Abstract Submitted
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Quasiparticle effects in the bulk and surface-state bands of Bi_2Se_3 and Bi_2Te_3 topological insulators[1] OLEG V. YAZYEV, UC Berkeley/LBNL/EPFL, EMMANOUIL KIOUPAKIS, U of Michigan, JOEL E. MOORE, STEVEN G. LOUIE, UC Berkeley/LBNL — We investigate the bulk band structures and the surface states of Bi_2Se_3 and Bi_2Te_3 topological insulators using first-principles many-body perturbation theory based on the GW approximation. The quasiparticle self-energy corrections introduce significant changes to the bulk band structures, surprisingly leading to a decrease in the direct band gaps in the band-inversion regime as opposed to the usual situation without band inversion. Parametrized "scissors operators" derived from the bulk studies are then used to investigate the electronic structure of slab models which exhibit topologically protected surface states. The introduction of self-energy corrections results in significant shifts of the surface-state Dirac point energies relative to the bulk bands and in enlarged gap openings from the interactions between the surface states across the thin slab, both in agreement with experimental data.

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