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Electronic structure and magnetocrystalline anisotropy of the Bi_2Se_3 topological insulator/ferromagnet interface JIA ZHANG, Physics and Astronomy, University of Nebraska, Lincoln, Nebraska 68588, USA, JULIAN P. VELEV, Department of Physics, University of Puerto Rico, San Juan, Puerto Rico 00931, USA, EVGENY Y. TSYMBAL, Physics and Astronomy, University of Nebraska, Lincoln — Interesting spin-dependent phenomena are expected to emerge when a topological insulator is interfaced with a magnetic material. In this work the magnetic properties of the interface between a topological insulator Bi_2Se_3 and ferromagnetic metals (FM) fcc (111) Ni and Co are investigated by first-principles calculations. Different interface terminations are considered, and the most stable interface termination is identified to be an interface Ni (Co) atom located atop the hollow site of the interfacial Se monolayer. We find that the proximity effect induces a small magnetic moment on the interface Se atom (0.028 μ_B for Ni and 0.023 μ_B for Co). The surface state in Bi_2Se_3 disappears due to the strong interface hybridization between FM and Bi_2Se_3 and metal induced gap states appear in the bandgap region of Bi_2Se_3. We find that both the Bi_2Se_3/Ni(111) and Bi_2Se_3/Co(111) interfaces exhibit an in-plane easy axis with the magnetic anisotropy energy of around 2 erg/cm^2 per interface. An interesting feature resulting from our calculations is a non-collinear k-dependent spin texture at the interface which may have important consequences for the spin-dependent transport properties, such as the spin transfer torque.

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