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A DFT+DMFT study of Orbital Physics in a Spin Orbital Lattice Coupled 2p Electron Mott System: KO_2 MINJAE KIM, B.I. MIN, Department of Physics, Pohang University of Science and Technology, DEPARTMENT OF PHYSICS, POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY TEAM — We have investigated the temperature (T)-dependent orbital physics in a typical spin-orbital-lattice coupled 2p electron Mott system KO_2, based on the electronic structures obtained by the dynamical mean-field theory as well as the density functional theory. KO_2 consists of K^+ cations and O_2^- molecule anions, and there are three electrons in the fourfold degenerate pi anti-bonding orbital of O_2^- anions. Hence, the orbital degeneracy occurs in a O_2^- anion with a magnetic moment. We have shown that KO_2 exhibits the orbital fluctuation phenomenon at high T due to the degenerate pi anti-bonding orbital. Upon cooling, this orbital fluctuation is suppressed by the Jahn-Teller (JT) type crystal field with lowering of the crystal structure symmetry, and then the ferro-orbital (FO) ordering emerges at low T. This FO ordering is compatible with the experimental antiferromagnetic spin order at low T in KO_2. We suggest that the suppression of the orbital fluctuation in KO_2 upon cooling is similar that in 3d transition-metal oxides such as $LaVO_3$.

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