Abstract Submitted
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Room Temperature Quantum Spin Hall Insulators with a Buckled Square Lattice WEI LUO, HONGJUN XIANG, None — Two-dimensional (2D) topological insulators (TIs), are excellent candidates for coherent spin transport related applications Currently, most known 2D TIs are based on a hexagonal lattice. Here, we propose that there exists the quantum spin Hall effect (QSHE) in a new tight-binding (TB) model for a two-orbital system with the buckled square lattices. We show that the band inversion is due to the hybridization between the$p_x$and$p_y$orbitals, while the spin-orbit coupling (SOC) induced nearest-neighbor effective hopping is responsible for a band gap opening at the Dirac cone. Through performing global structure optimization, we predict a new three-layer quasi-2D (Q2D) structure which has the lowest energy among all structures with the thickness less than 6.0 for the BiF system. It is identified to be a Q2D TI with a large band gap (0.69 eV). The electronic states of the Q2D BiF system near the Fermi level are mainly contributed by the middle Bi square lattice, which are sandwiched by two inert BiF_2 layers. This is beneficial since the interaction between a substrate and the Q2D material may not change the topological properties of the system, as we demonstrate in the case of the NaF substrate. Our analysis shows that the low-energy physics of the Q2D BiF system can be qualitatively described by our newly proposed two-orbital TB model. Our study not only predicts a Q2D QSH insulator for realistic room temperature (RT) applications, but also provides a new lattice system for engineering topological states such as quantum anomalous Hall effect.

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