

Metal-insulator transition in Hollandite-type $\text{K}_2\text{V}_8\text{O}_{16}$ and $\text{K}_2\text{Cr}_8\text{O}_{16}$

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The synthesis, structure and electromagnetic properties of Hollandite-type $\text{K}_2\text{Cr}_8\text{O}_{16}$ and $\text{K}_2\text{V}_8\text{O}_{16}$ are reported. In the crystal structures, the double chains of edge sharing MO_6 ($\text{M}=\text{V},\text{Cr}$) octahedra share corners with neighboring chains to form a M_8O_{16} stoichiometry framework that encloses large four-sided tunnels. The K^+ cation is located in the tunnels. These are mixed-valence compounds. Since the crystallographic site of vanadium and chromium atom is unique, the formal oxidation is $\text{M}^{3.75+}$ ($\text{M}=\text{V},\text{Cr}$). We successfully obtained $\text{K}_2\text{V}_8\text{O}_{16}$ and $\text{K}_2\text{Cr}_8\text{O}_{16}$ by a high pressure synthesis. Combining electrical resistivity, magnetic susceptibility, and x-ray diffraction, we found that $\text{K}_2\text{V}_8\text{O}_{16}$ exhibits a first order metal-insulator transition at 170 K, accompanied by charge order of V^{4+} and V^{3+} and the formation of $\text{V}^{4+}\text{-V}^{4+}$ singlet pairs and $\text{V}^{4+}\text{-V}^{3+}$ pairs in the low temperature insulator phase.¹ On the other hand, $\text{K}_2\text{Cr}_8\text{O}_{16}$ is a ferromagnetic metal with $T_c = 180$ K and shows a transition to an insulator at 95 K without an apparent structural change but retaining ferromagnetism.²

¹M. Isobe, S. Koishi, N. Kouno, J. Yamaura, T. Yamauchi, H. Ueda, H. Gotou, T. Yagi, and Y. Ueda, J. Phys. Soc. Jpn. **75**, 07381 (2006).

²K. Hasegawa, M. Isobe, T. Yamauchi, H. Ueda, J. Yamaura, H. Gotou, T. Yagi, H. Sato and Y. Ueda, Phys. Rev. Lett. **103**, 146403 (2009).