

Quantum Materials Modeling and Electronic Structure Prediction for Varying Mechanical and Chemical Boundary Conditions

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Invited Talk

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In quantum materials research, we have reached a stage where the exotic phenomena once predicted by quantum field theory are being observed in real materials. These developments bring significant expectations on computational materials science to reliably predict physical properties. Density functional theory (DFT) remains the most popular approach to modeling material systems in the computational materials domain. In this presentation, we will provide a comprehensive assessment of various DFT formalisms and their effectiveness in capturing the electronic structure of topological insulators (TIs), a class of quantum materials that has semiconducting properties in the bulk, but the surface develops a unique band structure. Our findings indicate that the generalized gradient approximation (GGA) and kinetic density functional (metaGGA) predict an outward relaxation of TI slabs, whereas the local density approximation (LDA) shows opposite behavior. Including van der Waals (vdW) interactions corrects the over-relaxations of the GGA, aligning the atomic positions closer to experimental findings. Based on a systematic computational study, we demonstrate that GGA with vdW treatment is an appropriate method for structural optimization. We show that mechanical boundary conditions (e.g., biaxial strain) and chemical boundary conditions (e.g., doping) can introduce TI properties in several layered tellurides, such as Bi_2Se_3 , Bi_2Te_3 , As_2Te_3 , ZrTe_5 , and SnTe . These two approaches are independent but can be combined to engineer TI states in high-Z and low-band gap compounds. Additionally, we will also briefly discuss our group's research efforts on optical qubits in 2D semiconductors with point defects.

Keywords: Quantum materials, Topological insulators, Telluride compounds, Qubits, 2D-semiconductors