Ab initio study on metal-insulator and magnetic transitions in correlated hollandites: $K_2Cr_8O_{16}$ and $K_2V_8O_{16}$

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1. Introduction

Hollandite-type TM oxides $A_2M_8O_{16}$ (A=alkali metal, M=TM element) have drawn recent attention due to their quasi-one-dimensional column structure made of four double MO chains. Despite the similarity in the crystal structures, these materials have different physical properties depending on the TM element. $K_2Cr_8O_{16}$ and $K_2V_8O_{16}$ exhibit the metal-insulator transition (MIT) and the structural transition concomitantly upon cooling [1,2].

In order to explore the driving mechanism of the concomitant metal-insulator and structural transitions in quasi-one-dimensional hollandite $K_2Cr_8O_{16}$ and $K_2V_8O_{16}$, electronic structures and phonon properties are investigated by employing the *ab initio* density functional theory (DFT) calculations. We have also investigated magnetic properties of $K_2Cr_8O_{16}$ and $K_2V_8O_{16}$.

2. Results and Discussions

For $K_2Cr_8O_{16}$, we have found that the Coulomb correlation plays an essential role in MIT and the structural transition. Above the MIT temperature, $K_2Cr_8O_{16}$ has ferromagnetism and a half-metallic nature. After MIT, $K_2Cr_8O_{16}$ goes ferromagnetic insulator. U effect facilitates the MIT and structural transition by increasing the hybridization between Cr d_{yz+zx} and O p_z. Thus we proposed the Mott-Peierls transition as the driving mechanism of the concomitant MIT and the structure transition in $K_2Cr_8O_{16}$. The unique feature of $K_2Cr_8O_{16}$ is that the Mott-Peierls transition occurs in the fully spin-polarized band.[3]

For $K_2V_8O_{16}$, we have obtained the insulating electronic structures with charge ordering (CO) and orbital ordering (OO). The optical conductivity and magnetic exchange interaction were calculated to investigate the ground state of $K_2V_8O_{16}$. The CO of V^{3+} and V^{4+} occurs in separate chains, preserving the inversion symmetry of the crystal. Thus, $K_2V_8O_{16}$ is to be a model system for investigating a spin-orbital-lattice coupled Mott system. The MIT of the system occurs via the orbital-selective Mott transition. The insulating ground state of $K_2V_8O_{16}$ arises from the interplay of on-site Coulomb interaction, the magnetic-exchange interaction, and tetragonal distortion, causing the CO of V^{3+} and V^{4+} and the OO of d_{xy} and d_{yz+zx}. We have separated the physics of MIT and Peierls-like distortions in $K_2V_8O_{16}$, whereby demonstrated that the Peierls physics is not essential in driving the MIT.

3. References

[1] T. Toriyama, A. Nakao, Y. Yamaki, H. Nakao, Y. Murakami, K. Hasegawa, M. Isobe, Y. Ueda, A.V. Ushakov, D. I. Khomskii, S. V. Streltsov, T. Konishi, and Y. Ohta, Phys. Rev. Lett. 107, 266402 (2011).

[2] M. Isobe, S. Koishi, N. Kouno, J.-I. Yamaura, T. Yamauchi, H. Ueda, H. Gotou, T. Yagi, and Y. Ueda, J. Phys. Soc. Jpn. 75, 073801 (2006).

[3] S. Kim, K. Kim, and B. I. Min, Phys. Rev. B 90, 045124 (2014)