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Temperature effects in spin-orbit physics from first principles

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The spin-orbit interaction drives a number of physical phenomena, including the spin splitting of electronic bands and the band inversion in topological insulators. In this work, we study the effects of finite temperature on such spin-orbit physics, including both thermal expansion and electron-phonon coupling effects [1].

First, we describe the temperature dependence of the inverted gap in topological insulators. We find that increasing temperature reduces the topological gap in the Bi_2Se_3 family of materials, and we predict a temperature-induced topological phase transition in Sb_2Se_3 [2].

Second, we study the temperature dependence of the Rashba split bands in the bulk bismuth tellurohalides, and we find that increasing temperature suppresses the Rashba splitting. We also show that in the topological insulating phase of BiTeI, which is stabilized under pressure, the temperature dependence of the Rashba split bands is opposite to that of the normal state, suggesting a novel signature for the experimental determination of pressure-induced topological phase transitions.

[1] J.H. Lloyd-Williams and B. Monserrat, Phys. Rev. B **92**, 184301 (2015).

[2] B. Monserrat and D. Vanderbilt, Phys. Rev. Lett. **117**, 226801 (2016).