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Electronic, magnetic, and structural properties of ferromagnetic insulator $K_2Cr_8O_{16}$ SOORAN KIM, KYOO KIM, B.I. MIN, Pohang University of Science and Technology — The hollandite-type material, $K_2Cr_8O_{16}$, exhibits a couple of phase transitions upon cooling: the first magnetic transition at T = 180K and the second metal-insulator transition at T = 95K. Namely, for 95K < T < 180K, $K_2Cr_8O_{16}$ is a ferromagnetic metal, while, for T < 95K, it is a ferromagnetic insulator. Moreover, the metal-insulator transition is accompanied by the structural transition from tetragonal to monoclinic structure. In order to explore the underlying mechanisms of these phase transitions, we have investigated systematically electronic, magnetic, and structural properties of $K_2Cr_8O_{16}$ based on the first principles DFT (density-functional theory) band structure calculations taking into account the on-site Coulomb correlation interaction U. The role of the electron-electron correlation on the magnetic, metal-insulator, and the structural transitions will be discussed by comparing the band structures of DFT and DFT+U.

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