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Filling-Enforced Quantum Band Insulators in Spin-Orbit Coupled Crystals HOI CHUN PO, University of California, Berkeley, HARUKI WATANABE, Massachusetts Institute of Technology, MICHAEL P. ZALETEL, Station Q, Microsoft Research, Santa Barbara, ASHVIN VISHWANATH, University of California, Berkeley; Materials Science Division, Lawrence Berkeley National Laboratories, Berkeley — While band insulators are usually described in wavevector space in terms of fully filled bands, they are sometimes also described in terms of a complementary Wannier picture in which electrons occupy localized, atom-like orbitals. Under what conditions does the latter picture break down? The presence of irremovable quantum entanglement between different sites can obstruct a localized orbital description, which occurs in systems like Chern and topological insulators. We collectively refer to such states as Quantum Band Insulators (QBIs). Here we report the theoretical discovery of a filling-enforced QBI - that is, a free electron insulator in which the band filling is smaller than the minimum number dictated by the atomic picture. Consequently such insulators have no representation in terms of filling localized orbitals and must be QBIs. This is shown to occur in models of certain cubic crystals with non-symmorphic space groups. Like topological insulators, filling-enforced QBIs require spin-orbit coupling. However, in contrast, they do not typically exhibit protected surface states. Instead their nontrivial nature is revealed by studying the quantum entanglement of their ground state wavefunction.

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