

Abstract Submitted
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Quasiparticle electronic structure of bulk and slab Bi_2Se_3 and Bi_2Te_3 ¹ BRADFORD BARKER, University of California-Berkeley, Lawrence Berkeley National Laboratory, JACK DESLIPPE, Lawrence Berkeley National Laboratory, OLEG YAZYEV, University of California-Berkeley, Ecole Polytechnique Federale de Lausanne (EPFL), STEVEN G. LOUIE, University of California-Berkeley, Lawrence Berkeley National Laboratory — We present ab initio calculations of the quasiparticle electronic band structure of three-dimensional topological insulator materials Bi_2Se_3 and Bi_2Te_3 . The mean-field DFT calculation is performed with fully relativistic pseudopotentials, generating spinor wavefunctions in a plane-wave basis. Quasiparticle properties are computed with a one-shot ab initio GW calculation. We use both bulk and slab forms of the materials to better understand the quasiparticle band gaps and Fermi velocities of the topological surface states of these materials.

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