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A Case Study Of Organic Dirac Materials – BENJAMIN COMMEAU, University of Connecticut, Storrs, CT, MATTHIAS GEILHUFE, Nordita, Center for Quantum Materials, KTH Royal Institute of Technology and Stockholm University, Stockholm, Sweden, GAYANATH FERNANDO, University of Connecticut, Storrs, CT, ALEXANDER BALATSKY, Nordita, Center for Quantum Materials, KTH Royal Institute of Technology and Stockholm University, Stockholm, Sweden — Dirac Materials are characterized by linear band crossings within the electronic band structure. Most research of Dirac materials has been dedicated towards inorganic materials, e.g., binary chalcogenides as toplogical insulators, the Weyl semimetal TaAs or graphene. The purpose of this study is to investigate the formation of Dirac points in organic materials under pressure and mechanical strain. We study multiple structural phases of the organic charge-transfer salt (BEDT-TTF)2I3. We numerically calculate the relaxed band structure near the Fermi level along different k-space directions. Once the relaxed ion structure is obtained, we pick different cell parameters to shrink and investigate the changes in the band structure. We discuss band structure degeneracies protected by crystalline and other symmetries, if any. Quantum Espresso and VASP codes were used to calculate and validate our results.

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