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Robustness, tunability, and functional properties of topological surface states in topological insulator heterostructures

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The recently discovered quantum materials of topological insulators (TIs), characterized by being insulating in the bulk but with topologically protected surface states (TSS), have been the focus of much current research effort. In particular, how robust such TSS are under diverse physical conditions and their functional properties are of significant fundamental and technological importance. In this talk, I attempt to review some of latest developments surrounding these two aspects of topological insulator heterostructures, as investigated using first-principles calculations within density functional theory and microscopic modeling. We first show how an overlayer of gold on a TI substrate modifies the vertical location of the TSS, and exploit the enhanced catalytic properties of the hybrid system due to the presence and robustness of the TSS. Next, we expand the monolayer systems to include different types of conventional insulators, and demonstrate counterintuitive tunability in the vertical location of the TSS enabled by their inherent robustness. Finally, we further expand the systems to include superconducting/TI interfaces, and reveal the role of the TSS in mediating ferromagnetic ordering of magnetic dopants and related quantum phase transitions associated with time reversal symmetry breaking. Collectively, these findings lay the foundation for precise manipulation of the real-space properties of TSS in various TI heterostructures of diverse technological significance.