Quantum Phase Transitions in Topological Insulator and Graphene Nanoribbon 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 such robust TSS behave under diverse physical conditions is of significant importance. Using first-principles calculations within density functional theory, we have investigated the influence of a monolayer of conventional insulator (CI) of ZnM (M = S, Se, or Te) adsorbed onto a TI substrate of Bi2Se3 or Bi2Te3 on the spatial properties of the TSS [1]. We found the vertical location of the TSS can be accurately tuned to the top of the CI, at the CI/TI interface, or even deeper into the TI. These contrasting behaviors imply a rich variety of possible quantum phase transitions in the hybrid systems, dictated by three key material-specific properties of the CI: the spin-orbit coupling strength, band gap, and work function. To further explore generic nature of the intriguing phenomena in related systems, we have investigated graphene nanoribbon (GNR) heterostructures consisting of topologically trivial and nontrivial GNRs of zigzagged or armchair edges, based on tight binding models. Here the topological phase diagrams can be further enriched by the different boundary types of the .GNRs. Collectively, these findings lay the foundation for precise manipulation of the real-space properties of TSS in various TI heterostructures of diverse technological significance.

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[1] Guangfen Wu, Hua Chen, Yan Sun, Xiaoguang Li, Ping Cui, Cesare Franchini, Jinlan Wang, Xing-Qiu Chen, and Zhenyu Zhang, Precise tuning of the vertical location of helical surface states in topological insulator heterostructures via dual-proximity effects, submitted (2012).
[2] Gufeng Zhang, Jie Wang, Guangfen Wu, Dimi Culcer, Xiaoguang Li, Efthimios Kaxiras, and Zhenyu Zhang, Quantum phase transitions in grapheme nanoribbon topological heterostructures, to be submitted (2012).