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First-Principles Investigation of Electrolyte–Electrode Interfaces: From Lithium Metal to Sodiated MoS_2

The electrode–electrolyte interface plays a critical role in the performance and stability of rechargeable batteries by governing the early stages of solid electrolyte interphase (SEI) formation. In this work, density functional theory (DFT) is used to investigate the interactions between electrolyte ions and two representative electrode systems: lithium metal and MoS_2 at different degrees of sodiation. Adsorption energies, charge transfer, electron localization, work function, and electronic structure analyses reveal how molecular orientation and electrode state influence interfacial stability and reactivity. Despite the different battery chemistries, both systems exhibit common mechanisms that govern electrolyte decomposition and SEI formation. These findings provide atomistic insights for the rational design of advanced electrolytes and electrode materials.

Primary author(s) : Prof. SELIS VASQUEZ, Luis Antonio (Universidad Nacional de Ingenieria)

Presenter(s) : Prof. SELIS VASQUEZ, Luis Antonio (Universidad Nacional de Ingenieria)

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