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Universal framework for identifying topological materials and its numerical implementation in Z2Pack software package DOMINIK GRESCH, MATTHIAS TROYER, ALEXEY SOLUYANOV, ETH Zurich, GABRIEL AUTES, OLEG YAZYEV, EPFL, ANDREI BERNEVIG, Princeton University, DAVID VANDERBILT, Rutgers University — Band structure topology has drastic effects on many observable phenomena in solids, and thus is a fundamental characteristic of a material. We present general framework for identifying various topologies of band structures and introduce a public software package –Z2Pack – for computing the associated topological invariants. Z2Pack works with first-principles calculations, tight-binding and k.p models. It can be used to identify both topological insulators and semimetals.

Dominik Gresch ETH Zurich

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