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Correlation effects on the different crystal structures of AO₂
(A=Na, K, and Ba) MINJAE KIM, CHANG-JONG KANG, B.I. MIN, Pohang University of Science and Technology (POSTECH) — In alkali superoxide (A=Na, and K), the structural phase transition from high symmetry to low symmetry structures occurs upon cooling. On the other hand, in BaO₂ peroxide, the crystal structure is always the high symmetry tetragonal structure of KO₂, independent of temperature. To resolve these different crystal structures of AO₂ (A=Na, K, and Ba), we have calculated phonon dispersions of AO₂, assuming the high symmetry tetragonal structure of KO₂ with first-principle band structure method in the generalized gradient approximation (GGA) incorporating the Coulomb interaction U (GGA+U). From softened phonon modes, we have shown that, in KO₂ and NaO₂, the degeneracy of the incomplete pi anti-bonding level is lifted with the symmetry lowering such as Jahn-Teller effect with help of Coulomb correlation U. In contrast, in BaO₂, the pi anti-bonding level of the peroxide is completely filled without degeneracy. Thus, U is not effective on the phonon structure so that the structural instability does not occur in BaO₂.

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