Surfaces and interfaces of topological insulators from relativistic many-body calculations\textsuperscript{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 $QSGW$ methods where the spin-orbit coupling is incorporated directly into the self-energy. This is critical to obtain reliable results for topological insulators (TIs) \cite{1}. Within the all-electron FLAPW formalism, we show calculations for Bi \cite{2} and TIs of the Bi$_2$Se$_3$ family \cite{3}. Comparison to photoemission spectroscopy \cite{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$_2$Se$_3$ is a direct gap semiconductor \cite{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. \cite{1} Aguilera et al., Phys. Rev. B 88, 165136 (2013). \cite{2} Aguilera et al., Phys. Rev. B 91, 125129 (2015). \cite{3} Aguilera et al., Phys. Rev. B 88, 045206 (2013). \cite{4} Michiardi et al., Phys. Rev. B 90, 075105 (2014). \cite{5} Nechaev et al., Phys. Rev. B 87, 121111(R) (2013). Correspondence: i.aguilera@fz-juelich.de

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