

Abstract Submitted
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Temperature dependence of the pressure-induced topological phase transition in BiTeI VÉRONIQUE BROUSSEAU-COUTURE, MICHEL CÔTÉ, Univ of Montreal — Tunable topological insulators are materials in which the band inversion can be turned on and off through an experimentally controllable parameter. Understanding the effect of temperature on these phase transitions becomes crucial for real devices intended to work in various conditions. This temperature dependence is directly related to the electron-phonon interactions, which induce a shift in the electronic band energies that may promote or suppress the topologically non-trivial phase. We investigate the temperature dependence of the pressure-induced topological phase transition in three-dimensional crystalline topological insulator BiTeI through first principles methods. We compute the electron-phonon coupling and the electronic bandstructure using density functional perturbation theory (DFPT).

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