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

Webinar

Electronic Properties of Cathode Materials in Lithium Ion Photobatteries

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Transition metal dichalcogenide (TMD)–based semiconductor heterojunctions, particularly type-II junctions, are central to many optoelectronic devices because they promote efficient separation of photo-generated charge carriers. This thesis develops computational and data-driven strategies to understand and engineer layered TMD cathodes for lithium-ion photobatteries. Barring the introduction and methods chapters, the thesis comprises primarily of three main chapters that highlight three independent, but related, studies. In the first project, we developed an alternative layering scheme in layered TMDs to realise type-II band alignment within the framework of most widely used density-functional-theory (DFT) functional. For the second project, the role of type-II heterostructure in lithiated MoS_2 is examined, partly using the design principles developed in the previous chapter. We showed that the heterostructure requires higher, as compared to MoS_2 alone, lithium ion concentration to induce metallization, which has huge implications regarding the role of heterojunctions as photocathodes. In the final completed work, we developed a machine learning model to predict the stable binding sites of lithium atoms on MoS_2 surfaces. This model is found to be quasi-transferable to other alkali metal ions and TMD systems. In the last chapter I have briefly described the ongoing projects. Building on the insights from the previous works, we developed a machine-learning screening workflow to accelerate the discovery of novel photocathode candidates. Finally, we investigate the dynamics of lithium transport upon photocharging from a partly discharged state.

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