Indian Institute of Technology Delhi

School of Interdisciplinary Research (SIRe)

SIRe Project Number

2022-01-35

(will be assigned by SIRe)

PhD Project

Project Details	
Project Title	**Two-Dimensional Nanomaterials as the Catalysts for Hydrogen Evolution Reactions: An Experimental and First-principles based Investigation**
Project Summary	On a global scale, clean energy generation needs to rapidly increase to meet rising energy demands and mitigate the effects of climate change from fossil fuel burning. In this regard, solar fuels such as hydrogen gas have emerged as a promising green energy source. Solar light-induced catalytic water splitting for hydrogen production using suitable semiconductors is an attractive approach due to low cost, environment-friendly by-products, etc. In recent times, two-dimensional (2D) nanomaterials have been explored widely as a photocatalyst for water hydrogen evolution reaction (HER). The appropriate band edge alignments, large surface area, high light absorption capability make these 2D materials ideal for photocatalytic applications. The heterostructures of 2D nanomaterials particularly those with transition metal chalcogenides (TMC) that are MX_2 (M = Mo, W; X=S, Se, Te), MX (M=Si, Ge, Sn) and carbides (M′Xenes that are M'_2C, M'_3C_2 and M'_4C_3; M= Ti, V, Nb) have demonstrated excellent photocatalytic activity. Nevertheless, with the recent discovery of a wide range of layered materials, we find considerable opportunities to strategically design 2D heterostructured nanomaterials for highly efficient photocatalytic performance. Particularly, the 2D heterostructures that possess constituent layers from different lattice systems, can be exciting to explore as the compositional search space is very wide and mostly unexplored so far. Considering these prospects, we propose to perform thorough state-of-the-art atomistic simulations and experimental synthesis, characterization, and catalytic activity study to identify the potential heterostructures for photocatalytic performance in HER. In this project, we will explore the various combinations of MX, MX_2, and M′Xenes based nanomaterials investigating their photocatalytic activity. Proposed work will further lead to provide a roadmap for designing heterostructures for other targeted catalytic reactions. Scope of the project: (1) To learn various state-of-the-art experimental synthesis, characterization, catalytic activity measurement techniques. (2) To learn various first-principles based methods such as density functional theory (DFT), *ab initio* molecular dynamics (AIMD) simulations, etc.

Ph.D. Supervisors			
Role	**Faculty**	**Academic Unit in IITD**	**Email ID**
Supervisor 1	Prof. Dibyajyoti Ghosh	Department of Material Science and Engineering [https://mse.iitd.ac.in/faculty-profile/19]	dibyajyoti@mse.iitd.ac.in
Supervisor 2	Prof. Sameer Sapra	Department of Chemistry [https://chemistry.iitd.ac.in/faculty/sapra.html]	sapra@chemistry.iitd.ac.in

Project requirements (Student qualifications, experience required, etc)

- MSc. / MTech. / Integrated BS-MS in Physics / Chemistry / Materials Science / Materials Engg. / Chemical Engg.
- BTech. in Engineering Physics / Materials Science / Materials Engg. / Chemical Engg.
- Candidates having PMRF / CSIR-UGC NET / GATE / DST Inspire are more encouraged to apply.

Source of funding (IRD/FITT Project details, if any)

1. PMRF/CSIR/UGC/DST Inspire fellowship
2. INSTITUTE fellowship with GATE qualification
3. Any other external funding available at the candidate's end

Role of Faculty Members involved:

The said project contains two parts (1) Building a robust first-principle-based computational model to screen a wide range of 2D heterostructure-based nanomaterials for HER photocatalytic activity and (2) experimental synthesis, characterization, and catalytic activity measurement of these screened heterostructured materials. While the initial part requires expertise in computational materials modeling the latter part needs expertise in experimental materials science.

Here Prof. D. Ghosh has extensive experience in theoretical materials modeling especially simulating electronic, optical, and catalytic processes in two-dimensional layered materials. And Prof. S. Sapra has expertise in synthesis, characterization, and catalytic performance measurements in a wide variety of materials including 2D-layered and heterostructure systems.

Considering these aspects of the proposed project, this will be a perfect interdisciplinary theory-experiment collaboration to fulfill the mentioned research effort.