Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Topological Quantum Chemistry II: Predicting topological materials in layered systems JENNIFER CANO, BARRY BRADLYN, ZHIJUN WANG, Princeton University, M. G. VERGNIORY, Donostia International Physics Center and University of the Basque Country, LUIS ELCORO, M. I. AROYO, University of the Basque Country, CLAUDIA FELSER, Max Planck Institute for the Chemical Physics of Solids, B. ANDREI BERNEVIG, Princeton University — We continue to develop a theory that describes the connectivity of a band structure based on the real space positions of atoms in the material and their relevant orbitals. We develop criteria to determine when a topological band structure is possible and identify several promising crystal structures to search for topological (or topological crystalline) materials. We then apply this result to layered systems, i.e., stacked layers of hexagonal (graphene) or square lattices and generalizations and show which orbitals need to be at the Fermi level to yield a topological insulator. Using this information, we predict candidate topological materials.

Jennifer Cano
Princeton

Date submitted: 11 Nov 2016 Electronic form version 1.4