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First-Principles Study of Electronic Structure in α-(BEDT-TTF)$_2$I$_3$ at Ambient Pressure and under Uniaxial Strains.[1] HIORI KINO, National Institute for Materials Science, TSUYOSHI MIYAZAKI — We calculate the electronic structure of α-(BEDT-TTF)$_2$I$_3$ at 8K and room temperature at ambient pressure and under the uniaxial strains along the a- and a-axes within the density functional theory. We discover *anisotropic Dirac cone dispersion* near the chemical potential. We also extract the orthogonal tight binding parameters to analyze physical properties. An investigation of the electronic structure near the chemical potential clarify that effects of the uniaxial strain along the a-axis is different from that along the b-axis. The Dirac cone dispersion yields the linear density of states to give T^2 dependence of the carrier density upto about 100K. It may explain the experimental findings not only qualitatively but also quantitatively.

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Hiori Kino
National Institute for Materials Science

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