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First-principles study of surface states of topological insulators[1]
KYUNGWHA PARK, Virginia Tech — Recently, three-dimensional topological insulators (TIs) with time reversal symmetry draw attention due to their unique quantum properties and device applications. Strong spin-orbit coupling in TIs induces metallic surface states within bulk band gaps. It has been known that Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 are TIs possessing a single Dirac cone in the dispersion of the surface states at a given surface. The surface states of TIs play a critical role in proposed novel physical phenomena and applications. We investigate the surface states of thin films of $Bi_2Te_3(111)$ and $Bi_2Se_3(111)$ using density-functional theory including spin-orbit coupling. We identify the surface states of the TI films from calculated band structures using the decay length of the surface states and electron density plots. We also present the electronic properties of the surface states of the films.

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