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Spin-Orbital-Lattice coupling in KO_2 superoxide MINJAE KIM, BEOM HYUN KIM, HONG CHUL CHOI, B. I. MIN, Department of Physics, PCTP, Pohang University of Science and Technology — In KO_2 superoxide, the magnetic ordering from the incomplete pi level emerges concomitantly with a symmetry lowering such as gyration of anions. The simultaneous structural and magnetic phase transitions suggest the spin-orbital-lattice coupling in correlated $2p$ electrons system. We have studied the interplay of the spin-orbital-lattice degrees of freedom in KO_2 by employing the first-principles electronic structure theory. We used generalized gradient approximation (GGA) for the exchange correlation potential incorporating the Coulomb interaction U and the spin-orbit coupling (GGA+U+SO). For the high symmetry phase of KO_2, we have found that the band gap opens by the spin-orbit coupling which splits the degenerate pi anti-bonding level. For the low symmetry phase of KO_2, we have found that the band gap opens by the strong Coulomb interaction and the crystal field effect from alkali cations. The simultaneous antiferro-spin and ferro-orbital orderings are found to occur with the band gap opening.

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