

Computational studies of Li adsorption, diffusion and voltage on a candidate anode material SnSe for rechargeable Li-ion batteries

Rechargeable lithium-ion batteries are pivotal in modern portable electronics and renewable energy storage, yet their performance depends critically on the efficiency and stability of electrode materials. Tin selenide (SnSe), which is a layered chalcogenide, has been reported to offer promising electrochemical properties due to its tunable structure and high electronic conductivity. Regardless of the known potential of SnSe, the atomistic and molecular mechanism guiding its role as a good anodic material in a voltaic cell has not been directly probed by experiments yet. This project seeks to investigate Li adsorption, diffusion, and intercalation energetics on SnSe using density functional theory (DFT) to elucidate and evaluate the potential of SnSe as an anode material. The study aims to uncover key atomic-scale insights governing lithium storage and mobility, guiding future design of high-capacity, fast-charging batteries.

In this project, we will determine whether the chosen material(s) can host Li stably, provide reasonable open-circuit voltage, and show low Li diffusion barriers using DFT.

TO DO.

Concrete calculations to perform (with formulas)

1. Bulk structure relaxation
 - Optimize lattice constants and cell (DFT geometry optimization).
 - Outputs: relaxed lattice parameters, total energy E_{bulk}
2. Surface/slab and adsorption calculations
 - Build a low-index slab (e.g., (001) or (100)), relax.
 - Compute Li adsorption energy at the most stable site:
3. Formation energy of lithiated phase
4. Average intercalation voltage
5. Li diffusion/migration barrier (NEB)
6. Density of states (DOS) and charge analysis