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Influence of the electron-phonon interaction on the topological phase transition in BiTeI

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The study of topological materials and their symmetry protected states has proven to be one of the most thriving fields of condensed matter physics of the last two decades, from both theoretical and applied point of views. Tunable topological phase transitions (TPT) have been identified in several materials, in which the variation of an external, experimentally controllable parameter can drive the system from a trivial to a topological insulating state. These phase transitions are intrinsically related to the bulk electronic structure and can be detected by tracking the variation of the bulk electronic band gap, which must vanish at the critical parameter.

However, like all other electronic properties of materials, the band gap is affected by the atomic motion through electron-phonon interaction, even at absolute zero temperature. As a consequence, this phonon-induced shift in the electronic eigenenergies can either promote or suppress the topologically non-trivial phase. Thus, when studying tunable topological phase transitions in real materials, the value of the critical parameter will be modified by finite temperature.

In this work, the temperature dependence of the pressure-induced TPT in Rashba semiconductor BiTeI is investigated through first-principles methods. A peculiarity of this material is that the lack of inversion symmetry imposes the existence of an intermediate Weyl semimetal (WSM) phase, resulting in two distinct gap-closing critical pressures that can be distinctly affected by temperature. I will first present an overview of electron-phonon interaction within the framework of density functional perturbation theory (DFPT). Then, by tracking both the pressure and temperature dependence of the bulk band gap, I will show how the WSM and topological insulator phases of BiTeI evolve with temperature, thus providing a guideline for experimental detection.

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