Prediction of topological bands from lattices

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Abstract

During this talk, I will examine topological metals and insulators stabilized by any of the 230 crystal symmetry groups. By defining the concept of elementary band representations of the double group augmented by time reversal, we can predict how many bands are connected in momentum space based on the lattice positions (Wyckoff multiplicities) and character (s,p,d) of the elements/orbitals existent in the material. This allows for the prediction of symmetry-enforced semimetals whenever the valence number of electrons that occupies the orbitals is a fraction of the band connectivity. Our theory also provides a set of rules of how bands can be connected in momentum space when the centre of charge is not at a Wyckoff position or when it does not respect local time reversal or spatial symmetries. In this sense we are able to predict new topological insulators (time reversal, crystalline, non-symmorphic). A set of new family of materials and its properties will be presented as well, some of them were reported trivial in the past.

References:
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