Students' Annual Seminar

Phase stability and binding sites of lithiated MoS$_2$

Raheel Hammad

Recent advancements in the field of photocathodes for photochargeable Li-ion batteries have led to the exploration of heterostructures such as MoS$_2$/MoO$_y$ and TiS$_2$/TiO$_2$. A type II setup has been proposed to generate spatially separated (longer-lived) excitons upon photo-exposure. The Li-intercalated MoS$_2$, generated during the discharge cycle of the battery, undergoes a phase transition from the semiconducting (2H) to a metallic (1T') phase, in contrast to its TiS$_2$ counterpart, casting doubt over the photocharging process. Utilising density functional theory (DFT) we show that an underlying band gap of Li$_x$MoS$_2$ is exposed in Li$_x$MoS$_2$/MoO$_3$ heterostructure, up to a certain value of x. Thus, dispersion of electron density from the conduction band of Li$_x$MoS$_2$ to MoO$_3$ can justify photocharging. Additionally, the heterostructure delays the transition from the semiconducting to the metallic phase, therefore enabling photocharging to occur at higher Li-ion concentrations. As the concentration of the intercalated Li-ion increases we need to find the corresponding low energy structures. However, solving this problem is easier said than done because the number of possibilities increases drastically with increasing number of Li-ions in a reasonably sized supercell. We propose a novel strategy integrating Point Charge Analyses and Machine Learning to forecast Lithium binding sites on monolayer H-MoS$_2$ accurately. By establishing a strong correlation between energy variation and electrostatic coupling of binding sites, our approach offers a scalable solution for predicting low-energy structures in various layered materials. This scheme significantly reduces the computational overhead associated with DFT calculations.

Thursday, Mar 28th 2024

14:00 Hrs (Tea / Coffee 13:45 Hrs)

Seminar Hall, TIFR-H