Hollandite ruthenate $K_2Ru_8O_{16}$ as a new Tomonaga-Luttinger-liquid system

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The electronic structure of hollandite ruthenate $K_2Ru_8O_{16}$ is calculated using the generalized gradient approximation (GGA) in the density functional theory, where the Hubbard-type repulsive interaction is taken into account (GGA+U). We find that the electronic structure near the Fermi level consists only of a single band coming predominantly from the $4d_{yz}$ and $4d_{zx}$ orbitals of Ru ions with strong admixture of the $2p_z$ orbitals of corner-shared O ions connecting the double RuO chains. The band structure near the Fermi level is highly quasi-one-dimensional, exactly at half filling, and has a pair of two nearly parallel sheetlike Fermi surfaces separated by π/c. The calculated results are consistent with observed quasi-one-dimensional transport properties of this material [1]. These results establish that $K_2Ru_8O_{16}$ belongs to a class of the simplest possible Tomonaga-Luttinger-liquid materials. See Ref. [2] for details.

Reference:
[1] W. Kobayashi, Phys. Rev. B **79**, 155116 (2009).
[2] T. Toriyama, M. Watanabe, T. Konishi, and Y. Ohta, Phys. Rev. B, in press (2011).