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Six-nearest-neighbor parameterized Slater-Koster tight-binding model for Bi

We report a six-neighbor Slater-Koster tight-binding model[1], with spin-orbit coupling included, to treat the electronic and topological properties of Bi crystals. We contrast two distinct parameter sets showing seemingly same electronic energy bands with different Z2 index of bulk Bi. The parameter set which shows trivial Z2 index (v=[0;0,0,0]) for Bulk Bi and nontrivial Z2 index (v=1) for few layer Bi reproduces semi metallic properties of bulk Bi and its topologically trivial surface states, while semiconducting nature of few layer Bi films and their topologically non-trivial edge states. This highlights that the topological index or parameter needs to be treated carefully for proper parameterization of first-principles energy bands of topological materials.

References

1. J. C. Slater and G. F. Koster, Phys. Rev., 94 (1954) 1498.

Figures

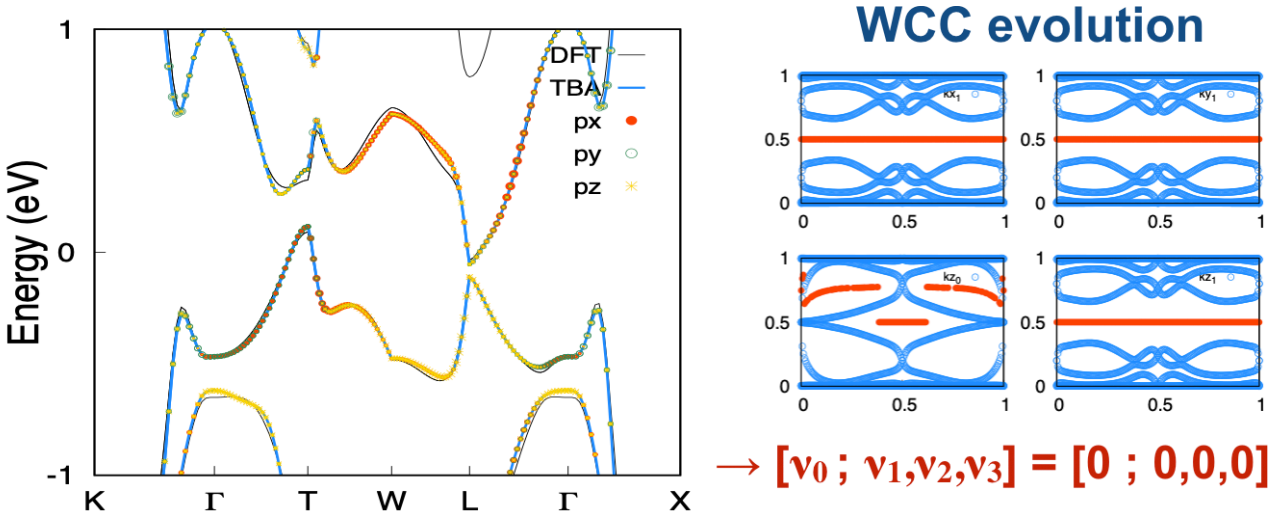

Figure 1: (Left pannel) Comparison of calculated band structure from density functional theory with rev-vdW-DF2 method (black solid line) and present tight-binding model with Z2=0. (Right pannel) The Wannier charge center (WCC) evolution.