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Complex Band Structure of the Topological Insulator Bi_2Se_3 SHIJIE LI, Univ of Nebraska - Lincoln, JESUAN BETANCOURT, University of Puerto Rico, J.D. BURTON, Univ of Nebraska - Lincoln, JULIAN P. VELEV, University of Puerto Rico, EVGENY Y. TSYMBAL, Univ of Nebraska - Lincoln — Recently there is a surge of interest in using topological insulators for electronic and spintronic applications. For applications it is important to understand the complex band structure (CBS) of the topological insulator, which determines the decay rate of the protected surface states into the bulk of the material. The Bi_2Se_3 family of three-dimensional topological insulators is the most studied and best understood. In this work we investigate the CBS of Bi_2Se_3 using first-principles density-functional calculations. We determine the decay rates and the symmetry of the evanescent states and we follow their evolution from those of the band insulator. We complement these results with Bi_2Se_3 (0001) slab calculations to explore the penetration depth, oscillatory behavior and spin texture of the surface states. The CBS provides a new insight into the topologically protected states and could be used for the search of new topological insulators and device concepts.

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