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First principles study of the charge transfer salt κ-(BEDT-TTF)$_2$Cu(CN)$_3$ HARALD O. JESCHKE, HEM C. KANDPAL, ROSER VALENTI, Institut fuer Theoretische Physik, Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — The charge transfer salt κ-(BEDT-TTF)$_2$Cu(CN)$_3$ has attracted a lot of attention due to experimental evidence that it is a realization of a spin liquid: no magnetic ordering was found down to 32 mK. For a good description of this behavior, it is crucial to consider the appropriate effective model for this system. Here, we present electronic structure calculations in the frame of density functional theory (DFT) and derive an effective model with the NMTO (N-th order muffin tin orbital) downfolding method and discuss its features. Since from X-ray diffraction, the structure of κ-(BEDT-TTF)$_2$Cu(CN)$_3$ has been determined without hydrogen positions, we first prepare a very similar structure including hydrogen atoms and carefully relax it using the projector augmented wave method. This structure is then used for the DFT and NMTO analysis.

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