Stability of Surface States of Topological Insulators upon Nonmagnetic Adsorption

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Topological insulators (TIs) draw great attention due to their unique quantum properties and various applications. TIs possess metallic surface states within bulk band gaps induced by strong spin-orbit coupling (SOC). TIs allow the surface states to cross Fermi level only an odd number of times for each surface, which was observed in angle-resolved photoemission spectra (ARPES) on Bi-based alloys. Recently, novel phenomena and applications have been proposed for TIs interfaced with other types of materials such as magnetic or superconducting materials. Here we present a systematic study of interface-induced effects in TIs Bi_2Te_3 and Bi_2Se_3, using density-functional theory including SOC self-consistently. Surface states are identified using the method discussed in Ref. [1].

Interfaces are simulated by Si adsorption only on top of Bi_2Te_3 and Bi_2Se_3 slabs. Even with nonmagnetic adsorption, dispersion of the top surface states is qualitatively affected by momentum-dependent coupling to bulk-like states, Si-dominated states, or Rashba-split quantum-well states, which depends on adsorption sites and topological insulator types. Our findings provide insight into engineering new heterostructures using interfaces for devices or discovering new phenomena.

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