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Topological Dirac line nodes in centrosymmetric semimetals YOUNGKUK KIM, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, USA , BENJAMIN WIEDER, CHARLES KANE, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6396, USA, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, USA , TI SEED TEAM — Dirac line nodes (DLNs) are one-dimensional lines of Dirac band-touching points, characterized by linear dispersion in only a single direction in momentum space. In the presence of inversion symmetry and time-reversal symmetry, crystals with vanishing spin-orbit coupling can host topologically protected DLNs. Recently, we have proposed and characterized a novel Z2 class of DLN semimetals [1]. We present Z2 topological invariants, dictating the presence of DLNs, based on the parity eigenvalues at the time-reversal invariant crystal momenta. Our first-principles calculations show that DLNs can be realized in Cu3N in an anti-ReO3 structure via a metal-insulator electronic transition, driven by transition metal doping. We also discuss the resultant surface states and the effects of spin-orbit coupling.

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