Anomalous electronic states of hollandite-type transition-metal oxides

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We make the electronic structure calculations of transition-metal oxides with the hollandite-type crystal structure $\text{A}_x\text{M}_8\text{O}_{16}$ 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 3\textit{d} series ($M=$Ti, V, Cr, Mn) as well as the 4\textit{d} 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 $\text{K}_2\text{Cr}_8\text{O}_{16}$ and quasi-one-dimensional electron conduction observed in $\text{K}_2\text{Ru}_8\text{O}_{16}$ by focusing on singularities in their calculated band structures and Fermi surfaces [1,2]. We also study the electronic structure of $\text{K}_2\text{V}_8\text{O}_{16}$ 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].