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High-Throughput, Multi-Scale Modeling of Bi2Se3 Topological Materials

This talk presents our progress in developing autonomous workflows that generate DFT data and fit both reactive and machine-learned force fields to guide the molecular beam epitaxial synthesis and characterization of the van der Waals–layered topological insulator Bi_2Se_3. I will introduce pyRMG, our Python package for high-throughput real-space multigrid (RMG) DFT calculations on Frontier, and show how it can be used to explore the potential-energy surface and electronic structures of Bi_2Se_3 films with variable twist angles on $NbSe_2$ superconductor substrates. Next, I'll describe our fitting approaches for ReaxFF and ML (MACE) force fields for the Bi-Se system, and how we've applied Bayesian optimization to navigate the complex MD parameter space for targeted synthesis (e.g., recrystallization pathways). Finally, I'll outline future directions for extending these highly-integrated computational methods to other low-dimensional topological materials and compositional systems.

Topical Area

Hard matter: quantum, electronic, semiconducting materials

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