,135(15).)

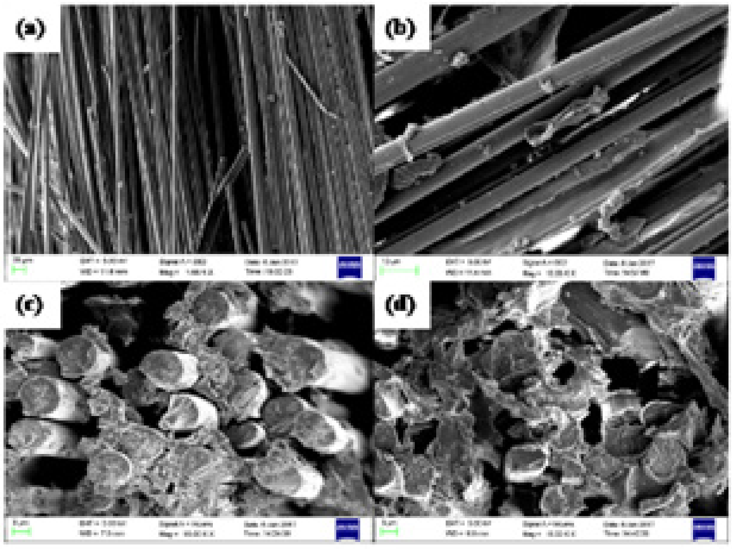


Fig 4: FE-SEM images of tensile fractured surfaces of (a) pure CF/epoxy and (b) 0.05 wt%, (c)0.1 wt%, (d) 0.2 wt% of GO reinforced CF/epoxy composite. (ref: Kuila et.al. J. Mat. Eng.Perfrom 27, 2018, Issue3, 1138-1147)

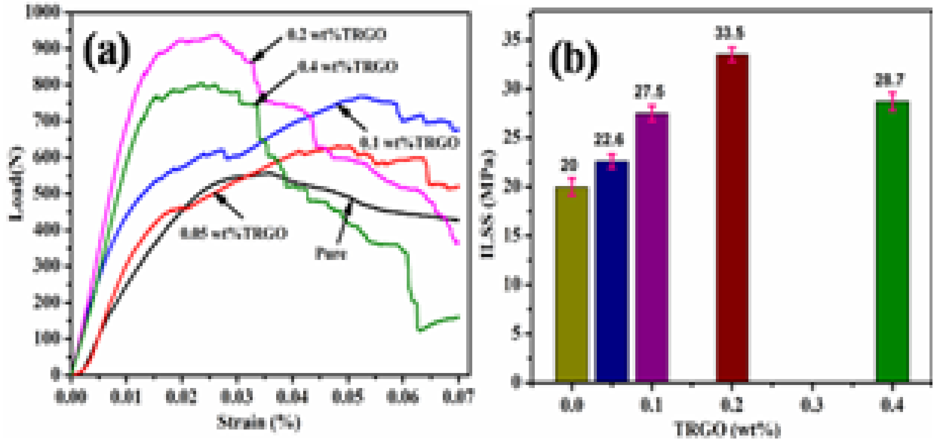


**Fig 5: (a) Load vs. displacement curves and (b) ILSS vs. TRGO content of the prepared CF/epoxy composites (ref: Kuila et. al., crystals 2018, 8(3), 111.)**


**Dr. Naresh Chandra Murmu**
**Senior Principal Scientist,**
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Dr. Naresh Chandra Murmu, Head, Surface Engineering and Tribology Divison, CSIR-CMERI received his B.E. (1992) from Bengal Engineering College, Shibpur, M.E. (1994) from Indian Institute of Science, Bangalore, and Ph.D. (2010) from Indian Institute of Technology (BHU). All are in mechanical Egnineering. He also worked as Visiting Scientist in University of Erlangen-Nuremberg, Germany during 2001-2003 and Northwestern University, USA during 2011-2012. He has been awarded prestigious VASVIK Industrial Research Award (2015), National Design Award (2012), CSIR-Raman Research Fellowship (2012), DAAD Fellowship (2001) & Co-Author of Best Paper Award from Material Science and Engineering-B Journal (2014). Dr. Murmu has published over 80 research papers in SCI journals, 4 book chapters and has filed 5 patents & 8 copyrights/design registration. He is currently Associate Editor, Journal of the Institute of Engineers (India) Series–C and Co-Guest Edited the Special Theme (2017): India's Reusable Launch Vehicle Technology Demonstrator: The Future of Space Transportation System with Shri Sivan, K., Chairman, ISRO. He supervised 6 PhD students and currently supervising 8 PhD students. Sucessfully transfered a couple of technologies to Industries. He has been elected as Fellow of Indian National Academy of Engineering (INAE) in year 2019 for his outstanding contribution in the areas of Additive and Micro Manufactuirng, Graphene Composite & Lubricants.

# 12 Room Temperature Aqueous Phase Alcohol Dehydrogenation with Electricity Generation

## Aim

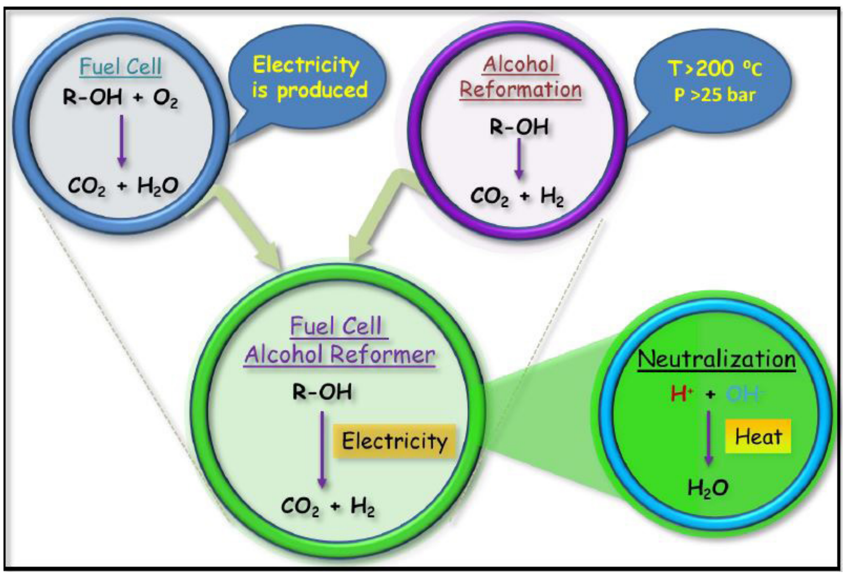
Development of the alcohol reformer operating at room temperature and pressure that combines the fuel cell features and the alcohol dehydrogenation features in a single device. The proposed device can simultaneously produce power like a fuel cell and hydrogen fuel like a dehydrogenator. The produced hydrogen is extremely pure and doesn't need extra module for purification. This is added advantage over the state of the art dehydrogenation processes where the hydrogen often contains other gases like CO, $CO_2$ etc., which is poisonous to $H_2$-$O_2$ fuel cell and thus needs purification before being used.

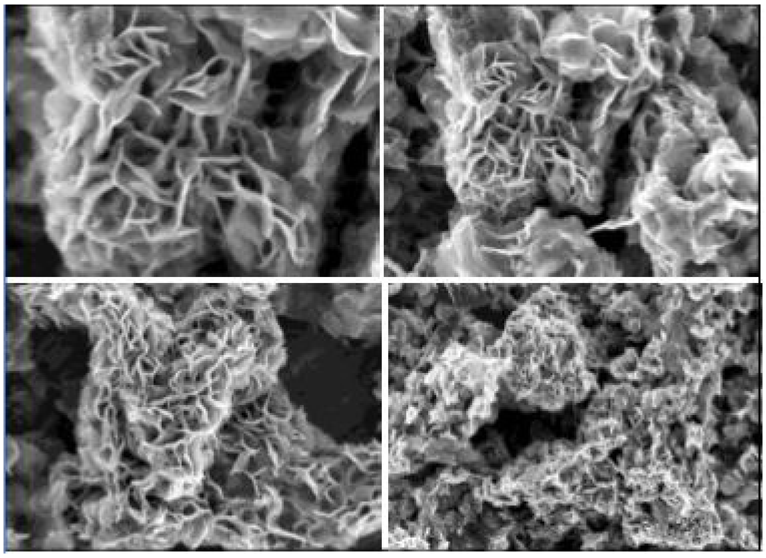
## Methodology

We propose a novel strategy wherein we can combine the alcohol fuel cell with the alcohol dehydrogenator in a single device. By the proposed strategy alcohol reformation can be made a thermodynamically downhill process. By harvesting the acid-base neutralization energy as the driving force alcohol dehydrogenation at room temperature along with electricity generation can be achieved. Since in the proposed device reformer compartment and fuel generation compartments are well separated by an ion selective membrane, the generated fuel is extremely pure and therefore could be directly pumped to PEMFC without any additional separation modules (Scheme 1). The online generation of fuel at room temperature along with electricity simultaneously boosts the integration of neutralization electrochemical reformer with a fuel cell in a tandem configuration.

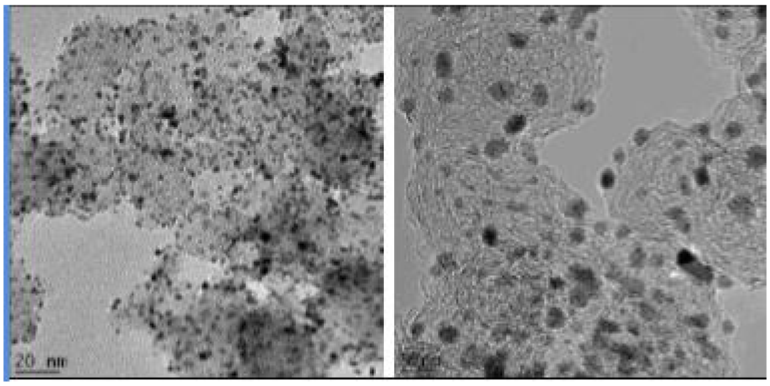
## Expected Outcome & Deliverables

- To develop a hybrid electrochemical dehydrogenator device this can produce electricity and extremely hydrogen fuel simultaneously.
- To increase the efficiency of the proposed hybrid device in order to achieve maximum dehydrogenation of alcohols.
- To design noble metal free inexpensive electrocatalyst for hydrogen evolution reaction (HER) possessing domains this can
- suppress parasitic chemistry of alcohols.
- To integrate the hybrid electrochemical device with proton exchange membrane fuel cells as its fuel reservoir.
- Proof of the concept to convert free energy of neutralization into electricity and fuel simultaneously.
- Hybrid fuel cell which will produce power and fuel simultaneously.
- An onboard hydrogen generation device for PEMFCs.





MoS2




Carbon Supported Platinum Nanoparticles (Pt/C)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**Associate Professor**
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**Email: musthafa@iiserpune.ac.in**


Dr. Muhammed Musthafa obtained his PhD in fuel cells from the Indian Institute of Science, Bangalore in collaboration with the Université Joseph Fourier, Grenoble, France. As a research associate at the University of St Andrews he investigated the fundamental (electro) chemistry of the aprotic Li– O2 battery. In 2014, he joined as an assistant professor at the Indian Institute of Science Education and Research (IISER), Pune, India. Presently he is working as an associate professor in Department of chemistry, IISER pune. His research interests include energy storage and conversion and semiconductor electrochemistry with special emphasis on solar fuel production.

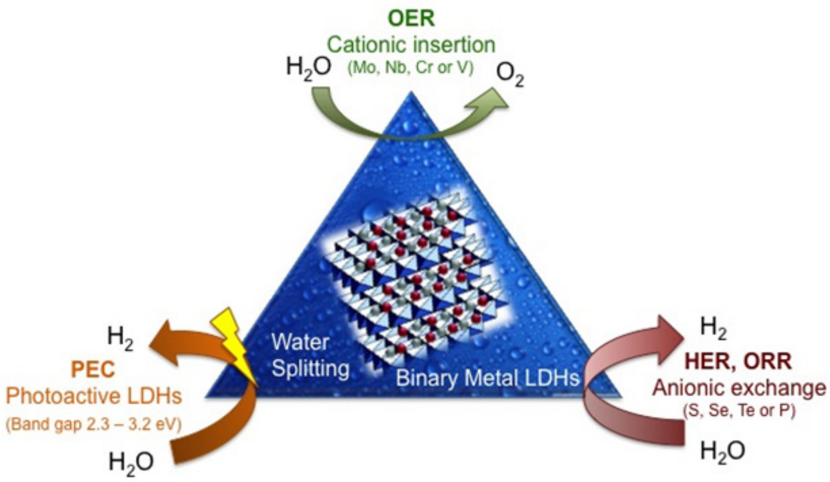
# 13 2D Transition Metal Layered Double Hydroxides: A Cost-Effective Catalyst for Hydrogen Production by (Photo) Electrochemical Water Splitting

## Aim

To deal with the energy crisis, hydrogen production as clean energy via electrocatalytic as well as photocatalytic water splitting are considered to be the major option. The proposed work has been focused on the development of binary metal layered double hydroxides (LDHs) as a family of versatile layered materials for effective water splitting. The unique structure and composition of M-LDHs allow for both metal insertion as well as interlayer anion exchange without disrupting the two-dimensional (2D) crystal structure. The aim is to manipulate the intrinsic properties of M-LDHs as catalyst to facilitate water splitting mechanism with a target of overall cell voltage of 1.5-1.6 V.


## Methodology

While development of trimetallic LDHs will be attempted to facilitate OER mechanism with the aim of overpotential value of 250-300 mV, anionic substitution with sulphide, selenide, teluride and phosphide are expected to be beneficial for HER mechanism with the overpotential value of 100-200 mV. The photoactive M-LDHs will also be developed with band gap engineering containing Ti3+ or other metal cations and will be combined with graphitic carbon nitrides to fabricate 2D-2D hybrid materials based on LDHs. Such photoactive 2D-2D hybrid materials are expected to produce hydrogen in the rate of 10-50 mmol g-1 scale over 500 h stability. It is needless to say that cost-wise such catalysts containing transition metals will be much economical (Fe: ~$0.0001/g, Co: ~$0.03/g, Ni: ~$0.02/g etc) compared to conventional noble metal catalysts (Pt: ~$50/g, RuO2: $2.50/g).

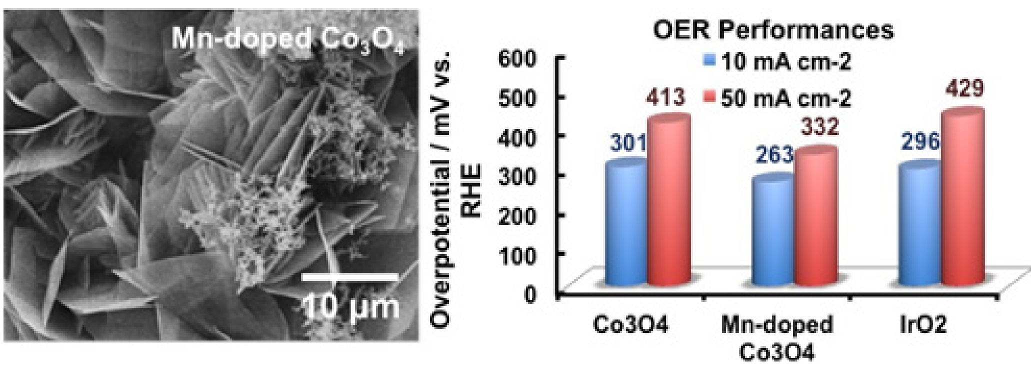



**Representation of transition metal LDHs as catalyst for efficient hydrogen production via water splitting in three different ways**

### Expected Outcome & Deliverables

- Development and designing of trimetallic LDHs for facilitating oxygen evolution reaction (OER) in alkaline electrocatalysis with the target of achieving overpotential in the range of 250-300 mV vs. RHE.

- Modification of binary LDHs via anionic exchange to develop catalyst for efficient hydrogen evolution reaction (HER) in alkaline electrocatalysis.
- To achieve the overall cell voltage of ≤ 1.6 V for electrocatalytic water splitting to generate H2 and O2 separately and utilize H2 in microsystem fuel cell device using vanadium as catholyte to generate energy.
- Designing of 2D-2D LDH-based hybrid photoelectrodes with band gap < 2.2 eV to split water with 7-10% QE and hydrogen evolution rate of 10-50 mmol g-1 scale over 500 h stability.




**Mn-doped Co3O4 nanosheets deposited on Ni foam as effective catalyst for OER performance (Raj et al. ACS Sustainable Chem. Eng. 2019, 7, 9690−9698)**

**Dr. Poulomi Roy**
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Dr. Poulomi Roy is a Senior Scientist at CSIR – Central Mechanical Engineering Research Institute. Before joining CSIR – CMERI, she was working as an Assistant Professor at Birla Institute of Technology Mesra for about 5 years. Dr. Roy is a Fulbright Fellow under Fulbright-Nehru Academic and Professional Excellence Award 2016-17 and visited University of Wisconsin – Madison, USA. Dr. Roy obtained her PhD on Inorganic Nanomaterials from Indian Institute of Technology Kharagpur, India in 2007. She spent 2008-2011 at Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany as a postdoctoral research fellow, where she worked on the development of self-organized TiO2-based nanostructures and their various energy applications. Her research interests comprise of the development of nanomaterials based on metal oxides, chalcogenides and hybrid materials for their applications in energy conversion to storage devices, including photocatalysis, electrocatalysis, water splitting, dye-sensitized solar cells, supercapacitors, batteries etc. She has published several research articles in various high impact international journals with very high citation to her credit.

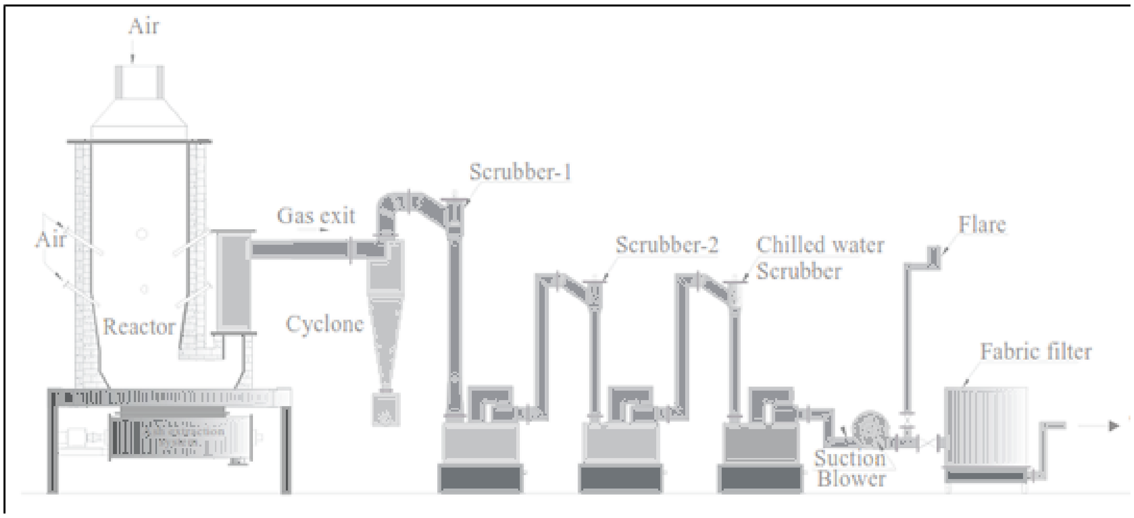
# 14 Use of bio-hydrogen for PEM fuel stacks – research and demonstration

## Aim

To generate bio-hydrogen from thermo-chemical conversion of biomass is an oxy-steam gasifier and condition the gas to PEM fuel cell quality as per ISO 14687:2019 and test a fuel cell/stack with the bio-hydrogen.

## Methodology

With a focus on generating PEM fuel cell quality hydrogen, it is proposed to use variety of carbonaceous matter like biomass, other residues including MSW in a patented gasification system to generate bio-syngas. The generated bio-syngas is subsequently separated in a downstream a swing adsorption system to generate pure $H_2$ with volumetric composition greater than 99.97%. Subsequently, the generated Hydrogen is analysed for quality and conditioned to generate $H_2$ of quality as per as per ISO 14687:2019 using recommended protocols. Further, in order to explore contaminant tolerance, PEM fuel cells are set to be operated at higher temperatures. Stacks of up to 100 kWe are planned to be tested as per standard test protocols under both low and high temperature mode. Experimental investigations will be supplemented with multi-dimensional and multi-physics numerical simulation models.



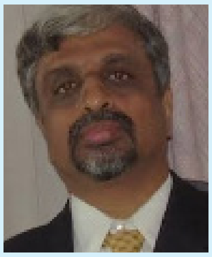

## Expected Outcome & Deliverables

- Establishing gas quality for the PEM fuels cells from sources other than reforming of Natural gas/Naptha. An important aspect for national program on fuel cells
- Bio-to- electricity technology package using bio-hydrogen starting from biomass/sorted MSW as fuel
- PEM fuel cell characterization under both high and low temperature operating condition
- Testing of cells and stacks of capacity up to 100 W using bio-hydrogen
- Long duration and cyclic operation testing
- A program for large scale dissemination for deploying PEM fuel cells using bio-hydrogen for various applications.

| | |
|---|---|
| Water ($H_2O$) | 5 µmol/mol |
| Total hydrocarbons [b] *(Methane basis)* | 2 µmol/mol |
| Oxygen ($O_2$) | 5 µmol/mol |
| Helium (He) | 300 µmol/mol |
| Total Nitrogen ($N_2$) and Argon (Ar) [b] | 100 µmol/mol |
| Carbon dioxide ($CO_2$) | 2 µmol/mol |
| Carbon monoxide (CO) | 0,2 µmol/mol |
| Total sulfur compounds [c] *($H_2S$ basis)* | 0,004 µmol/mol |
| Formaldehyde (HCHO) | 0,01 µmol/mol |
| Formic acid (HCOOH) | 0,2 µmol/mol |
| Ammonia ($NH_3$) | 0,1 µmol/mol |
| Total halogenated compounds [d] *(Halogenate ion basis)* | 0,05 µmol/mol |
| Maximum particulates concentration | 1 mg/kg |

ISO 14687:2019 standard for PEM quality Hydrogen. Contaminant limiting concentrations

Fuel cell test station



**Dr. S Dasappa**
**Professor**
**Indian Institute of Science, Bangalore**
**Email : dasappa@iisc.ac.in**

Prof. S Dasappa is a faculty at the Centre for Sustainable Technologies, Indian Institute of Science. He had his education at the Indian Institute of Science and obtained Masters and Ph. D degree in the faculty of engineering. His area of research has been solid, liquid and gaseous fuel combustion science and technology. Research in the area of internal combustion engine using alternate fuels has resulted in addressing impact of fuel properties on engine in-cylinder performance. Some of the specific areas of research are; Oxy-steam gasification for producing hydrogen rich syngas and hydrogen, Catalyst development and FT process, SOFC & PEMFC using alternate fuel, In-cylinder diagnostics for alternate fuel, Hydrolysis during biological conversion, Modeling of renewable energy systems, Waste to Energy.

# 15 Development of Micro Solid Oxide Fuel Cells (μ-SOFC) in Low Temperature Co-fired Ceramic (LTCC) Technology

## Aim

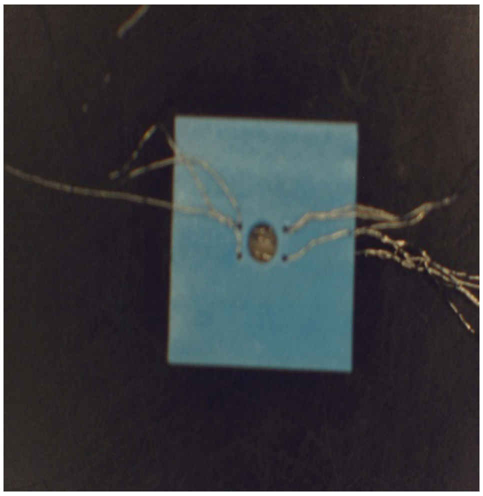
The aim of this work is to develop of Low Temperature Co-fired ceramic ( LTCC) integrated micro-SOFC with integrated heaters, temperature sensors and passive microfluidic channels for handling fuel and the by-product together with external fuel supply system or fuel cartridge and power management system. The objective is to take advantage of LTCC's capability of micro level integration of electrical and fluidic components, good sealing and conductors with high conductivity and develop an innovative product. The project is a collaboration between C-MET and industry partner, h2e power systems P. Ltd. CMET, Pune facilities primarily dedicated for component fabrication, integration and testing and h2e will look into the powe management of the cell.

## Methodology

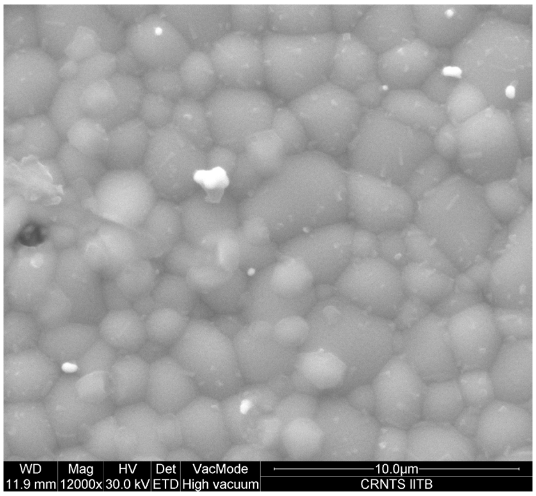
The development plan for is based upon three aspects. First is to synthesize innovative materials for SOFC which will integrated effortlessly with LTCC materials and fabrication process. It is planned to develop cathode, anode as well as electrolyte for such SOFC. Second, is to uses these materials along with standard LTCC materials and develop detailed fabrication process for such SOFC. The third aspect is to develop and independent power and fuel management system for the μ-SOFC cells.

## Expected Outcome & Deliverables

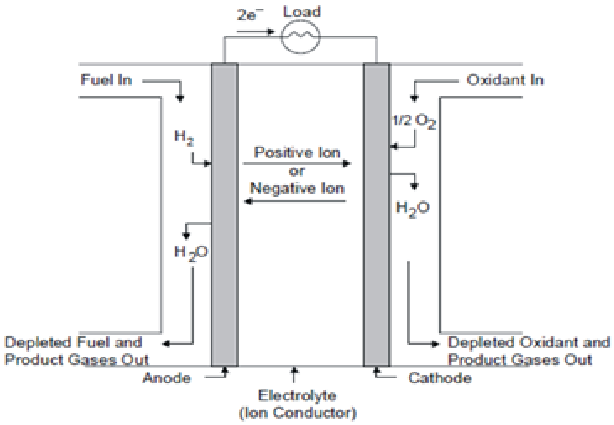
- One of the major outcome of this project will be development of flat and thin SOFC that can be used for micro scale power delivery to a variety of standalone applications across various sectors, such as, defence, logistics, agriculture etc.
- The project will deliver a technology demonstrator device through prototype development of integrated planar SOFC (μ-SOFC) integrated into LTCC.
- The proposed specifications of the LTCC integrated SOFC cell are:
    a. Size: 40 × 40mm
    b. Integrated fuel distribution and reactants removal channels
    c. Integrated current collection
    d. Integrated heaters and temperature sensors
    e. Operating temperature: 550 to 600$^o$C
    f. Power output: 100 to 250mW/cm$^2$
- The project will deliver a total of 5 devices



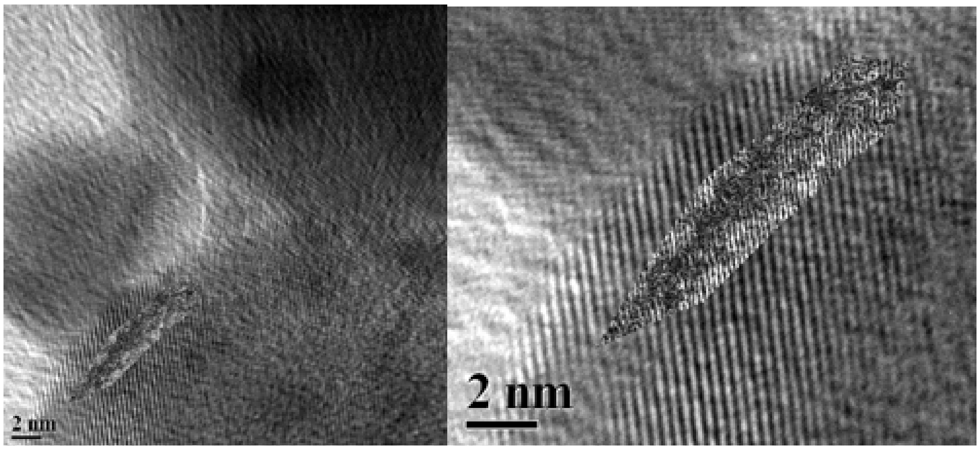
Pellet based SOFC with LTCC packaging and external heaters




SEM image of 1350$^o$C sintered pure Gadolinium doped ceria




**Schematic showing of basic fuel cell operation**




**FE-TEM images of GDC-glass composite powder showing lattice planes and distortion of lattice plane due to glass re-crystallization**


**Late Dr. Girish J. Pathak**
**Senior Scientist**
**C-MET, Pune**
**Email : gjp@cmet.gov.in**


Dr Girish J Phatak is a senior scientist at C-MET, Pune. After his initial work in microelectronics at IIT Bombay and University of Pune, he shifted to the area of Hybrid Micro Circuit (HMC) and Surface Mount Technology (SMT) materials. He has contributed to the development of paste families of Ag and Ag-Pd based conductor pastes, resistor pastes and solder pastes for HMC. The Solder paste technology has since been has been transferred to the Industry. He has been a pioneer in setting up Low Temperature Co-fired Ceramic (LTCC) fabrication facility at prototype scale. He is currently involved in several projects of national importance where he is contributing in development of special packages and circuits. He has also pursued state of the art and futuristic materials development for LTCC applications. He has more than 40 research papers in renowned journals, 4 book chapters and 10 patents, including US and EU patents, to his credits. He also has more than 100 contributions to International and National conferences. Four students have completed PhD under his guidance and few more are pursuing PhD in the area of LTCC and Packaging Materials.

# 16 Hydrogen Storage Materials: Optimization of known materials, developing new storage materials and finding exploratory application.

## Aim

- To develop new hydrogen storage alloy materials: High Entropy Alloys (HEA) e.g. Mgx(MnAlZnCu)100-x. Exploration of increase in storage capacity of HEAs. Exploration of occupation of Tetrahedral as well as octahedral sites for achieving high hydrogen storage capacity
- To investigate the synthesis, characterization and hydrogenation of Rare Earth Aluminium Hydride ($RE(AlH4)_3$, RE = Y,Sc)
- Detailed Study of new Li-Mg-N-H system with LiBH4/NaBH4 (source of in-situ quaternary catalyst $Li_4BH_4(NH_3)_2$). Studies of effect of $Li_4BH_4(NH_3)_2$ together with intermetallic catalyst (FeTi and other intermetallic compound including quasicrystalline and Mxenes ($Ti_3AlC_2$).
- Synthesis of air stable version of potential hydrides (e.g. $LaNi_5$, $MgH_2$ and their derivatives) through encapsulation by reduced graphene Oxide/Graphene wrapping.
- Finding of optimum catalyst/additive (including dual catalyst: separate catalyst for absorption/desorption) and their role for improving the de/re-hydrogenation properties of hydrogen storage materials as mentioned in 1 (e.g. binary, tertiary, quaternary alloy of transitions metal as catalyst for $MgH_2$).
- Proposed studies on the Indigenous Synthesis of $MgH_2$ (A Frontier Hydrogen Storage Material).
- Studies on HS through adsorption (as close to Room temperature as possible) in

porous carbon material including graphene and carbon aerogel (storage capacity ~ 4 to 5 wt.% at liquid Nitrogen temperature and more than 1-2 wt.% at room temperature).

## Methodology:

### M 2.1. Structural / Microstructural, thermal induced phase transformation, BET surface area and hydrogen sorption & other techniques to be employed in the proposed studies.

- Phase identification, phase transformation, catalytic activity, thermal properties gross structural characterization microstructural characteristics will be done by employing X ray diffractometer (Pan-Analytical Empyrean equipped with area de tector, with in situ specimen heating arrangement), Fourier Transform Infrared (FTIR) Spectrometry (Spectrum-100 Perkin Elmer), SEM (Quanta 200), RAMAN Spectrometer DSC 8000 (Perkin Elmer), TEM (Technai G 20).

### M 2.2. Methodology for Proposed studies on Magnesium Hydride:

- To overcome the limitations of slow kinetics (<1wt% per min) and high sorption temperature (>200°C), for the presently favoured hydride $MgH_2$, multiple attempts like alloying methods: targeting thermodynamic issue (i.e. to reduce hydride stability) and /or use of catalysts like transition metals, their oxides, alloys, carbon nanostructures etc. have been done. We have used mechanical milling method for preparing the nanoparticle of catalyst.

### M2.2.1. Methodology for development of Graphene templated Catalyst for improving the de/rehydrogenation properties of MgH2.

- To overcome the limitations in hydrogen sorption characteristics arising from agglomeration of catalyst a novel approach will be the immobilization of catalysts on a template. Among many materials, graphene sheets (GS) and its derivatives are best suited as a template possesses all the specification needed for a template. It is very light (~ 0.3 gm/cc), it is stronger than steel (1.3×1011 Pascals) and has high thermal conductivity. Also graphene does not undergo hydrogen sorption under the pressure, temperature conditions used in the present studies for hydrogen sorption in $MgH_2$. In the present studies graphene will be used as the base for temptation.

### M2.2.2. Methodology for: Use of quasicrystalline catalyst for improving hydrogen sorption (de-re hydrogenation) or MgH2

- A variety of catalysts ranging from transition metals and alloys, through transitions metal compounds oxides, chlorides, fluorides etc., to rare earths elements and their compounds have been used to improve the hydrogen storage properties of MgH2. Quasicrystalline materials often contain more than one transition metals. This is particularly true for Al bearing quasicrystalline alloys e.g. $Al_{65}$ $Cu_{20}$, $Fe_{15}$, $Al_{65}Cu_{20}Ru_{15}$ etc. The deployment of these qc alloys as catalysts will be very interesting and will be studied in the present investigation.

### M 2.2.3. Methodology for of Li-Mg-N-H Hydrogen Storage Material:

- In view of the very low storage capacity of the intermetallic storage material, the attention has shifted to light weight hydrides. We have made extensive studies of the light weight hydride Li-Mg-N-H system. Pure (devoid of impurities) Mg $(NH_2)$-L-H has been synthesized by deploying Zr $Fe_2$ as pulverize cum catalyst storage capacity of ~5 wt% has been achieved.

### M2.2.4. Methodology for Studies on formation of in situ catalyst using $LiBH_4$ as additive and effect of in situ catalyst (with and without intermetallic alloy catalyst) on hydrogenation behaviour.

- It is known that Li-Mg-N-H ($Mg(NH_2)_2/LiH$) system is very flexible and can a commodate and react with other similar compounds such as $LiBH_4$ reaction path followed is expected to correspond to following:
- $2LiNH_2$ + $1MgH_2$ + 0.1 $LiBH_4$ (ball milling) --------->$LiNH_2/MgH_2$ + $Li_4BH_4(NH_2)_3$ (Annealed)---------> $Mg(NH_2)_2$ / 2LiH + $Li_4BH_4(NH_2)_3$.
- Under the influence of additive cum catalyst Zr $Fe_2$ and in situ formed quaternary catalyst the onset desorption temperature, sorption kinetics and cycalbility has significantly improved for Mg $(NH_2)_2$-Li storage material.

### M2.2.5. The methodology for confinement of Mg/MgH2 will be carried out as per the following protocol:

- Protocol to be followed for nano-confinement of $MgH_2$.

(a) Mg will be dissolved in suitable solvent (Heptane or Teta Hydro Furan ) to form a solution.

(b) High purity porous carbon (preferably Graphene , Graphene Aerogel )(BET > 450 $m^2/g$, pore size <20- 100nm, total pore volume= 0.65 $cm^3/g$)(60-75 wt.% ) will bemixed in the solution (through stirring or by sonication)

(c) The resulting solution will be dried by drying the above mentioned solution below the boiling point of solvent taken in first step. The as synthesized material will be hydrogenated at higher temprature and pressure to obtain $MgH_2$ confined in porous support.

### M 2.2.6. Methodology for Studies: on High-Entropy alloys: Why HEA for Hydrogen Storage?

- Recently high entropy alloys have shown interesting hydrogen storage capability. Here high entropy alloys ZrTiVCrFeNi HEAs will be synthesized.
- Keeping the above aspect in view in the proposed studies, ZrTiVCrFeNi HEAs will be synthesized through mechanical milling (MM) and arc (induction) melting of Ti, Fe, Ni, Cr, Zr, V (purity of 99.9% and particle sizes less than 50 μm) as constituent elements. The viability of HEA may revive the interest in intermetallic hydrides which show hydrogen sorption at nearly room temperature and have very high cyclability.

### M 2.2.7. Methodology for Synthesis of Air Stable Hydride

- The protocol for synthesis of air stabile hydride ($AB_5$; $LaNi_5$ and $AB_2$:Zr $Fe_2$), will be done as per the following.

First of all, the binder (Ethyl Cellulose (EC) or polymer (P)) solution will be prepared by taking 10ml butyl carbitol (pye-kam Lab, Noida) with 30mg ethyl cellulose (EC) (Sigma Aldrich). This solution (binder solution) will be sonicated for 1 hour.

After this, 20mg of reduced graphene oxide (rGO) will be added to binder solution. The rGO will be dispersed in binder solution by sonication for 1 hour followed by addition of 2gm LNF. Afterwards, the above obtained sample will be sonicated for 2 days continuosly followed by stirring through the mixer for 10 minutes.

The process could be repeated to increase the rGO-EC encapsulation over hydride. The process can be repeated number of times to increase the loading of rGO-EC

### M2.2.8. Methodology for Proposed Research on Graphene Aerogel Synthesis and development of Graphene aerogel.

- The details for the synthesis of graphene aerogel are the following:
- Take solution (a) and solution (b);
- (a). Graphene oxide (GO) 100mg Deionised water 10g Sonication time 24 hrs + (b). Deionised water 7.1g
- Resorcinol 0.625 g Formaldehyde 0.9g, Anhydrous sodium carbonate 3mg.
- Mix (a) + (b)
- (c) Then combine 1.83 g of solution (A) with 1 g of solution {B}; (d). Keep the mixture of solution A and B in furnace at $90^0$C for three; (e). Supercritical Drying of wet gel with liquid $CO_2$ to produce organic; (f). Pyrolysis ($1000^0$C) of organic aerogel to obtain Graphene aerogel.

### M2.2.9. Methodology for Proposed Research on Carbon Aerogels : Chemical and Hydrogen Sorption Characterizations.

- Similar to synthesis of Graphene Aerogel synthesis of carbon aerogel are outlines at the following:

- For Hydrogen sorption characterization and also for such specific cases where the functionalization or doping / admixing of porous carbon / carbon aerogel will be involved for example for enhancement of storage capacity through spill over and carbon matrix polarization effect.

## Expected Outcome

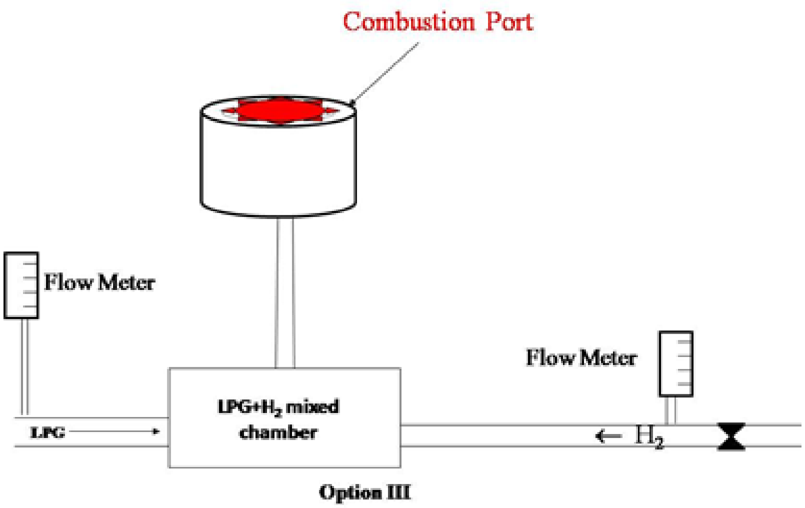
- Upgraded Hydride materials with new catalyst or additive so as to become compatible with the required storage specification (Please see Annexure -1) For example new catalyst/additive or both.
- Only Partially (For example Hydrogen (hydride as a source) based fuel cell device. Use of Hydride for replacement of LPG in home cooker and development of hydride based room warming system.).
- New Synthesis method like Hydrothermal , Sol-gel Synthesis will be used for the synthesis of graphene template catalyst, Ball milling will be used for the synthesis of Hydride.
- Analysis of storage capacity of Hydrogen Storage Material with reference to US DOE target.
- Development of new Hydrogen Storage Materials, optimization of known Hydrogen Storage materials so as to meet the US DOE target for exploratory application in fuel cell based devices and hydrogen fuelled Home cooker and Hydride based Room Warmer.

## Deliverables

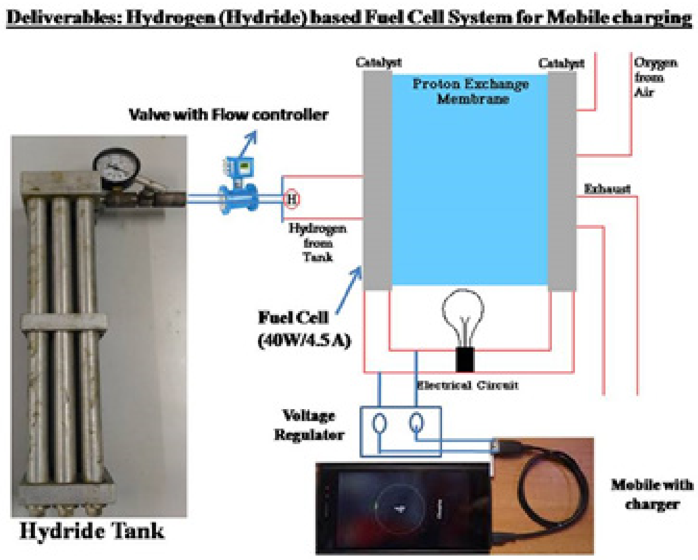
**Home Cooker and Room Warmer**

- Home Cooker: Schematic diagram of hydrogen fueled home cooker is shown in the following (details are given on the project write up). Home cooker can be converted into room warming system by using it to boil water and making hot water flow in the pipes around the roomtube.

## a. Scheme of hydrogen based home cooker (being developed)




## b. Fuel Cell based Charging System




# Papers published:

List of Publications from this Project (including title, author(s), journals & year(s):

(A). Papers published only in cited Journals (SCI)…………

- Sweta Singh, Ashish Bhatnagar, Vivek Shukla, Alok K Vishwakarma, Pawan K

Soni, **Satish K Verma**, M A Shaz, A S K Sinha and O N Srivastava; Ternary transition metal alloy FeCoNi nanoparticles on graphene as new catalyst for hydrogen sorption in $MgH_2$; International Journal of Hydrogen Energy, Volume 45, Issue 01, Page 774, 2020; doi.org/10.1016/j.ijhydene. **(Impact Factor: 4.939, ISSN:0360-3199).**

- Vivek Shukla, Ashish Bhatnagar, Sweta Singh, Pawan K Soni, **Satish K Verma**, T P Yadav M A Shaz and O N Srivastava; A dual borohydride (Li and Na borohydride) catalyst/additives together with intermetallic FeTi for the optimization of the hydrogen sorption characteristics of $Mg(NH_2)_2/2LiH$; Dalton Transactions, Volume 48, Issue 30, Page 11391, 2019; doi.org/10.1039/C9DT02270H **(Impact Factor: 4.174, ISSN: 1477-9234).**
- Formation and stability of $C_{14}$ type Laves phase in multi components high entropy alloy: SS Mishra, TP Yadav, ON Srivastava, NK Mukhopadhaya and K Viswas; IJHE 832 (2020) 153764 (0925-8388;2020), **(Impact Factor: 4.939, ISSN:0360-3199)..**
- Synthesis of pure $MgH_2$ with reversible hydrogen storage capacity, Ashish Bhatangar, MA Shaz, ON Srivastava; IJHE (2019), 44 (13) 6738-6747. **(Impact Factor: 4.939, ISSN:0360-3199).**

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**Professor**
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Onkar Nath Srivastava (born 1942) is an Indian material physicist, an Emeritus professor of Banaras Hindu University and the vice president for India and South Asia of the International Association for Hydrogen Energy, who is known for his contributions to the disciplines of nanotechnology and hydrogen energy.He is the author of two books and over 440 scientific papers[2] and a recipient of several honors including Shanti Swarup Bhatnagar Prize, the highest Indian award in the science and technology categories.[3] The Government of India awarded him the fourth highest civilian honour of the Padma Shri, in 2016, for his contributions to science and engineering.

# 17 Demonstration And Validation Of Hydrogen Ecosystem For Stationary Power Backup Application For Telecommunication Towers

## Aim

To develop, demonstrate and validate an indigenous know-how for PEM fuel cell-based power backup solution for telecom towers that is economically viable because of its potential for reduced initial capex and reduced opex. This development is expected to pave the way for wide-spread deployment of Fuel Cell based power backup, replacing anthropogenic diesel generators which rely on imported fuels costing upwards of a billion dollars every year.

## Methodology

Developing and testing new Membrane Electrode Assembly (MEA) and Cell design for self-humidified operation to eliminate expensive, complex external humidification Developing and testing optimal stack design of up to 3-kWe along with operational details and Standard operating protocols for robust performance with (i) low-to-no fuel and oxidant humidity, (ii) low air pressure component for oxidant and cooling supply and (iii) uniform mass-and-heat transfer.

Integration of 3-kWe self-humidified system with hydrogen generation for testing under simulated tower conditions

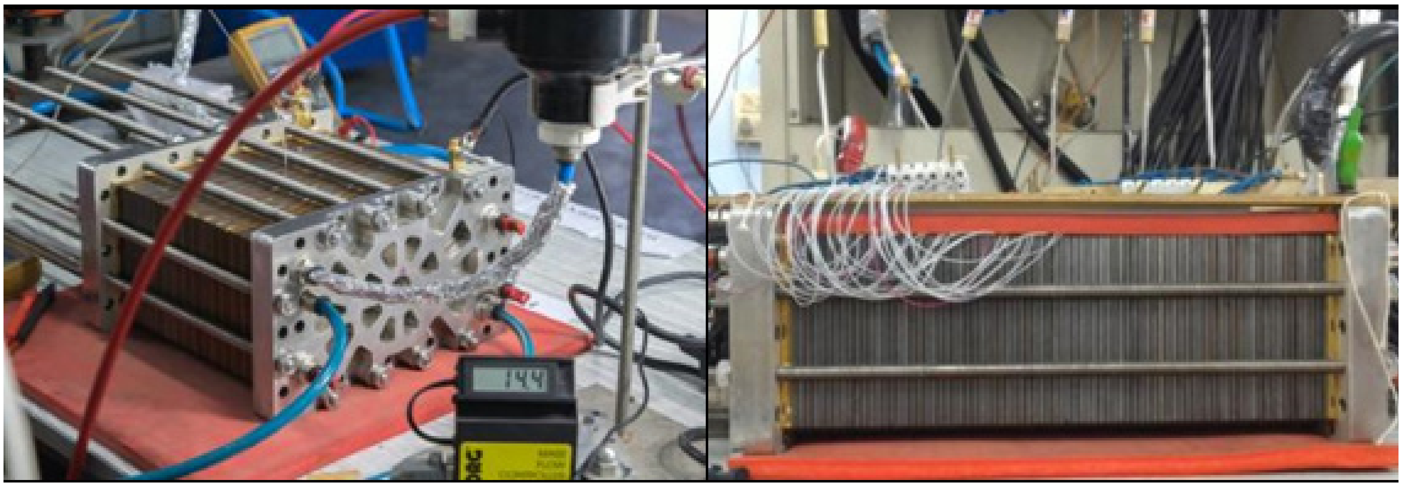
## Expected Outcome & Deliverables

**Hydrogen utilization through Fuel Cell**

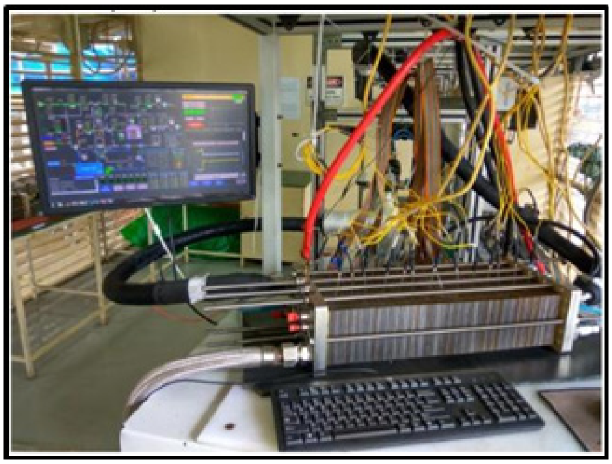
- Self-humidified stack of innovative cell design.
- Testing stacks and prototype systems on simulated telecom towers.

**Target performance:**

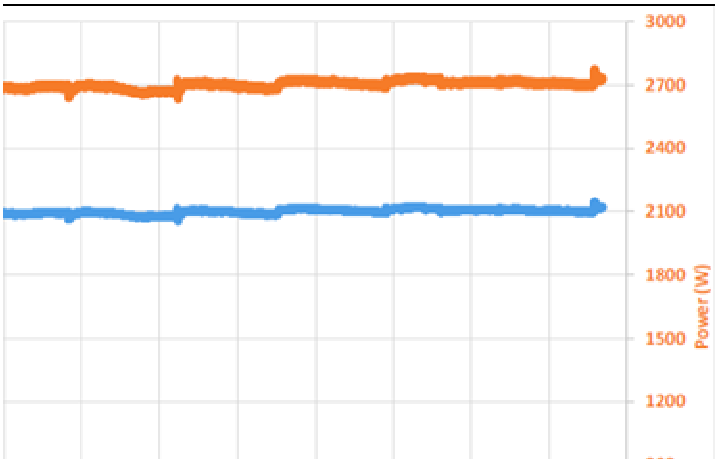
- 150 mW/cm$^2$ at 0.65 V.
- 45% electrical efficiency at stack level.
- 35% electrical efficiency at system level.
- 100+ h accelerated stress test at 10-50% and 10-90% humidity at anode and cathode, respectively.



1-kW and 2-kW water cooled LT-PEMFC stack of 30 and 60 cells respectively



Validation of 90 cell 2.7 kW fuel cell stack at Reliance test bed site




Life test (durability) for 55  h of 3-kW water cooled stack with shut-down/start-up sequences.

**Dr. Santoshkumar D. Bhat**
**Principal Scientist**
**CSIR, Madras**
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Dr Santoshkumar D. Bhat received his M.Sc in 2001 and he was a project assistant in National Chemical Laboratory in a NMITLI Programme from 2001-2003. He then completed his Ph.D in Polymer Chemistry in 2007 from Karnatak University Dharwad. He then joined CSIR-Central Electrochemical Research Institute-Madras Unit, Chennai and worked as a Scientist Quick Hire Fellow from 2007-2009 on the development of composite membranes for fuel cells and humidification applications. In 2009, he subsequently was selected for a regular position from CECRI as a Scientist at CSIR-CECRI Madras Unit at Chennai to work especially on the design and development of membrane electrode assembly for fuel cell applications. Dr. Bhat was initially granted projects from DST-Fast Track Scheme and CSIR- EMPOWER Scheme for developing various components for fuel cells. He also led the major 12th Five year plan Hydrogen Energy Programme (HYDEN) from CSIR-CECRI. He was also given a major grant for the development of anion exchange membranes and catalysts for alkaline polymer electrolyte fuel cells from 2013-19 as a part of recipient of CSIR Young Scientist Award in 2013. Dr. Bhat has led IOP-NMITLI Projects with NMITLI from CECRI in collaboration with Reliance from 2013, KPIT and Thermax in 2016. He has recently received a major grant from DST-HFC to work on the hydrogen eco system in 2019. His current research interests are membrane electrolytes and electrocatalysts for polymer electrolyte fuel cells.

# 18

## Unraveling The Potential Of Graphene Quantum Dots For Hydrogen Storage In Fuel Cells

## Aim

To achieve high hydrogen adsorption capacities in graphene exploiting the existing and inherent grain boundaries and defects in high specific surface area (SSA) graphene quantum dots (GQDs).

## Methodology

1. In the first, we will focus on the development of molecular dynamics (MD) models to determine the SSA, energetic stability, and $H_2$ adsorption and mobility of GQDs accounting strain, edge, GBs and temperature effects. Then, we will identify the most energetically favourable doped monolayer GQD considering different dopants (Li, K, Ti, V, Ni, S and Pd). The novelty of the proposed research lies in the fact that it is considering all possible routes for enhancing the $H_2$ storagecapacity of GQDs whereas the existing studies focus on only on one or two routes for graphene layers with small SSA.
2. In the second, using input from the step 1, we will determine the energetic stability, self-adhesion, and $H_2$ adsorption and mobility of functionalized bilayer GQDs and multilayer GQDs (MGQDs) via MD. Emphasis will be placed on varying interlayer distance between MGQDs with different stacking sequences via stable functionalization strategies so that the most energetically favourable MGQDs for occupying significant amount of $H_2$ molecules can be obtained.
3. In the third, we will try to achieve the target for $H_2$ storage capacity of MGQDs

on the order of 10–15% by optimizing the functionalization, edge and strain strategies, and physisorption mechanisms of $H_2$ adsorption. We also plan to modify the existing thermodynamic models accounting the geometry of GBs and absorbed molecular $H_2$, which is suitable for optimization of topology and geometry of nanostructure materials and included in the model effects accounting for the non-ideality of molecular $H_2$.

4. Finally, we will focus on the development of nonlinear continuum and MD models of MGQDs, absorbing $H_2$ atoms, subjected to thermal perturbation, and will analyse their stochastic stability. We will obtain the stress-strain curves of MGQDs under compression loads to capture their nonlinear hysteretic characteristics by deriving the new model based on the existing differential Van der Pol hysteretic model.
5. An integral part of this research program is the nanoscopic experimental validation. We will synthesize the graphene oxide and reduced graphene oxide for hydrogen storage applications based on the computational & numerical outcomes.

## Expected Outcome & Deliverables

- Materials Design and Development: This project aims to study the $H_2$ storage capacity in novel 2D architectures of GQDs in fuel cells using multiscale and experimental strategies. It will also present the perspectives of the next-generation, lightweight and high-performance fuel cells made of 2D materials.
- Performance Advancement: This project aims to achieve performance advances of $H_2$ fuel cells in terms of adsorption and mobility by right combination of engineered GQDs considering various dopants, strain, edges, GBs and temperature effects, and stacking configurations.

- Computational Material Modelling: This research will serve as a go-to-guide for designers, engineers, and researchers attempting to address the challenges associated with the multifaceted aspects related to the $H_2$ storage in nanomaterials and nanostructures. The outcome of this research project will have a direct bearing on the design and development of new-generation $H_2$ storage technologies.
- Cost Effectiveness: Large-scale MD models of $H_2$ storage in MGQDs will be very useful to determine atomistic information that is difficult or too expensive to capture experimentally.
- Scientific Data Generation, Analysis and Evaluation: Accurate and reliable multiscale strategies will provide a huge scientific data on $H_2$ storage in nanomaterials as well as deep insight into otherwise unexaminable aspects of different influencing parameters.

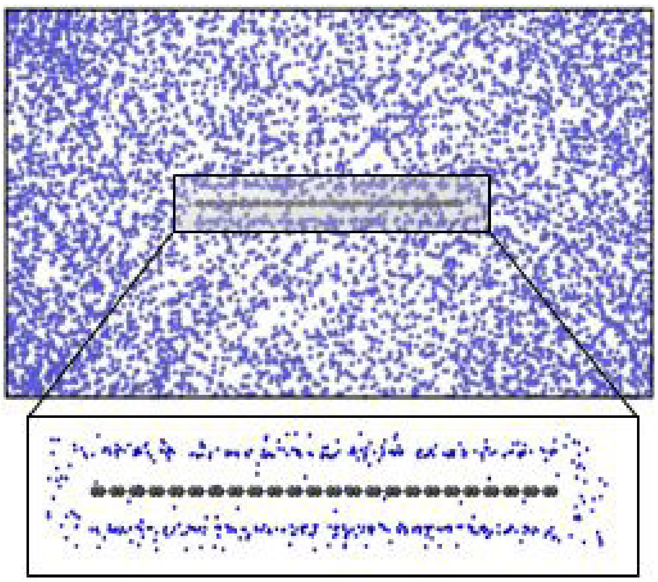

**Fig. 1. Hydrogen adsorption on pristine graphene**

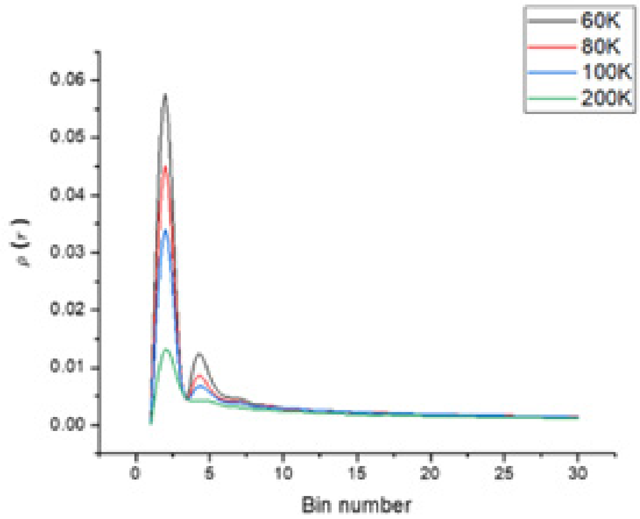


**Fig. 2. Hydrogen adsorption density at different temperatures**

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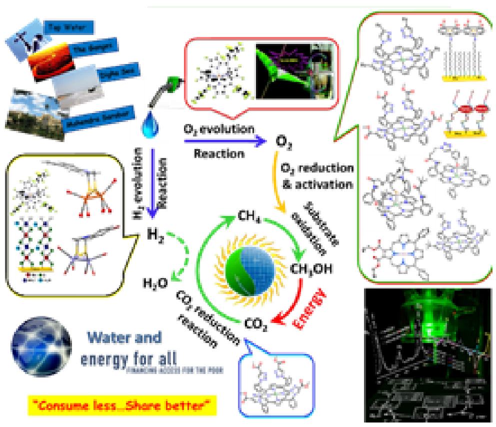
**Associate Professor**
**IIT Indore**
**Email: kundalwal@iiti.ac.in**

Dr. Shailesh I. Kundalwal is an Associate Professor in the Discipline of Mechanical Engineering at Indian Institute of Technology (IIT) Indore. Prior to joining IIT Indore in 2017, he was the Banting Fellow at the University of Toronto. He earned his Master of Technology and PhD degrees from IIT Kharagpur, both in Applied Mechanics. Immediately after his PhD, he did three postdoctoral fellowships: two at the University of Toronto and one at Masdar Institute in collaboration with Massachusetts Institute of Technology (MIT). He founded Applied and Theoretical Mechanics (ATOM) Laboratory at IIT Indore which undertakes research primarily in the following areas: Mechanics of Nanostructures, Nanomechanics and Micromechanics, and Nanotechnology in Engineering. He has authored more than 40 research articles (excluding conference papers and chapters) in reputed international journals. He is also contributing as a reviewer on several international journals (> 20) and Elsevier books in the broad field of mechanics.

# 19 Bio-Inspired Hydrogen Evolution from Water: Trouble-shooting Practical Limitations

## Aim

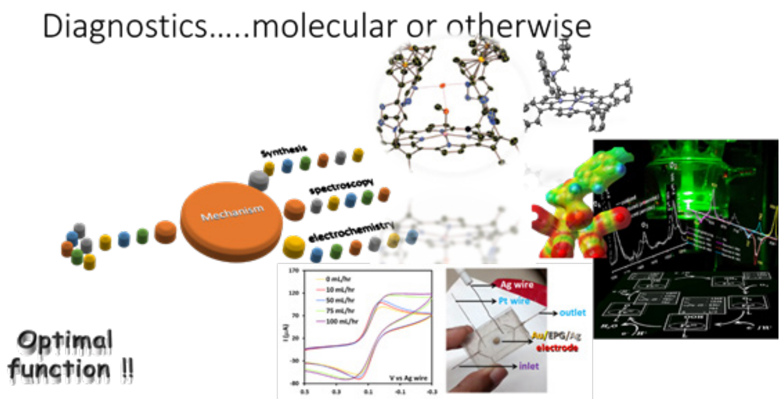
New bio-inspired electrocatalysts for hydrogen production will be delivered. These materials will be cheap and readily accessible. These will translate the finesse of metallo-proteins that produce hydrogen to artificial system. Previous work from this PI has demonstrated that these bio-inspired materials surpass catalytic performance of other conventional materials. Now a library of such bio-inspired material will be developed to generate hydrogen from saline water and waste water. The proposed solution also includes hydrogen generation coupled to detoxification of dissolved organics in waste water.




## Methodology

A long-standing impediment to hydrogen evolution is the sensitivity of catalysts to oxygen. The standard reduction potential of hydrogen is 0 V vs NHE in 1N $H_2SO_4$. The reduction potential for Oxygen under the same condition is 1.23 V vs NHE. Thus, at the cathode, where proton is reduced to hydrogen, the dissolved oxygen in the electrolyte will be reduced as well as the thermodynamics indicate. Oxygen is seldom reduced to water easily; that in itself is a major research area in fuel cell industry. Partial reduction of oxygen produced reactive oxygen species like hydrogenperoxide ($H_2O_2$) and superoxide ($O2^{\bullet -}$) which degrade the catalyst for hydrogen evolution. This is the reason why most hydrogen evolution catalysis reported till date use degassed water for testing. This is a major impediment towards achieving water splitting under practicable applications and needs to be addressed directly.

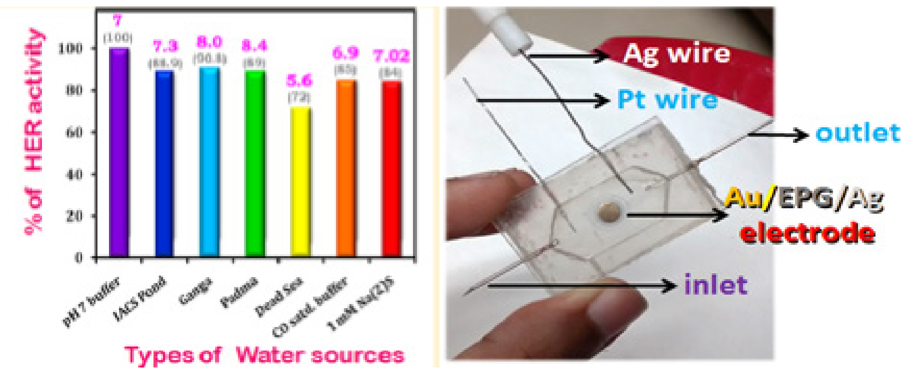
A lucrative option is to obtain hydrogen from industry waste water. In Indiatremendous amount of waste-water containing dissolved organic wastes are generated from the pharma, textile and chemical industry. Even in the organized sector, only 60% of this waste water is treated. To be able to use industry waste water for hydrogen generation, these catalysts must tolerate brine, sulfide and CO. Apart from that, waste water containing dissolved organic wastes (dyes etc.) needs to be utilized for hydrogen generation and, if possible, decontaminate the organic waste along with hydrogen generation.




## Expected Outcome & Deliverables

The proposal aims to develop a testing platform for in operando investigations of heterogeneous electrocatalysts using easily available FTIR instrument. The PI has previously developed a Raman based technique for such purposes which was proved to be very useful for diagnosing oxygen reduction electrocatalysts. Such a set up will be unique in the world and can be utilized by any heterogeneous catalyst group in the country for troubleshooting their catalytic system.

- Rapid hydrogen evolution at neutral pH
- Troubleshoot oxygen sensitivity of hydrogen evolution catalysts and develop oxygen tolerance to produce hydrogen from abundant natural water sources and waste-water.



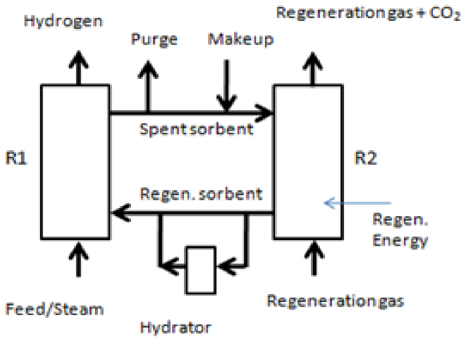

**Dr. Abhishek Dey**
**Professor**
**Indian Association for the Cultivation of Science, Kolkata**
**Email : abbeyde@gmail.com**

Abhishek Dey has a background in electronic structure and synthetic inorganic chemistry. His research aims at emulating the reactivity of enzyme active sites in synthetic analogues using the geometric and electronic structure function relationships present in natural systems. His current area of interest includes multi-proton and multi-electron transformations that are key for clean energy and environment and development of new analytical techniques to spectroscopically investigate heterogeneous electrocatalysts.

# 20 Improved Hydrogen Production From Biogas Using -Sorption - Enhanced Reforming

## Aim

Exploration of new materials for cheap hydrogen production via sorption-enhanced steam reforming (SESR) of biogas




## Methodology

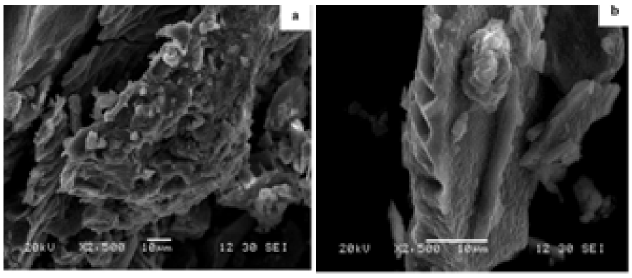
Nickel-based hybrid materials (containing calcium-based oxides, or promoted hydrotalcite, or alkali metal ceramics) will be synthesized, characterized and tested for biogas reforming in a vapour-phase flow reactor.

Reactor details

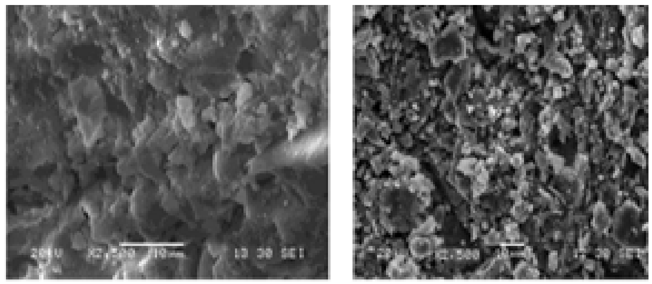
Vapour-phase flow reactor setup

## Expected Outcome & Deliverables

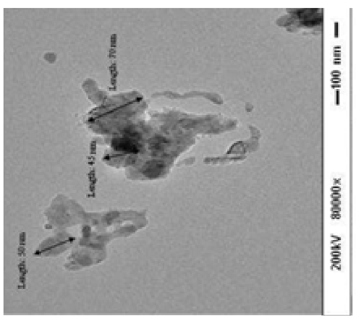
New materials (with high $CO_2$ loading capacity, breakthrough time and multi-cyclic durability) for the production of pure $H_2$ (>95 mol %) from biogas reforming at low temperature (T<600$^0$C) and low cost (25% less than traditional steam methane reforming) will be developed.



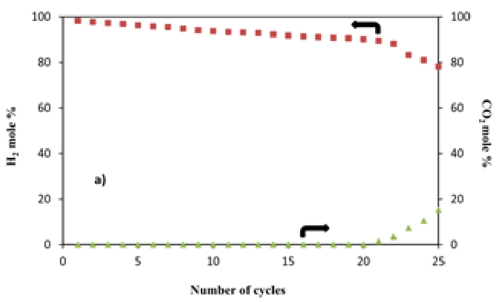
SEM photographs of new materials



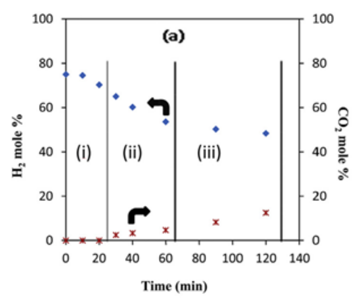
Typical SEM photographs of spent materials



Sample TEM photographs of spent materials




Sample TEM photographs of spent materials




Typical SEM photographs of spent materials

**Dr. P. D. Vaidya**
**Professor**
**Institute of Chemical Technology, Mumbai**
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Professor Prakash Vaidya teaches chemical engineering at the Institute of Chemical Technology in Mumbai since the past 12 years. He is an expert in separation and reaction engineering. His research interests are biomass conversions, CO2 capture and recycling, and wastewater treatment. So far, he has authored 85 research papers (citations: 2600, h-index 25) and 2 patents, and guided 22 PhD researchers. He is presently working on 5 research projects related to sustainability.

# 21 Development and testing of Nano-doped hybridized biodiesel as pilot fuel for Hydrogen duel fuel operation in a Stationary CI engine.

## Aim

Development of Nano-doped hybridized biodiesel extracted from tree borne vegetable oil available in North East India. Stability analysis of Nano-doped hybridized biodiesel. Evaluation of the performance, combustion, and emission characteristics of hydrogen run diesel engine with and without the hybrid biodiesel as pilot fuel. Techno-economic analysis of Nano-doped hybridized biodiesel as a sustainable alternative fuel.

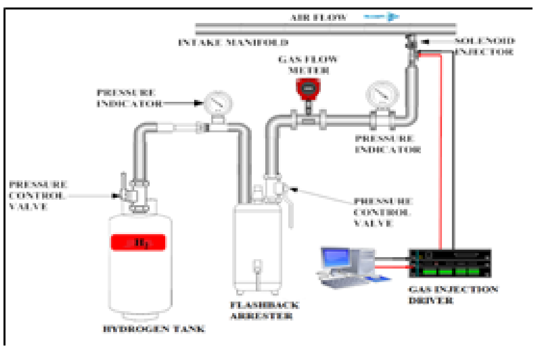
## Methodology

The present work plans to undertake a methodical approach to alter the properties of biodiesel by Nano additive doping to make it more suitable as a pilot fuel for Hydrogen dual fuel operations. It is expected that Nano doped hybridized biodiesel will significantly improve the efficiency of the engine with minimal exhaust emission. Moreover, it is also expected that the modified pilot fuel will allow higher flow rates of Hydrogen to be injected in the combustion chamber, thus reducing dependability on liquid fossil based fuels.

### Expected Outcome & Deliverables

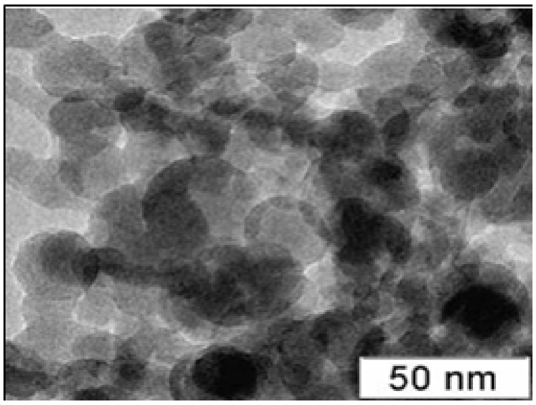
- Modified fuel blends with suitable composition of Biodiesel and inorganic Nano Additives to supplement diesel.
- Combustion and emission characteristics of different Nano Additives viz. $Al_2O_3$, $CeO_2$ etc under dual fuel mode is to be investigated.

- An upgraded CI engine system with optimum injection timing, pressure, and amount of gaseous fuel and liquid fuels to be unveiled.
- Correlations are to be developed to predict and optimize the performance for the given set of parameters.
- Feasibility of maximum replacement of commercial diesel with hybrid fuel as CI engine fuel without effecting the engine performance and emissions to be attempted.
- The developed technology of modified engine will be kept open for the other researchers for awareness, at the same time results will also be reported in the form of report, research paper to share with the scientific community.

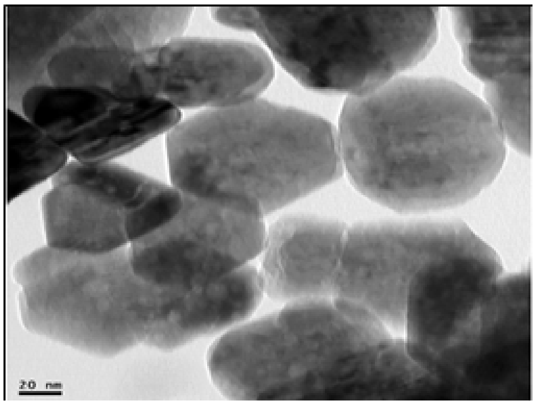


Typical hydrogen injection system

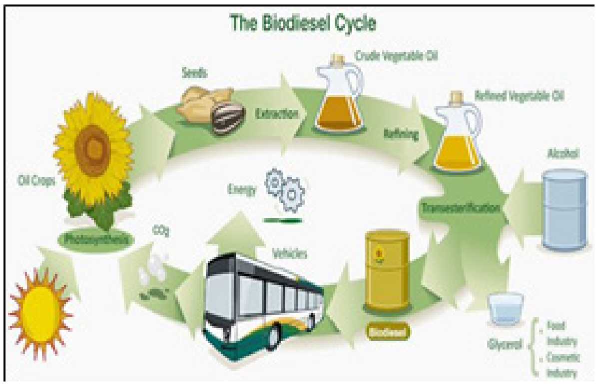
DAF Truck with Gas-Diesel engine.



Al2O3



ZnO




Biodiesel Cycle


Biodiesel fueled bus in Nebraska, USA

**Dr. Abhishek Paul**
**Assistant Professor,**
**Mechanical Engineering Dept. NIT Silchar**
**Email- v1.abhishek@gmail.com**

Dr. Abhishek Paul did his B.E in Mechanical Engineering from NIT Agartala (2008), M.Tech in Thermal Science and Engineering from NIT Agartala (2011) and Ph.D from NIT Agartala (2015). He joined Mechanical Engineering Department of NIT Silchar as Assistant Professor in 2018. His primary research area is IC engine combustion and alternative fuels. He has more than 17 research articles in his research field till date in various prestigious International Journals. He is a regular reviewer of various Energy related SCI indexed journals.

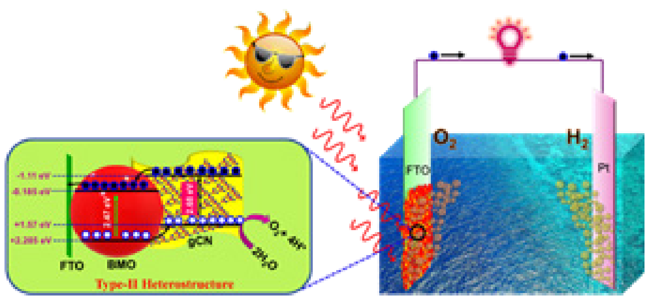
# 22 Development of Visible Light Active Functional Materials for Efficient Photocatalytic and Photoelectrocatalytic Generation of Hydrogen

## Aim

To design and develop a facile method to synthesize graphitic carbon nitride based hybrid catalytic materials with metal oxides, metal chalcogenides and metal phosphates and its potential application as photocatalysts for the photocatalytic and photoelectrochemical water splitting. The charge transfer dynamics of G-$C_3N_4$ based hybrid catalytic materials and correlating the photocatalytic and photoelectrocatalytic performance with the charge transport, electron life time and recombination process.

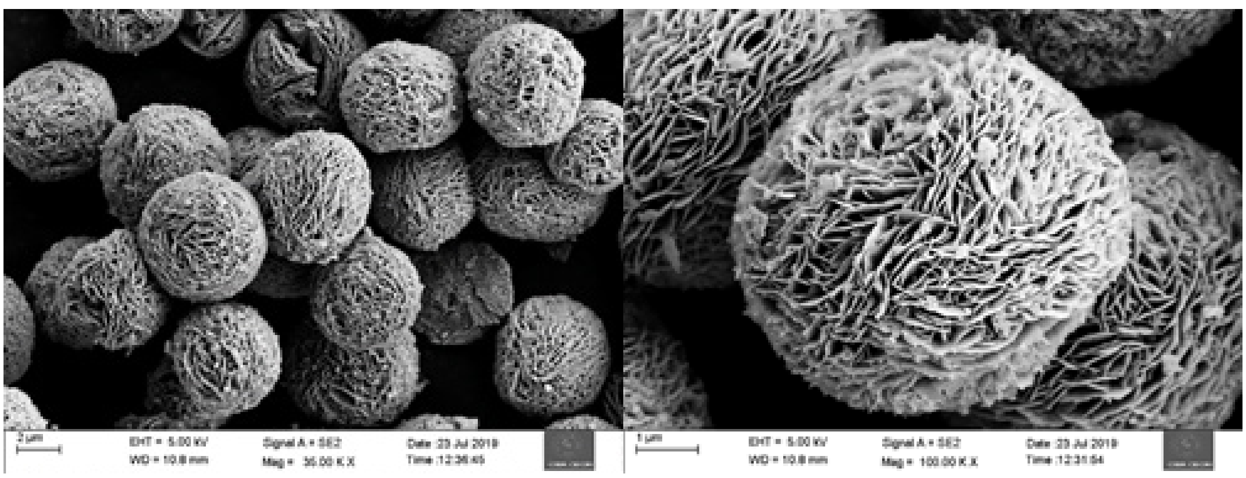
## Methodology

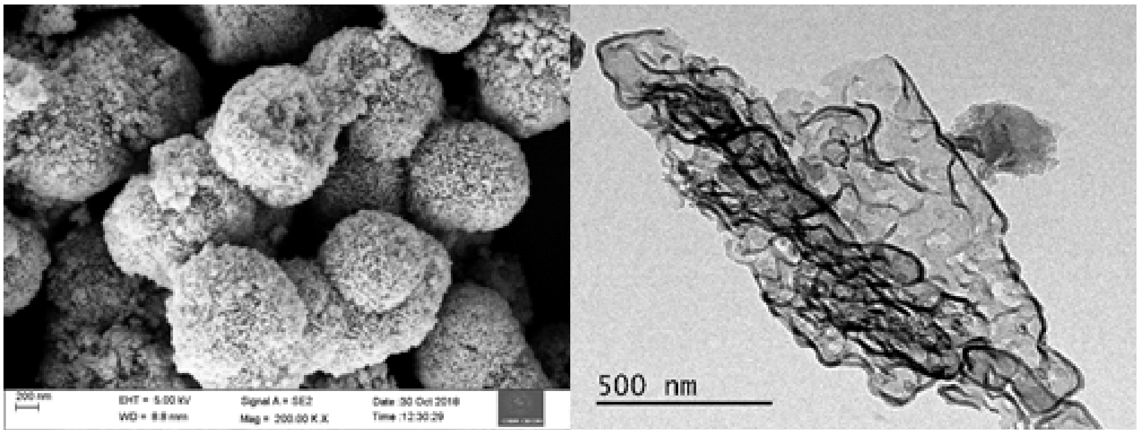
In this project, incorporation of metal oxides, metal chalcogenides and metal phosphate with G-$C_3N_4$ by hydrothermal method will be adopted and this leads to enhance the charge separation and transfer during the photo-induced process and it will be used as efficient visible light active photocatalyst for photocatalytic and photoelectrochemical generation for hydrogen. Also, a durable and more efficient photoelectrochemical cell will be developed by implementing a holistic approach of integrating novel G-$C_3N_4$ based hybrid catalytic materials.

## Expected Outcome & Deliverables

- Developing a simple synthetic route for visible light active g-$C_3N_4$-metal oxide, g-$C_3N_4$-metal chalcogenide,g-$C_3N_4$-metal phosphate based hybrid materials by hydrothermal approach.
- Investigation on the charge transfer dynamics of g-$C_3N_4$-based hybrid materials under illuminated condition for better utilization of visible light for hydrogen production.
- The optimization of best catalyst to achieve a high hydrogen production rate of 1,25,000 mol h-1g-1 with the g-$C_3N_4$ based hybrid catalytic materials.
- In spite of the large volume of activities devoted to these strategic areas of research and development, an economically viable process for the production of H2 via photoelectron/catalytic splitting of water is yet to be seen, this scenario needs to be changed to serve the country.



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M. Sathish received his PhD in Chemistry (2006) from Indian Institute of Technology Madras (IIT Madras) India. He was working on “Photocatalytic and Electrochemical Processes for Generation of Hydrogen and Decontamination of Water”. Then, he moved to Fullerene Engineering Group (2006-2008) and Supermolecules group (2008-2009), National Institute for Materials (NIMS), Japan. He was working on the development of fullerene based nanostructures using liquid-liquid interfacial precipitation method. After having three years of experience as a postdoctoral researcher, he moved to National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba (2009-2010) where he developed graphene-based materials for supercapacitor and Li-ion battery applications. When his research group moved to Tohoku University, Sendai, Japan, he also moved as JSPS research fellow (2010-2012) and continued the same work. From April 2012, he joined at CSIR-Central Electrochemical Research Institute (CSIR-CECRI), Karaikudi, as Scientist in Functional Materials Division. His research is focused on the development of carbon based materials for supercapacitor, nanocomposite materials for photocatalytic hydrogen production and supercritical fluid processing for 2D layered materials.

# 23 Development Of Earth Abundant Heterostructured Photocatalyst Based Solar $H_2$ Generation Reactor/Process

## Aim

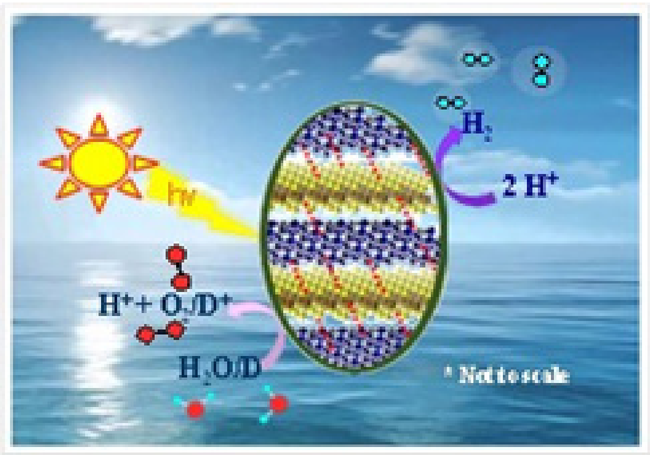
The synthesis of Earth abundant 2-D layered material based photocatalysts by wet-chemical approaches. Co-catalysts modification of synthesized 2D cross linked Earth abundant layered photocatalysts to reduce the activation energy/overpotential and improving charge carrier separation. The evaluation of the developed modified photocatalysts for solar hydrogen generation with overall improved efficiency, stability and optimization of solar hydrogen generation reactor to achieve (IPCE: ˜35 %, STH ≥ 4 %). The efforts will also be made to utilize the sea water as the water/proton source.

## Methodology

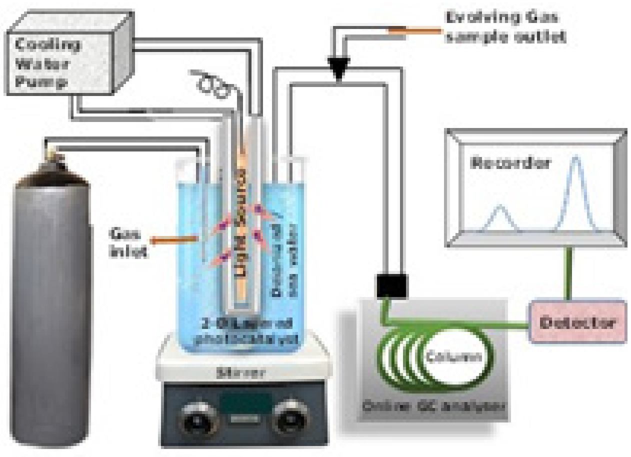
A versatile synthetic approach (soft chemistry based) will be developed to synthesize Earth abundant semiconductor nanostructures. In order to introduce porosity, the hard template will be used while synthesizing these photocatalysts. Co-catalysts modification of synthesized 2D cross linked Earth abundant layered photocatalysts to reduce the activation energy/overpotential and improving charge carrier separation will be undertaken. The structural, optical and electronic characterization of synthesized photocatalysts will be undertaken. To underpin the photogenerated charge carrier separation and their transfer kinetics phenomena for the developed photocatalysts, steady-state and time resolved photoluminescence studies were undertaken. These photocatalysts will be subjected to assess their activity for solar $H_2$ generation. Further optimization of overall efficiency, stability and scale-up trials for solar $H_2$ generation reactor/process will be undertaken.

## Expected Outcome & Deliverables

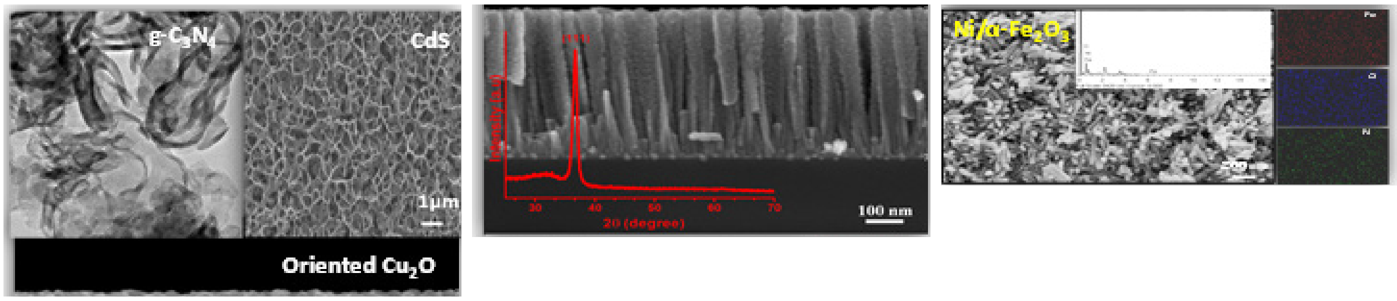
- Development of relatively low cost heterojunction photocatalysts based on Earth abundant elements to drive solar $H_2$ generation with overall improved efficiency.
- Fundamental understanding of the charge carrier dynamics of 2D cross linked Earth abundant layered photocatalysts.
- Introduction of novel materials design for the solar hydrogen generation.
- Solar $H_2$ generation process using the deionized water and also using sea water as proton source.
- Reinforcement of the visibility of CSIR-IMMT and India on the global stage among prestigious organization.




Schematic showing the solar hydrogen generation




Schematic showing the proposed solar H2 generation process and design of solar hydrogen generation reactor




Photocatalysts for solar $H_2$ Generation

Tata's $H_2$ powered bus trial by IOCL in 2018

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Dr. Yatendra S. Chaudhary is Principal Scientist at CSIR-Institute of Minerals & Materials Technology, Bhubaneswar, India and Associate Professor at the Academy of Scientific and Innovative Research (AcSIR), India. He earned Ph.D. for the research work focused on nanostructured photo-catalysts for solar-driven water splitting in 2004 from DEI, Agra. Subsequently, he moved to Tata Institute of Fundamental Research (TIFR), Mumbai, India, where he carried out research in Materials Chemistry. He designed enzyme-semiconductor based photocatalysts for visible light driven CO2 reduction and H2 production while working at University of Oxford, UK. His research accomplishments in the area of nanomaterial and solar fuel research have brought him many recognitions such as Green Talent-2011 Award from the Federal Ministry of Education and Research (BMBF), Germany, CSIR-Young Scientist Award-2013 in Chemical Sciences section from the Council of Scientific & Industrial Research, India and prestigious Marie Curie Fellowship by the European Union. He has edited a book - "Solar Fuel Generation" 1st ed. New York: CRC Press Taylor & Francis Group, 2017. His current research interest is energy conversion- solar fuels, direct white light emitting materials and nanomaterial synthesis.

# 24 Transition Metals Doped Strontium Zirconate And Strontium Manganite Perovskite For Solid Oxide Fuel Cell Applicatons

## Aim

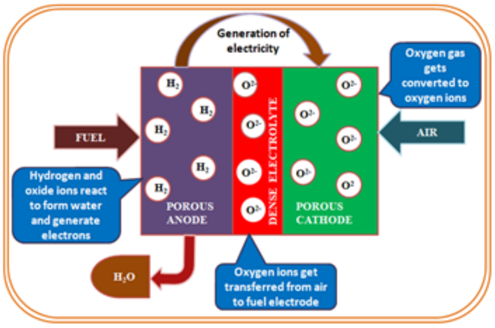
Synthesis of transition metals doped strontium zirconate and manganite using the solid-state reaction method. Study of the structural, thermal, electrical and mechanical properties using different characterization techniques. Interaction study of the selected samples with glass sealants and interconnect materials would be carried out to check their suitability as cathode/electrolyte materials for solid oxide fuel cells.

## Methodology

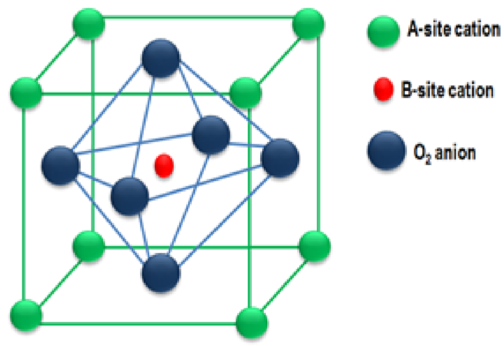
The focus of the proposed research work is to synthesize and characterize perovskite structured materials and study the effect of doping transition metal oxides. The proposed materials would be tested for their applicability as cathode/electrolyte materials for solid oxide fuel cell (SOFC) applications.

### Expected Outcome & Deliverables

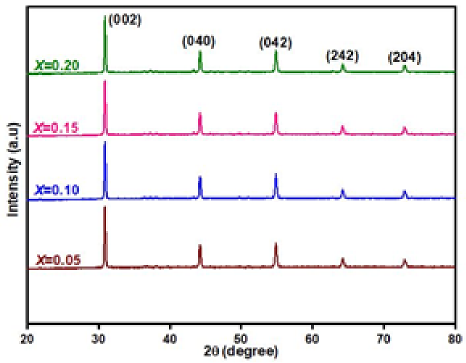
- Development of Nickel and Copper doped $SrZrO_3$ and $SrMnO_3$ for SOFC applications.
- Materials with appreciable conductivity to be used as cathode/electrolyte in SOFCs.
- Collaborative work with other departments within India to make the materials applicable for industrial applications.
- Publication of the results in peer reviewed journals or filing for the patent.



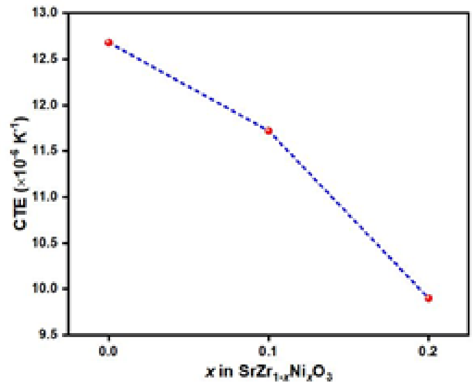

Schematic of an SOFC



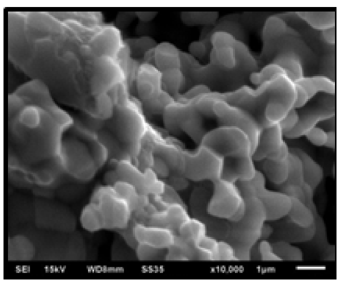

Basic perovskite structure

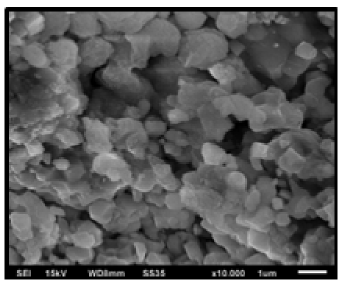


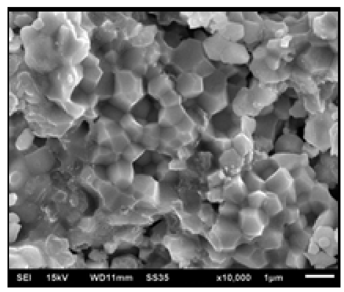

X-ray diffraction patterns of Ni-doped $SrZrO_3$




Variation of the coefficient of thermal expansion (CTE) with Ni concentration







**Dr. Kulvir Singh**
**Professor**
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**E-mail:kusingh@thapar.edu**

Dr. Kulvir Singh has completed his PhD in 1995 from HP University Shimla (IIT Bombey). He has 30 years research and 21 years teaching experience in various institutes of India and abroad such as research center, Forschungszentrum- Juelich, Germany, IIT Bombay, IIT Kanpur, HP University, Thapar University, Patiala. He has published more than 200 research articles in reputed SCI journals. More than 20 students have been awarded the PhD degree under his guidance. He is a reviewer of very prestigious SCI journals and CSIR, DST, India. He served as the head of the School of Physics and Materials Science, Associate Dean Strategy, Thapar Institute of Engineering and Technology (TIET), Patiala. Currently, he is working as a Professor and Associate Dean of Research & Sponsored Projects at TIET, Patiala.

# 25 Biomass Derived Heteroatom Doped Graphene and Hard Carbon Composites for Energy Storage Application

## Aim

This proposal aims to explore biomass (marine and terrestrial) derived carbon (functionalized graphene and hard carbon) for energy conversion (electrocatalyst for Fuel cell) and storage (electrodes for Na-ion Battery supercapacitor hybrid)
application.

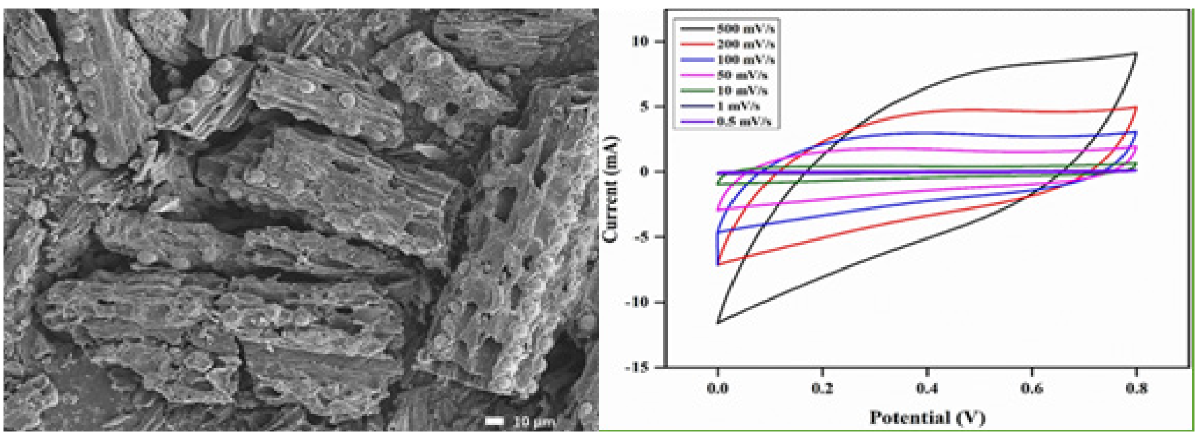
1. Tuning heteroatoms composition in biomass to suit fast electron transport and rapid ion/mass diffusion for energy storage and catalytic conversion of fuel to energy.
2. Synthesis and characterizations of biomass derived functionalized hard carbon aiming fast Na+ intercalation kinetics.
3. Fabrication and optimization of Membrane Electrode Assemblies (MEAs) for the electrochemical performance test for energy conversion.
4. All biomass derived carbon based full cell Na-ion battery supercapacitor hybrid fabrication and optimization of the electrochemical performance.

## Methodology

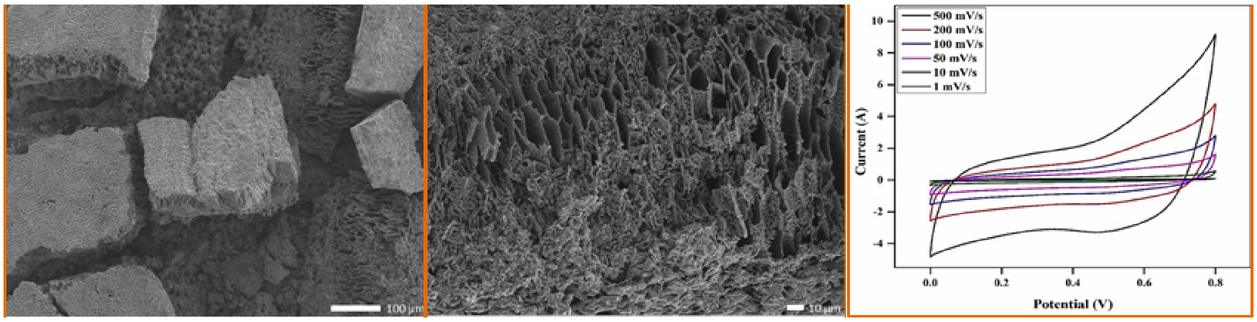
The project will focus on designing and modification of biomass derived heteroatom doped graphene as electrocatalyst in fuel cell. The other part of the project will explore the development of high energy high power Na-ion BSH devices targeting improvements upon all supercapacitor/battery components, i.e. cathode and anode. Biomass derived heteroatom doped functionalized graphene composites with high surface area will be used as cathodes and heteroatom doped functionalized hard carbon with fast Na+ intercalation kinetics will be used as anodes. Graphene or hard-carbon will be produced from lignocellulose and protein-rich biomass wastes, and agricultural lignocellulose wastes. After suitable pre-treatment (drying, mixing, grinding), task specific annealing of the dried mass will be carried out. Depending on the end application suitable activation step will be developed to obtain high surface area graphene or hard carbon.

## Expected Outcome & Deliverables

- Fabrication of biomass derived graphene with dual role of catalyst as well as support for high performance fuel cell and fabrication of MEAs with target energy density >50 $Whkg^{-1}$
- Fabrication of biomass derived graphene based capacitive electrode with target capacitance (>150 $F/cm^3$) and hard-carbon as high capacity $Na^+$ intercalation anode with target capacity (>150 mAh/g)
- Fabrication and prototype demonstration of full cell Na-ion battery supercapacitor hybrid coin cell.



Areca CATECHU derived carbon and its CV analysis




**Pisum SATIVUM derived carbon and its CV analysis**

**Dr. S.K. Nataraj**
**Professor**
**CNMS, Jain University**
**Email: sk.nataraj@jainuniversity.ac.in**

Dr. S.K. Nataraj is currently working as Professor at Centre for Nano and Material Sciences (CNMS), Jain University, Bangalore, India. He obtained his PhD in 2008 in Polymer Science from Karnatak University, Dharwad, India. Immediately after completion of PhD, he pursued three Postdoctoral Associate assignments at Chonnam National University, South Korea to (2007-2009), Institute of Atomic Molecular Sciences, Academia Sinica (2009-10), Taiwan and Cavendish Laboratory, University Cambridge, UK (2010-2013), respectively. He was awarded DST-INSPIRE Faculty Award (2013-2015) at CSIR-CSMCRI, Bhavnagar. His main areas are to develop sustainable materials and processes for Energy and Environmental applications including water treatment.

**Dr. Debasis Ghosh**
**Assistant Professor**
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**Email: g.debasis@jainuniversity.ac.in**

Dr. Debasis Ghosh obtained his PhD from Materials Science Centre, IIT Kharagpur in 2014 and after more than two years of postdoc experience in energy storage technology in reputed foreign Institutes, he joined CNMS, JAIN University as Assistant Professor in 2017. His research interest is designing functional nanomaterials and nanocomposites for electrochemical energy conversion and storage (supercapacitors and rechargeable batteries, e.g. metal ion, Lithium-sulfur and metal-air batteries).

# 26 Non-Pt Based Alloys And Intermetallics As Efficient Electrode Materials For The Energy Conversion In Fuel Cell

## Aim

Synthesis of nanomaterials such as intermetallics, oxides and chalcogenides for electrochemical applications such as watersplitting and fuel cells.

## Methodology

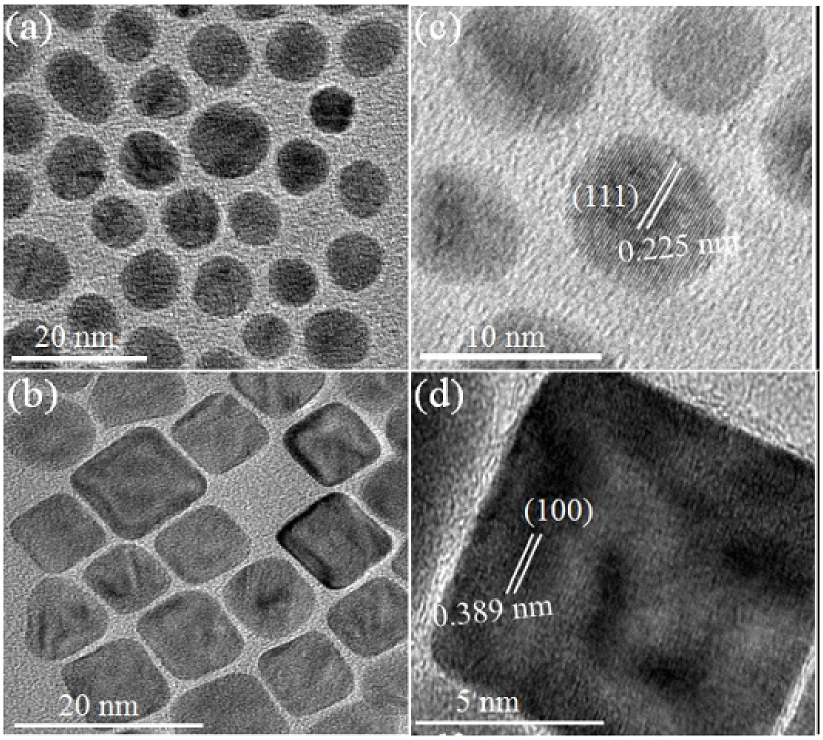
The focus of the proposed research is to develop catalyst for water electrolyzer and also for fuel-cells. Hydrothermal and colloidal techniques are few of the common synthesis method for electrocatalysts. Exsitu, in-situ and DFT analysis are used for probing the catalyst surface. Electrocatalysts are then screened in a three electrode configuration followed by testing in a dedicated test station.

### Expected Outcome & Deliverables

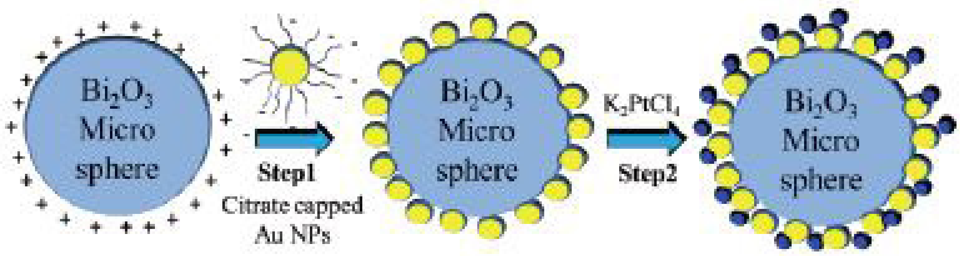
- Development of non-Pt based electrocatalyst for hydrogen generation and fuel-cell reactions.
- Design and fabrication of highly active and stable electrocatalyst.
- Achieving high-current density at a lower overpotential.
- Scaling up of electrocatalyst for fuel cell testing.
- Developing full-cell testing protocol for hydrogen generation and fuel-cell in a dedicated 2-electrode setup.
- Development of fuel cell systems that are able to reach 75% power density

(W/L) as compared to the current state-of-the-art running for at least 30 minutes at a temperature of 60 °C.

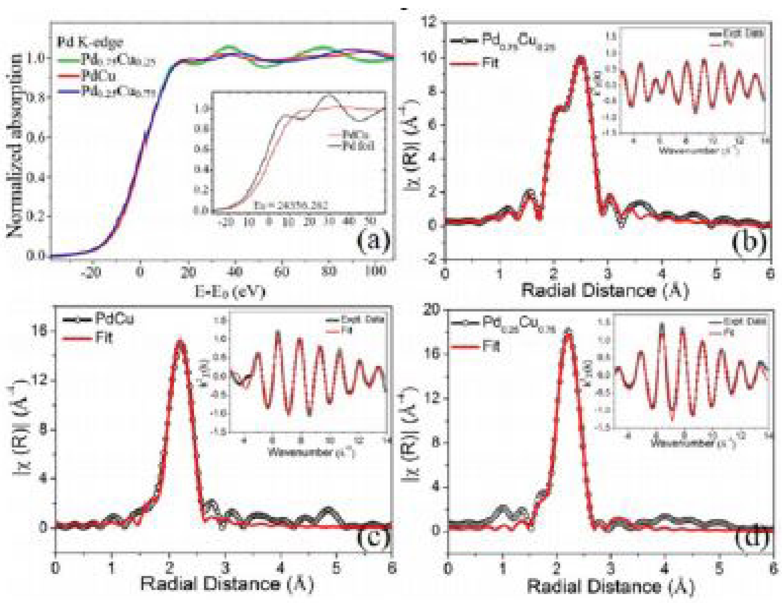
- Modification of catalyst to achieve target set by Department of Energy, US.




**Surfactant-assisted Sphere and Cubic PdCu3**



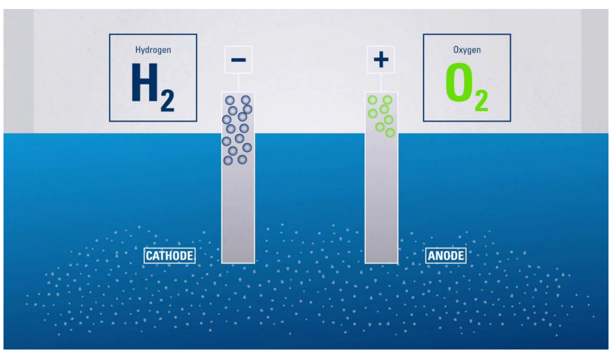

**Facile Aqueous Phase Synthesis of PtAu/Bi Hybrid Catalyst**




XAFS analysis of PdCu compound

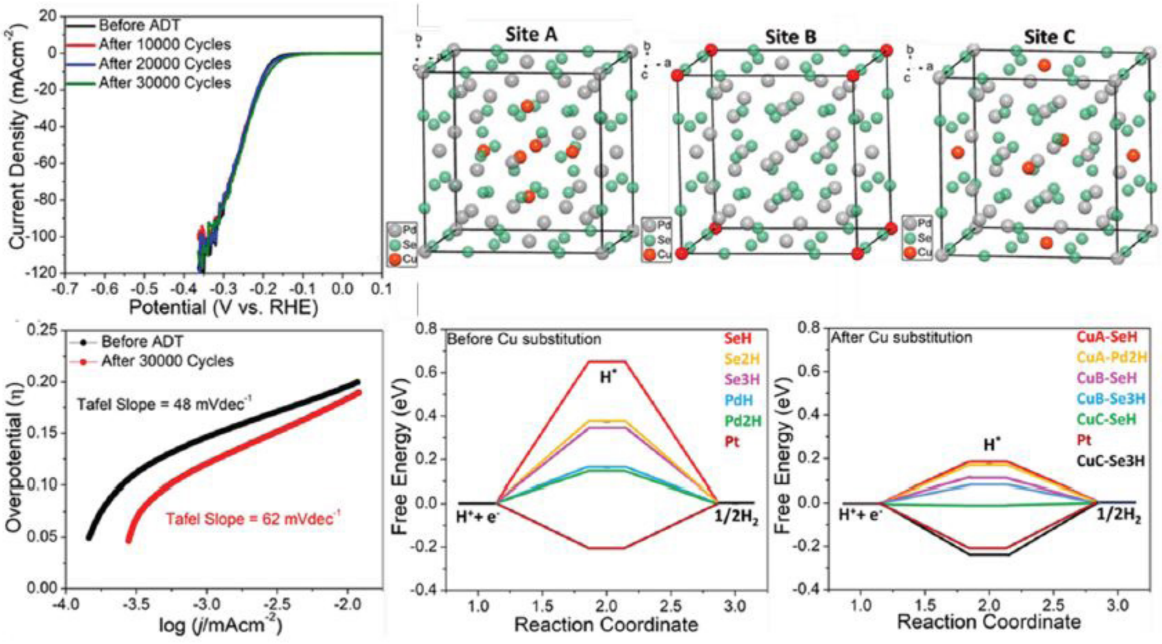
QBEAK DMFC car

Yamaha DMFC Scooter




Electrolysis: Producing Hydrogen from Water

Fuel-Cell Test Station




**Dr. Sebastian C. Peter**
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Prof. Sebastian C. Peter received his M.Sc. degree from Calicut University (India), and M. Tech. degree from CUSAT (India). He received his Ph.D. degree from the University of Münster, Germany in 2006 and was a postdoctoral researcher at Max Plank Institute for Chemical Physics of Solids, Dresden, Germany and Northwestern University, U.S.A. He is presently an Associate Professor at Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India. His research interests include fuel cells and CO2 reduction. He received prestigious Swarnajayant Fellowship in 2018-19. He is the founder and director of the start-up BREATHE Applied Sciences Pvt. Ltd.

# 27 Synthesis of MOF/ZIF for fuel cell application

## Aim

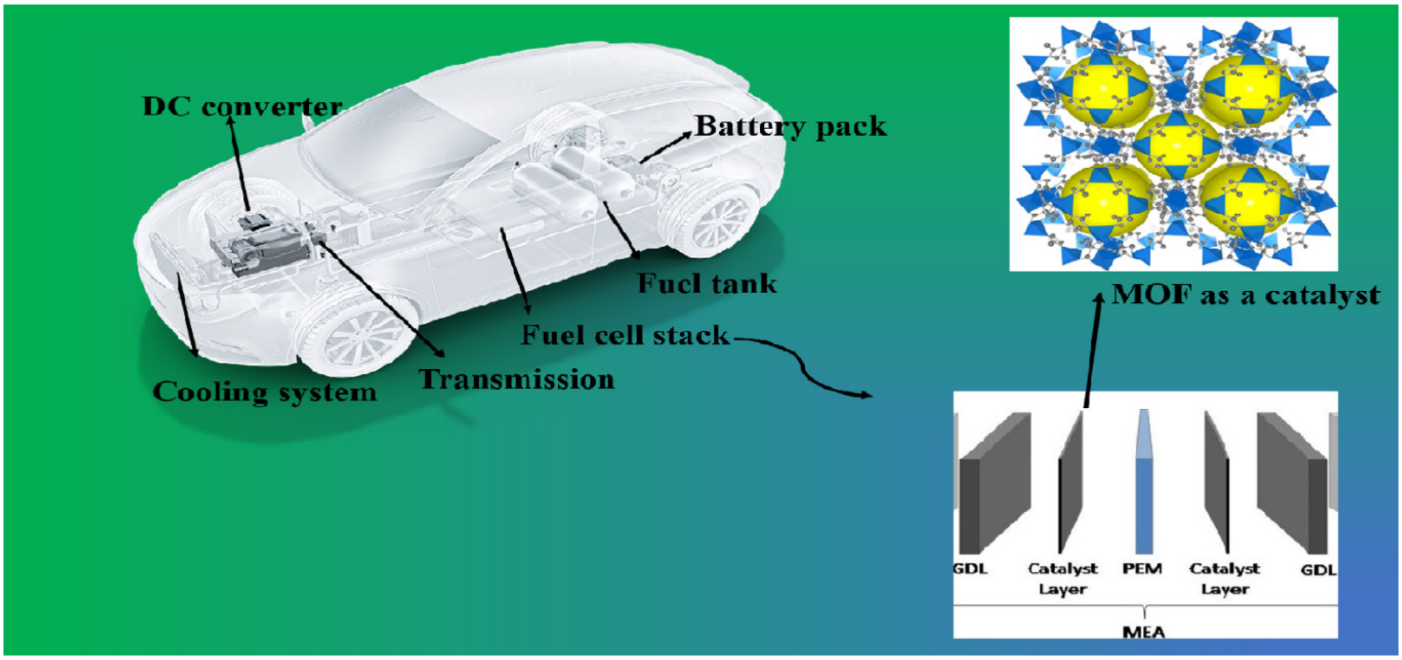
Development of highly porous Metal Organic Framework (MOF) / Zeolite Imidazolate Framework (ZIF) based electrocatalyst via chemical/hydrothermal method for electrochemical Oxygen Reduction Reaction (ORR) in fuel cell applications.

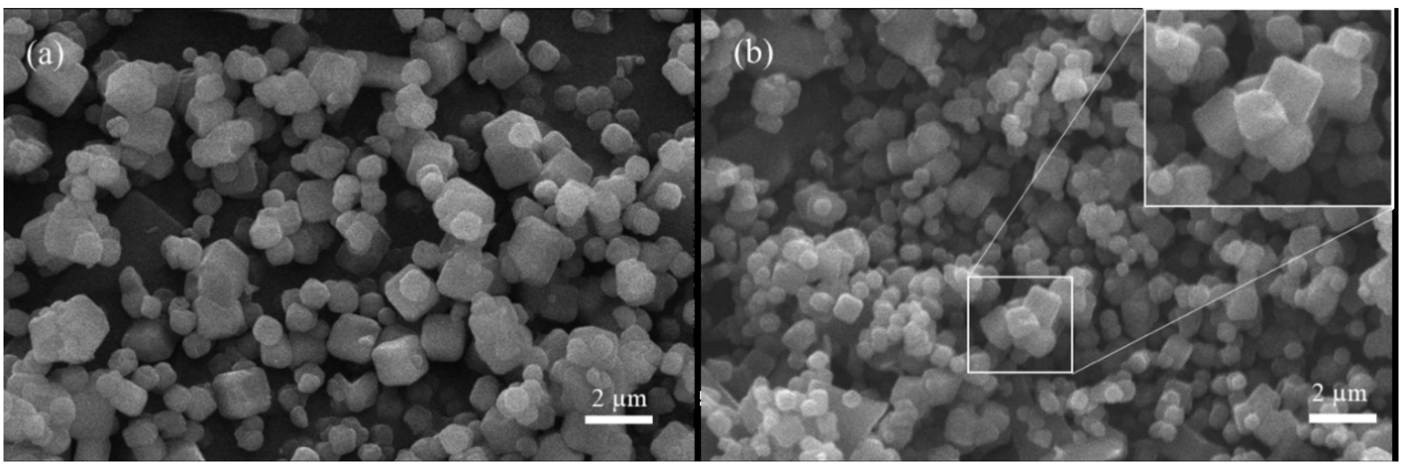
## Methodology

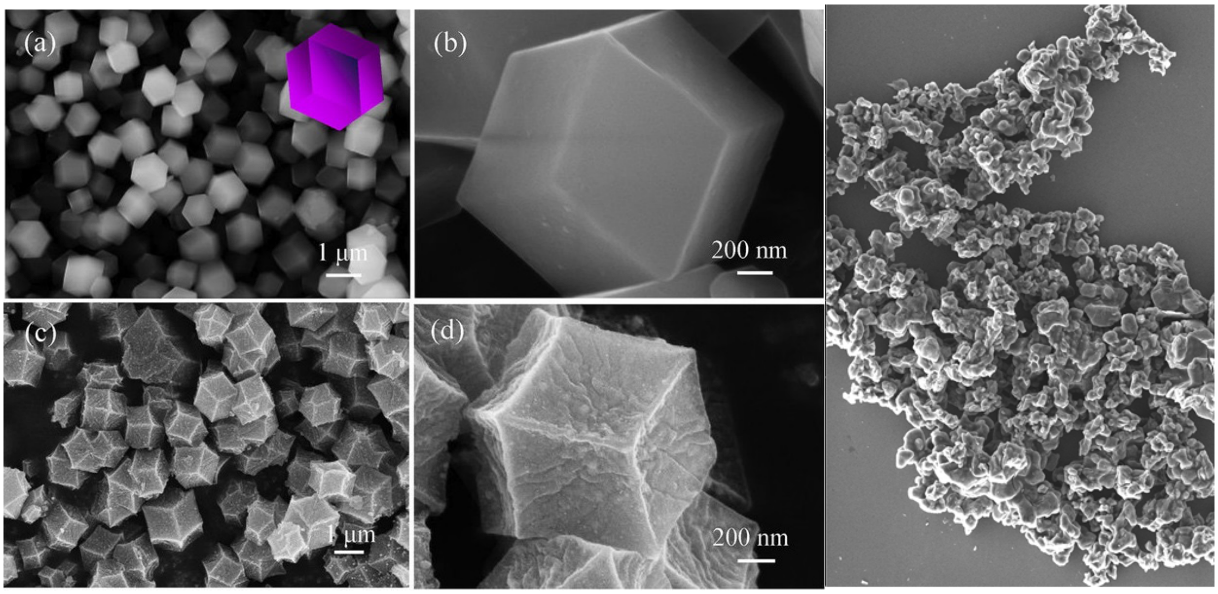
The proposed research plan mainly focuses on the synthesis and characterization of fundamental and applied aspects of metal based cage like highly porous MOF materials (conducting polymer and composite materials) to study their electrochemical activity, stability and durability for fuel cell and energy storage devices. Further modification will be incorporated focusing the improvement of electrical conductivity, tuning porosity and surface area of material.

### Expected Outcome & Deliverables

- Development of high performance and relatively low cost highly porous 2D/3D Pt free.
- electro catalyst material for ORR based fuel cell applications.
- Introduction of unique methods for the synthesis of nanocomposites at low cost and large scale which will be beneficial in the field of energy storage.
- Synthesis of highly stable and durable electrocatalyst, comparable with commercial PT/C material which is highly expensive.


DC converter
Battery pack
Fuel tank
Fuel cell stack
Cooling system
Transmission
MOF as a catalyst
GDL
Catalyst Layer
PEM
Catalyst Layer
GDL
MEA


(a)
2 µm
(b)
2 µm




**Dr. Neetu Jha**
**Assistant Professor,**
**ICT Mumbai**
**Email : jha.neetu@gmail.com**

Dr. Neetu Jha did her M.Sc in Physics from the Department of Physics, BHU in 2004. Then she joined the Department of Physics, Indian Institute of Technology Madras for PhD followed by postdoc from the University of California Riverside. She joined ICT Mumbai in 2012 and working here since then. Her main research interest is in the area of development of novel electrode materials for energy applications, where she is involved in developing green techniques for the development of nanocomposites and studying their applications in energy devices like fuel cells, battery and supercapacitors. She is also actively involved in the development of energy efficient water purification techniques like capacitive water desalination and photothermal materials for solar steam generation.

# 28 Noble-Metal free Advanced Catalysts for Hydrogen Generation and Fuel Cell Applications

## Aim

The main objective is to carry out technology oriented research in the frontier area of hydrogen energy and to set up a strong research base to deliver highly efficient and advanced noble metal-free catalysts for hydrogen generation and fuel cells. In this approach we plan to make noble metal-free catalysts based on metal nitrides, hydroxides, chalcogenides and phosphides and their composites with other 2D layered materials such as graphene, towards water electrolysis.

## Methodology

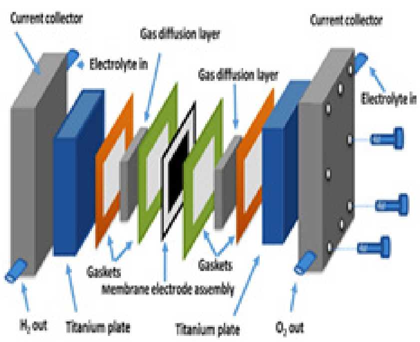
We propose to undertake an in-depth study on the electro- and photo-catalytic performance of nanocomposites of doped graphene with certain metal chalcogenides, metal phosphides, metal nitride system towards various energy converting reactions like Oxygen Evolution (OER), Hydrogen Evolution (HER), Oxygen Reduction (ORR) and Hydrogen Oxidation (HOR). The main advantage of this method in comparison with the current techniques are (i) reduction in cost of the cells by replacing the noble metal catalysts with low-cost non-noble metal based materials and (ii) bi-functionality of the catalysts to function as both cathode and anode. Nanocomposites will be prepared either by thermal annealing of graphene oxide or other 2D material with corresponding precursors or by solvothermal route. Exfoliation of bulk counterparts to attain few layered nanocrystals of 2D layered materials will be attempted via liquid phase or electrochemical routes. The physicochemical properties of the materials will be characterized by various spectroscopic and microscopic methods. Performance of the electrocatalyst including electrode kinetics will be analyzed using rotating ring disc electrode (RRDE) voltammetry technique. Further, prototype fuel cells and water electrolysers using optimized electrode materials, with high efficiency and stability, will be fabricated.

## Expected Outcome & Deliverables

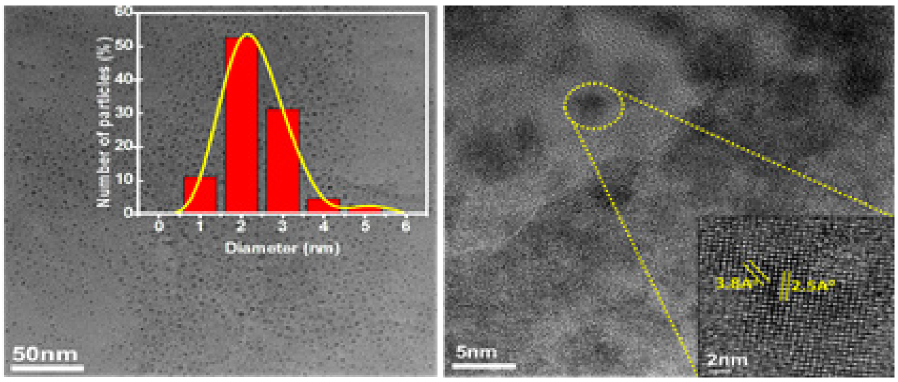
- Developing effective approaches for the rational design of efficient noble metal-free catalysts based on certain metal chalcogenides, nitrides or metal phosphides and their graphene composites for large-scale production of hydrogen through electro-and photocatalysis.
- Design and fabrication of polymer electrolyte membrane based prototype Fuel cells and Water electrolysers based on the developed catalysts.
- Electrochemical characterization of doped graphene metal chalcogenides, metal phosphides, metal nitride system towards various energy converting reactions like oxygen evolution (OER), hydrogen evolution (HER), Oxygen reduction (ORR) and Hydrogen oxidation.

Toyota's Fuel Cell Car

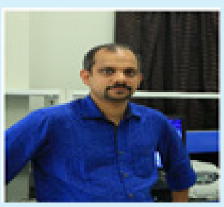

**SEM images of cobalt phosphides**




**Schematic of a PEM Fuel cell**




**Low and High resolution images of Phosphorene quantum dots synthesized through electrochemical exfoliation method**



**Dr. M. M. Shaijumon**
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Dr. Shaijumon obtained his Ph.D in Physics from Indian Institute of Technology Madras. He spent more than 3 years in the United States as a postdoctoral research fellow at Rensselaer Polytechnic Institute, Troy, New York and Rice University, Houston, Texas. Later he spent nearly a year and half as a senior postdoctoral researcher at Paul Sabatier University, Toulouse, France. He joined IISER Thiruvananthapuram as an Assistant Professor in School of Physics in 2010 and he is an Associate Professor since 2017. Dr. Shaijumon's research interests are in the area of nanomaterials and energy storage and conversion, focusing on the synthesis of novel nanostructures, design and development of efficient energy storage devices, mostly looking at the materials science and physics of these systems. He has three US patents and two Indian patents filed. He has published more than 65 journal papers with more than 5000 citations and with an h-index of 33. He received the MRSI medal in 2019 and DAE Young Scientist Research Award in 2012.

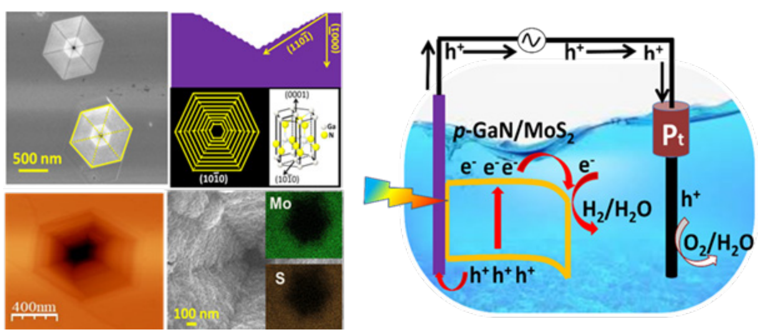
# 29 DEEP: Development of an Efficient Photoelectrode for Hydrogen Fuel from Water

## Aim

This Project aims at the growth of ordered nearly defects free (In)GaN NSs by Plasma Assisted-MBE (PAMBE) and also by other growth techniques like PVD or CVD etc., as photoelectrodes (PEs) for water splitting PEC devices. The incorporation of different In compositions allowing fabrication of tendam NSs photo-electrodes with further enhanced efficiency, would be investigated.

## Methodology

This project aims the growth of the ordered (In)GaN NSs, their electrical, optical, chemical & structural characterization and optimizations for the efficient photoelectrode for water splitting to produce hydrogen fuel. The strategy is to use MBE technique to obtain a high quality (In)GaN alloys with the adequate compositions for water splitting application (2D layers and ordered NSs) followed by the p-doing and the decoration with differently suitable co-catalyst to improve the efficiency of the proposed photoelectrodes. Further the modification with different cocatalyst is proposed for the efficiency and stability enhancement.



## Expected Outcome & Deliverables

- A process for optimized ordered InGaN/GaN NSs growth for device
- Integration of III-nitrides photoelectrodes with other cocatalysts to develop hybrid photoelectrodes
- A prototype of a highly efficient and stable photoelectrode with efficient of > 10% for hydrogen fuel generation

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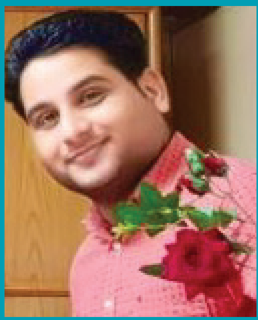
Dr. Praveen Kumar is an working as an Assistant Professor at IACS-Kolkata. He is also a Chair of Marie Curie Alumni Association (MCAA) Indian Chapter funded by European Commission. He received his PhD from Department of Physics, Indian Institute of Technology, Delhi in 2011. He is a recipient of several recognized awards and fellowships, few of them are BRICS Young Scientist Award, Marie Curie Postdoctoral Fellowship from European Commission, INSPIRE Faculty Award from Department of Science and Technology Delhi, 05 Best oral/poster award in various international conferences and Gold Medal in M. Sc. (Physics) From Rajasthan University. He is elected as a sectional committee member for Materials Science in the Indian National Science Congress Association. Dr Kumar's research contribution covers a broad spectrum of Materials Synthesis including III-V semiconductors, Oxides, Sulphides, Carbon Nanostructures, metal/semiconductor interfaces etc for LED emitters & solar cells, photoelectrodes, Broadband self-powered photodetectors, and sensors applications. He has authored 03 books, 72 publications in peer-reviewed international journals, more than 50 in conference proceedings, and delivered around 35 invited/oral talks at various conferences/institutes around the globe.

# Acknowledgement


Anu K Raj


Manoj Sharma


Vaibhav


Thakur Prithvi Pal Singh Negi


Mukul Sharma

**Technology Mission Division ( Energy & Water )**
**Department of Science & Technology**

**Cover page photograph:**

"Molecular Catalysts For Clean and Sustainable Energy and Environment"

**Courtesy :**
Dr. Abhishek Dey, Indian Association for the Cultivation of Science (IACS), Kolkata

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