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Data Mining for 3D Organic Dirac Materials[1] R. MATTHIAS GEILHUFE, STANISLAV S. BORYSOV, Nordita, KTH Royal Institute of Technology and Stockholm University, Sweden, ADRIEN BOUHON, Department of Physics and Astronomy, Uppsala University, Sweden, ALEXANDER V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory, USA; Nordita, KTH Royal Institute of Technology and Stockholm University, Sweden — The study of Dirac materials, i.e. materials where the low-energy fermionic excitations behave as massless Dirac particles has been of ongoing interest for more than two decades. Such massless Dirac fermions are characterized by a linear dispersion relation with respect to the particle momentum. A combined study using group theory and data mining within the Organic Materials Database leads to the discovery of stable Dirac-point nodes and Dirac line-nodes within the electronic band structure in the class of 3-dimensional organic crystals. The nodes are protected by crystalline symmetry. As a result of this study, we present band structure calculations and symmetry analysis for previously synthesized organic materials. In all these materials, the Dirac nodes are well separated within the energy and located near the Fermi surface, which opens up a possibility for their direct experimental observation.

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