Seminar

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Institute for Plasma Research

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Title: Advancing Energy Materials through Computational and Experimental Synergy

Speaker: Dr. Amit K Bhojani
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Date: 28th February 2025 (Friday)

Time: 10.30 AM

Venue: Seminar Hall, IPR

Abstract

The development of next-generation energy materials requires a seamless integration of computational and experimental approaches to unlock their full potential in terms of efficiency, stability, and real-world applicability. A key challenge in this field is optimizing energy conversion materials to achieve higher performance and stability. In this manner, two-dimensional (2D) materials exhibit unique structural, electronic, optical and thermoelectric properties that make them promising candidates for advanced energy applications. Among various novel 2D materials, carbon-based chalcogenides emerge as a highly promising class of materials due to their superior light absorption, high electron mobility, and excellent transport properties, showing potential for energy applications. Density functional theory (DFT)-based investigations have confirmed their structural stability and reveal unique properties that contribute to enhanced energy harvesting efficiency. Key findings include anomalous lattice thermal conductivity, which plays a crucial role in thermoelectric performance, and strong energy conversion capabilities, paving the way for their integration into sustainable energy technologies. Here, the utilized DFT technique is a powerful tool for predicting material properties at the atomic scale, enabling the design of novel materials with tailored functionalities. However, the true potential of any material can only be realized through experimental validation, which bridges the gap between theoretical predictions and real-world applications. By combining DFT simulations with advanced spectroscopic and surface characterization techniques, cryogenic systems, and temperature dependent adsorption studies, this research aims to unravel the complexities of molecular interactions and surface dynamics under extreme conditions. This synergy between computation and experiment is crucial for developing next-generation energy materials that meet the growing global demand for efficient and sustainable energy solutions.