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First-Principles Study on New Spin Liquid Candidate κ-H_3(Cat-EDT-TTF)$_2$ TAKAO TSUMURAYA, RIKEN/National Institute for Materials Science, HITOSHI SEO, RIKEN/JST-CREST, REIZO KATO, RIKEN, TSUYOSHI MIYAZAKI, National Institute for Materials Science — A new class of molecular conductors based on catechol with ethylenedithiote-tetrathiafulvalene, (H_2Cat-EDT-TTF) has been synthesized recently. Among them, κ-type H_3(Cat-EDT-TTF)$_2$ is considered to be a dimer-type Mott insulator at ambient pressure and emerges as a candidate of realizing quantum spin liquid down to lowest temperature.[1] In this crystal, two H_2Cat-EDT-TTF molecules share a hydrogen (H) atom, and face-to-face dimers are formed in a anisotropic triangular lattice. Differently from conventional charge transfer salts, this compound does not have insulating layers. Here we study κ-H_3(Cat-EDT-TTF)$_2$ based on first-principles density-functional theory (DFT) calculations. We evaluate inter-dimer hopping integrals by fitting to the DFT bands, and find a quasi-one-dimensional anisotropy in the effective dimer-dimer interactions with frustrated inter-chain couplings. Furthermore, the inter-layer hopping integrals are non-negligible compared to the intra-layer couplings and the Fermi surface shows a warped cylinder, indicating their three-dimensionality of the electronic structure. Lastly, we report sensitivity of the electronic structure depending on the position of the shared H atom. [1] T. Isono et al, Nature Comm. 4 (2013) 1344; Priv. comm.

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