

Abstract Submitted
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Accurate Tight-Binding Hamiltonians : Topological Insulators

MARCIO COSTA, Universidade Federal do ABC, ROBERTO BECHARA, Universidade Federal Fluminense, MARCO NARDELLI, North Texas University, ADALBERTO FAZZIO, Universidade Federal do ABC — In this work we report results of transport calculations for Topological Insulators using the recently developed pseudoatomic orbital projection technique(1-2). We construct a tight-binding Hamiltonian extract from an first-principles calculation. The Spin-Orbit effect is considered in two different forms. Direct from a DFT calculation, which involves a non collinear, and computational demanding, calculation. A more efficient approach, with comparable accuracy, is to introduce the SOC in a scalar relativistic tight-binding Hamiltonian using first order perturbation theory. We applied this methodology for 2D and 3D Topological Insulators. [1]- Phys. Rev. B 94, 165166 (2016). [2]- Phys. Rev. B 88, 165127 (2013).

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