

Stuttgarter Max-Planck-Institute, Heisenbergstraße 1, 70569 Stuttgart-Büsnau

The role of crystalline symmetries in topological materials

Maia G. Vergniory

Max Planck Institute for the Chemical Physics of Solids, Dresden

Abstract

Since the theoretical proposal of the first 2D and 3D topological insulators (TIs) more than 15 years ago, solid-state realizations of topological materials have been discovered at a rapid pace. The recently developed theories of Topological Quantum Chemistry and Symmetry-Based Indicators (SIs), based on symmetry eigenvalues and irreducible representations have in particular facilitated high-throughput materials discovery and revealed that topological phases in band structures are more common than originally thought. Indeed, over half of all of the known stoichiometric, solid-state, nonmagnetic materials are topological at the Fermi level, over 85% of the known stoichiometric materials host energetically isolated topological bands, and that just under 2/3 of the energetically isolated bands in known materials discovery in nonmagnetic and magnetic crystalline solids from the prediction based on TQC. We will also show that for a subset of the topologically trivial insulators, knowing only their electron number and the Wyckoff positions of the atoms we can separate them into two groups: the obstructed atomic insulator (OAI) and the atomic insulator (AI). The interesting group, the OAI, have a center of charge not localized on the atoms and therefor, surface states can be displayed at certain surfaces.