Anomalous electronic states of hollandite-type transition-metal oxides

Y. Ohta[a], T. Toriyama[a], M. Sakamaki[b], and T. Konishi[c]

[a]Department of Physics, Chiba University, Chiba 263-8522, Japan
[b]Photon Factory, IMSS, KEK, Tsukuba 305-0801, Japan
[c]Graduate School of Advanced Integration Science, Chiba University, Chiba 263-8522, Japan

We make the electronic structure calculations of transition-metal oxides with the hollandite-type crystal structure $A_xM_8O_{16}$ using the generalized gradient approximation (GGA) in the density functional theory, where the Hubbard-type repulsive interaction is taken into account (GGA+U). We examine the $3d$ series (M=Ti, V, Cr, Mn) as well as the $4d$ series (M=Mo, Ru, Rh) to discuss generic aspects in the electronic structure of hollandites first. Then, we in particular study the origins of the metal-insulator transition observed in $K_2Cr_8O_{16}$ and quasi-one-dimensional electron conduction observed in $K_2Ru_8O_{16}$ by focusing on singularities in their calculated band structures and Fermi surfaces [1,2]. We also study the electronic structure of $K_2V_8O_{16}$ to consider the origins of the observed anomalous electronic states and metal-insulator transition and find that the effect of electron correlations plays an essential role in the metal-insulator transition of this material [3,4].

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