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Electronic structure of a dual-layered organic charge transfer salt HARALD JESCHKE, MICHAELA ALTMEYER, ROSER VALENTI, Goethe-Universitaet Frankfurt — We examine the electronic properties of polymorphs of (BEDT-TTF)₂Ag(CF₃)₄(TCE) (1,1,2-trichloroethane) within density functional theory (DFT). While a phase with low superconducting transition temperature $T_c = 2.6$ K exhibits a κ packing motif, two high T_c phases are layered structures consisting of α' and κ packed layers. We determine the electronic structures and discuss the influence of the insulating α' layer on the conducting κ layer. We find that the stripes of high and low charge in the α' layer correspond to a stripe pattern of hopping parameters in the κ layer. This finding is the basis for studying the effect of the different underlying Hamiltonians on the superconducting properties.

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