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Electronic structure from relativistic quasiparticle self-consistent *GW* calculations[1]

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Most theoretical studies of topological insulators (TIs) are based on tight-binding descriptions and density functional theory (DFT). But recently, many-body calculations within the *GW* approximation attract much attention in the study of these materials. We present an implementation of the quasiparticle self-consistent (QS) *GW* method where the spin-orbit coupling (SOC) is fully taken into account in each iteration rather than added a posteriori. Within the all-electron FLAPW formalism, we show DFT, one-shot *GW*, and QS*GW* calculations for several, well-known TIs. We present a comparison of the calculations to photoemission spectroscopy and show that the *GW* corrected bands agree much better with experiment. For example, we show that Bi_2Se_3 [1,2] is a direct gap semiconductor, in contrast to what was believed for many years by interpreting experimental results on the basis of DFT and that small strains in Bi can lead to a semimetal-to-semiconductor or trivial-to-topological transitions [3]. Quasiparticle calculations for low-dimensional systems are still very demanding. In order to study the topological surface states with an approach based on *GW*, we use Wannier functions to construct a Hamiltonian that reproduces the many-body band structure of the bulk, and that is used to construct a slab Hamiltonian. With this approach, we discuss the effect of quasiparticle corrections on the surface states of TIs and on the interaction between bulk and surface states. [1] I. Aguilera *et al.*, PRB **88**, 045206 (2013), *ibid.*, PRB **88**, 165136 (2013). [2] M. Michiardi *et al.*, PRB **90**, 075105 (2014). [3] I. Aguilera *et al.*, PRB **91**, 125129 (2015).

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