Structural and Electronic Structure of the Topological Insulator Bi_2Te_3 and Bi_2Se_3 from Density-functional Study

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Bismuth telluride (Bi_2Te_3) and bismuth selenide (Bi_2Te_3) compounds attract much attention recently as atopological insulator. By means of thedensity-functional theory based on general gradient approximation, we studied the structural and electronic properties of Bi_2Te_3 and Bi_2Se_3. Being consistent with experiments, the total energy calculations showed that the optimized lattice parameters a and c of the hexagonal unit cell are 4.44 and 32.20 Å for Bi_2Te_3, those of Bi_2Se_3 are 4.18 and 31.50 Å. Bulk band gaps of 0.09 eV for Bi_2Te_3 and 0.3 eV for Bi_2Se_3 are calculated in consistent withexperimental values. To elucidate thenature of topological insulator, we have taken into account the surface states with spin-orbit coupling interaction. Te(Se)-termination with Bi-subsurface is found to be most stable, where a metallic state is realized in contrast to its insulating in bulk.