Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Topological quantum chemistry I: Global band topology and topological phases BARRY BRADLYN, JENNIFER CANO, Princeton Center for Theoretical Science, ZHIJUN WANG, Princeton University, MAIA VERGNIORY[1], LUIS ELCORO, MOIS AROYO, University of the Basque Country, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, B. ANDREI BERNEVIG, Princeton University — For the past century, chemists and physicists have advocated fundamentally complementary perspectives on materials: while chemists have adopted a "local" viewpoint, through the theory of chemical bonding and hybridization, physicists have thought about materials predominantly through band-structures in a nonlocal, momentum-space picture. The contrast between these two descriptions has been highlighted by the advent of topological insulators, the understanding of which overwhelmingly used the momentum-space picture. In this talk, I will present our method for unifying these two descriptions. By exploiting the constraints of symmetry on the relation between Bloch and Wannier functions, I will show how simple chemical input can be used to constrain the global band topology for materials in all 230 space groups. From this I will derive a predictive classification of topological insulators and semimetals.

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Date submitted: 11 Nov 2016 Electronic form version 1.4