Dirac line nodes in centrosymmetric crystals. YOUNGKUK KIM, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, BENJAMIN J. WIEDER, CHARLES KANE, Department of Physics and Astronomy, University of Pennsylvania, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — Dirac line nodes (DLNs) are one–dimensional nodal lines of electronic energy bands with linear dispersion away from the line nodes. We propose new Z_2 topological characterization of semimetals hosting bulk DLNs, protected by inversion and time–reversal symmetries with vanishing spin–orbit interaction. aZ_2 topological invariants are introduced based on parity eigenvalues at the parity–invariant points in reciprocal space, dictating the presence of bulk DLNs and two-dimensional (2D) nearly-flat surface states. Using first-principles calculations, we predict that DLNs occur in Cu_3N near the Fermi energy when doped by transition metal atoms, such as Zn and Pd. The 2D surface states are demonstrated to emerge in the projected interior of the DLNs, and the effects of spin–orbit interactions and symmetry-breaking are briefly discussed.

Youngkuk Kim
Univ of Pennsylvania