A DFT+DMFT study of Orbital Physics in a Spin Orbital Lattice Coupled $2p$ Electron Mott System: KO$_2$ MINJAЕ 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 3$d$ transition-metal oxides such as LaVO$_3$. 

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