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Spin polarization and transport of surface states in the topological insulators Bi_2Se_3 and Bi_2Te_3 from first principles[1] OLEG YAZYEV, JOEL MOORE, STEVEN LOUIE, UC Berkeley and LBNL — We investigate the band dispersion and the spin texture of topologically protected surface states in the reference bulk topological insulators Bi_2Se_3 and Bi_2Te_3 by using a first-principles approach. Exceptionally strong spin-orbit interaction in these materials entangles the electronic states across broad energy ranges thus reducing the spin-polarization of the topologically protected surface states to $\sim$50% in both cases. This reduction is absent in simple phenomenological models but of important implications to essentially any application of bulk topological insulators in spintronics and likely to some other phenomena. We further propose a way of controlling the magnitude of spin polarization associated with a charge current in thin films of topological insulators by means of an external electric field. The proposed dual-gate device configuration provides new possibilities for electrical control of spin.

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