Mechanism of the metal-insulator transition of hollandite vanadate $\mathbf{K_2V_8O_{16}}$

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We make the electronic structure calculations of hollandite vanadate $K_2V_8O_{16}$ using the generalized gradient approximation (GGA) in the density functional theory, where the Hubbard-type repulsive interaction is taken into account (GGA+U). We in particular calculate the electronic structure of the low-temperature phase of this material using the crystal structure reported by Komarek [1]. We thereby find that the electronic wave functions near the Fermi level are predominantly of the d_{xy} character and form the quasi-one-dimensional energy bands. The energy bands are made of the single chains of the VO_6 octahedra rather than the double chains. The effects of strong electron correlations play an essential role here. Based on these results, we discuss the origins of the observed metal-insulator transition of the material. Details will be reported in Ref. [2].

References:
[1] A. Komarek, PhD Thesis, Univ. zu Köln (2009).
[2] T. Toriyama, T. Konishi, and Y. Ohta, in preparation.