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First-Principles Study on Dirac Cones in a Single-Component Molecular
Crystal Under High Pressure TAKAO TSUMURAYA, RIKEN/NIMS, HENG-BO CUI, RIKEN, HIORI KINO, NIMS-MANA, TSUYOSHI MIYAZAKI, NIMS, REIZO KATO, RIKEN — Most single-component molecular crystals show insulating or semiconducting properties at ambient pressure. Recently, metal dithiolene complexes have attracted much attention ever since a metallic state was realized in $Ni(tmdt)_2$ at ambient pressure. Even if the system is insulating at ambient pressure, it possibly turns into a metallic or superconducting state by application of pressure. In this study, we have found anisotropic linear (tilted Dirac cone) dispersions near the Fermi level in a single-component molecular crystal, $Pd(dddt)_2$ at 8 GPa by first-principles density functional theory calculations. Recent electrical resistivity at 12.6 GPa shows temperature independent behavior as is observed in the massless Dirac fermion system, α-$(BEDT\text{-}TTF)_2I_3$. Our analysis of the electronic structure indicates that the band structure at ambient pressure has quasi-one-dimensional character, which corresponds to the stacking of $Pd(dddt)_2$ molecules along the b-axis, and the dimensionality of the band structure near the Fermi level is changed under the pressure of 8 GPa, where intermolecular hybridization increases due to the reduced intermolecular distances. We also discuss anisotropy of the Dirac cones and their possible origin in the multi-orbital system.

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