

Abstract Submitted
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Interface-driven magnetism in topological insulators Bi₂Te₃ and Bi₂Se₃¹ KYUNGWHA PARK, Virginia Tech, Blacksburg, VA 24061 — Topological insulators (TIs) draw great attention due to their unique quantum properties and applications. TIs possess metallic surface states within band gaps induced by spin-orbit coupling (SOC), and they allow only an odd number of Dirac cones in dispersion of the surface states at a given surface. Novel physical phenomena and applications proposed including TIs, critically rely on stability and topological nature of the surface states when TIs are interfaced with other types of materials. Despite many studies on TIs, it still remains unclear how the surface states of TIs behave in contact with other materials. In this talk, we present our study of an effect of interfaces on the surface states of TIs Bi₂Te₃ and Bi₂Se₃, using density-functional theory including SOC self-consistently. We simulate interfaces using adsorption layers on TI films in an asymmetric fashion. We discuss unexpected results on stability and topological nature of the surface states, as well as changes in their spin structure and energy gaps at zero momentum. Our findings reveal importance of interfaces and a possibility of engineering new hybrid TI structures using adsorption layers.

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Kyungwha Park
Virginia Tech, Blacksburg, VA 24061

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