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Quasiparticle electronic structure of Bi_2Se_3 via the sc-COHSEX+GW approach[1] BRADFORD A. BARKER, University of California-Berkeley and Lawrence Berkeley National Laboratory, JACK DESLIPPE, Lawrence Berkeley National Laboratory, OLEG YAZYEV, University of California-Berkeley and Ecole Polytechnique Federale de Lausanne (EPFL), STEVEN G. LOUIE, University of California-Berkeley and Lawrence Berkeley National Laboratory — We present ab initio calculations of the quasiparticle electronic band structure of three-dimensional topological insulator material Bi_2Se_3 using the full spinor GW approach. The mean-field is initially computed at the DFT level in the local density approximation (LDA) using fully-relativistic pseudopotentials. We then improve the mean-field electronic structure by solving Dyson's equation in the static COHSEX approximation, self-consistently updating the eigenvalues, eigenvectors, and dielectric screening. After a few iterations, we then perform a GW calculation to determine the quasiparticle energies. We compare our calculated results to experimental values of the band gaps and effective masses.

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