FIRST PRINCIPLE STUDY OF ELECTRONIC STRUCTURES ON MULTIFERROIC MATERIALS ($YMnO_3$, $BiCrO_3$)

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ABSTRACT

FIRST PRINCIPLE STUDY OF ELECTRONIC STRUCTURES ON MULTIFERROIC MATERIALS ($YMnO_3$, $BiCrO_3$)

In this first principle study of electronic structure on multiferroic materials, $YMnO_3$ and $BiCrO_3$ employed density functional theory (DFT). Computational techniques for calculations are performed via the Local Density Approximation (LDA). The calculated electronic structures were made in the high-symmetry cubic perovskite structure. There two parts to be considered in calculating the electronic structures, which are density of state (DOS) and energy band structures. B-site of perovskite structure for $YMnO_3$ was influenced by Jahn-Teller effect as the results of crystal field splitting by oxygen anions.