Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

Electronic Properties of Cathode Materials in Lithium Ion Photo Batteries

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Transition Metal Dichalcogenide (TMD)–based semiconductor heterojunctions, especially type-II, have been widely employed in optoelectronic devices for their ability to efficiently separate photo-generated charge carriers. This talk focuses on the development of computational and data-driven approaches to understand and engineer the layered transition metal dichalcogenide cathodes for lithium-ion photobatteries. I will begin by discussing an alternative layering scheme in layered TMDs that we developed to achieve type-II band alignment within the framework of GGA based density-functional-theory. This will be followed by a discussion on how the type-II heterostructure delays metallization in lithiated MoS_2 and its implication on the photobattery performance. Afterwards, I will discuss a separate but related study focused on predicting stable alkali adsorption sites on 2D TMDs using electrostatic features derived from point charge analysis. Building on the insights gained from these studies, we have developed a machine learning-based approach to screen novel photo-cathode materials. Finally, I will delve into the hybrid model—combining atomistic simulations and graph neural networks—that we are developing to predict lithium dynamics in a photobattery during simultaneous discharging and photocharging.

Friday, Jul 18th 2025

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Auditorium, TIFRH