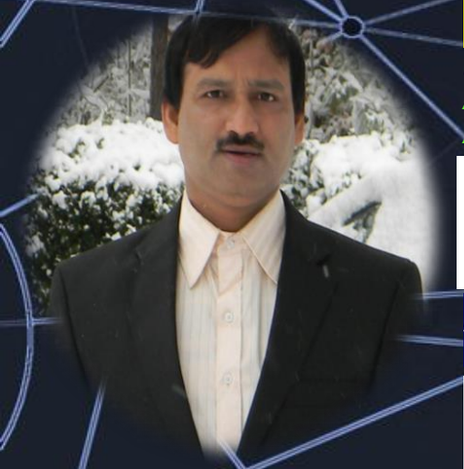
ACCMS-Global Research Center
SRMIST, Chennai India

Webinar #23



Dr. Brahmananda Chakraborty

High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai;
Associate Prof. Homi Bhabha National Institute, Mumbai

Title: 2D Nanomaterials for Hydrogen Storage and Electro-chemical Energy Storage: Insights From DFT Simulations

Registration link: http://tinyurl.com/5n8kz3r4
**Zoom details will be shared with the registered participants*

January 30, 2024,
11.30 am– 1.00 pm
Indian Standard Time

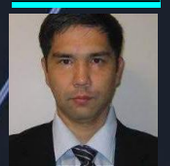
Short biography

Dr. Brahmananda Chakraborty is a scientist in High Pressure & Synchrotron Radiation Physics Division of Bhabha Atomic Research Centre, Mumbai and Associate Professor in Homi Bhabha National institute. His current research interest includes Density Functional Theory (DFT) & Molecular Dynamics (MD) simulations of materials for energy materials, bio-Sensors, reactor fuel and structural materials, nanomaterials and behavior of materials under high pressure. Dr. Chakraborty got his Ph.D degree from IIT, Bombay for his research topic on 'Irradiation Effects and Hydrogen Storage on Carbon Nanotubes'. He did two years Post-doctoral research in North Carolina State University, USA. He received International Association of Advanced Material (IAAM) Scientist Medal in 2017. He has published more than 250 papers in reputed international journals. He has published one book in 2022 (Editor as well as author) on "2D Metallic Transition Metal Dichalcogenides: Fundamentals and Applications" published by NOVA Publisher (Newyork, USA). Based on single year performance, he was selected among top 2% influential researchers by Elsevier in 2022 as well in 2023.

Abstract

Various 2D nanomaterials have drawn immense attention as energy storage devices (hydrogen energy & electro-chemical energy) due to their high surface area, high conductivity and high mechanical strength. For pristine carbon nanostructures H_2 adsorption is due to weak Van der Waals interactions and it can't hold H_2 at room temperature. The adsorption energy can be increased by: (i) attachment of metals, (ii) Applying strain, (iii) By substituting B and N in place of C. Carbon nanostructures functionalized by transition metals are most promising candidates as adsorption energy can be increased through Kubas interactions. This presentation will describe Density Functional Theory (DFT) results on interaction, charge transfer mechanism and hydrogen storage capability of various 3d and 4d transition metals attached on various carbon nanostructures (graphene, graphyne, holey graphene, biphenylene etc.). The effect of strain on 2D materials for enhancing the hydrogen storage capability will also be addressed. This talk will also highlight electro-chemical energy storage performance of various hybrid 2D structures based on graphene, transition metal dichalcogenides and MXene, e.g., MoO_3/RGO, VSe_2/RGO, VSe_2/MXene etc. as electrodes for supercapacitors. Recent synthesized 2D materials MXene and their hybrid structures are more promising for energy storage applications. Some of our recent work on MXene based materials will also be described.

Panelist



Prof. Talgat Inerbaev

Head of the Laboratory of computational materials science for energy application, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan

Convener:
Prof. Yoshiyuki Kawazoe
Head, ACCMS-GRC
SRMIST, KTR

Organizers:
Dr. V.J.Surya & Dr.S. Yuvaraj
ACCMS-GRC Center-in-Charges
Dept. of Physics and Nanotechnology, SRMIST, KTR

NAAC A++ | Category 1 with 12B Status | (2022) Ranked 19th University | (2023) World Ranking one among 41 Indian Universities | (2023) World Ranking one among 75 Indian Universities | (2021) Ranked 4th | (2023) World Ranking one among 14 Indian Universities