Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Surfaces and interfaces of topological insulators from relativistic many-body calculations[1] IRENE AGUILERA, CHRISTOPH FRIEDRICH, STEFAN BLUGEL, Peter Gruenberg Institute and Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — We introduce the *GW* and QS*GW* methods where the spin-orbit coupling is incorporated directly into the self-energy. This is critical to obtain reliable results for topological insulators (TIs) [1]. Within the all-electron FLAPW formalism, we show calculations for Bi [2] and TIs of the Bi_2Se_3 family [3]. Comparison to photoemission spectroscopies [4,5] shows that the many-body bulk and surface electronic structures agree much better to experiments than the ones from density functional theory (DFT). For example, we show that Bi_2Se_3 is a direct gap semiconductor [5], in contrast to predictions by DFT. For the description of surfaces of TIs as well as interfaces between TIs and between a TI and a trivial material, we use a basis of Wannier functions to construct slab Hamiltonians. This approach allows us to study very large systems with a high accuracy. [1] Aguilera *et al.*, Phys. Rev. B **88**, 165136 (2013). [2] Aguilera *et al.*, Phys. Rev. B **91**, 125129 (2015). [3] Aguilera *et al.*, Phys. Rev. B **88**, 045206 (2013). [4] Michiardi *et al.*, Phys. Rev. B **90**, 075105 (2014). [5] Nechaev *et al.*, Phys. Rev. B **87**, 121111(R) (2013). Correspondence: i.aguilera@fz-juelich.de

[1]Financial support from the Virtual Institute for Topological Insulators of the Helmholtz Association.

Peter Gruenberg Institute and Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 5242

Date submitted: 09 Nov 2016 Electronic form version 1.4