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First-principles study of the pressure effects on (BEDT-TTF)2XCl2 (X= I or Au) TSUYOSHI MIYAZAKI, HIORI KINO, National Institute for Materials Science (JAPAN) — We have calculated the lattice parameters, internal coordinates, and electronic structures of (BEDT-TTF)$_2X$Cl$_2$ (X = I or Au) using the density functional theory within the generalized gradient approximation (GGA). Although these two salts both show non-metallic behaviors at ambient pressure, their transport properties at high pressures are completely different. ICl$_2$ salt shows nonmetal-metal and superconducting transitions under the pressure around 8 GPa, while the AuCl$_2$ salt keeps its non-metallic behavior even when the pressure of 10 GPa is applied. We first show that the calculated structures at ambient pressure agree well with the experimental ones for both materials, implying that GGA is reliable for the theoretical determinations of the crystal structure. Then we report that the inter-molecule interactions exhibit various and complex pressure dependence, contrary to the simple suggestions made so far. Although we cannot find sensible differences in the pressure effects on the crystal structures, we have found that the pressure dependence of their band structures is qualitatively different between these two salts. We will show the dimensional change of Fermi surfaces, increase of the band width, and the pressure dependence of TB parameters which reproduces our present DFT results.

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