Topological Crystalline Kondo Insulator in Mixed Valence Ytterbium Borides

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The electronic structures of two mixed valence insulators YbB6 and YbB12 are studied by using the local density approximation (LDA) supplemented with the Gutzwiller and DMFT (dynamic mean field theory) methods. We find that YbB6 is a moderately correlated Z2 topological insulator, similar to and with bulk band gap much larger than SmB6; while YbB12 is a strongly correlated topological crystalline Kondo insulator, which can be characterized by its non-zero mirror Chern number (although its Z2 invariant is trivially zero). The surface calculations find odd (three) and even (four) number of Dirac cones for YbB6 and YbB12, respectively.