Correlated Topological Insulators with Mixed Valence

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Abstract

We propose the LDA+Gutzwiller method incorporating green's function scheme to study the topological physics of correlated materials from the First-principles. Applying this method to typical mixed valence materials SmB6, we found its non-trivial Z2 topology, indicating that SmB6 is a strongly correlated topological insulator (TI). The unique feature of this compound is that its surface states contain three Dirac cones in contrast to most known TIs.