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Ab Initio Studies of the Tunability of Topological Phases of Complex Materials RU CHEN, University of California, Berkeley and Lawrence Berkeley National Lab, ASHVIN VISHWANATH, University of California, Berkeley, JEFFREY NEATON, University of California, Berkeley and Lawrence Berkeley National Lab — Recently, there have been intensive studies of new existing and hypothetical, as-yet-unsynthesized materials with topological phases. Using density functional theory-based approaches, we perform detailed calculations on several promising candidate compounds, including Bi- and Cd- based Dirac and Weyl semimetals and oxide topological insultaors, that are predicted to exhibit topological or near-topological states. We compute surface states of candidate materials such as Dirac semimetals Na3Bi and Cd3As2 along various surfaces. For systems with strong correlations, we examine the efficacy of DFT-based hybrid functionals and the GW approximation for accurate prediction of band inversion. For a selection of systems, we also explore quantitatively the tunability of topological phases via hydrostatic pressure, biaxial strain, broken crystal symmetry, or doping.

Ru Chen
University of California, Berkeley and Lawrence Berkeley National Lab

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