Quasiparticle electronic structure of Bi$_2$Se$_3$ 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$_2$Se$_3$ 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.

$^1$This work was supported by NSF grant No. DMR15-1508412 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at LBNLs NERSC facility and the NSF through XSEDE resources at NICS.