

FIRST PRINCIPLE STUDY OF ELECTRONIC STRUCTURES ON
MULTIFERROIC MATERIALS (YMnO_3 , BiFeO_3)

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ABSTRACT

FIRST PRINCIPLE STUDY OF ELECTRONIC STRUCTURES ON MULTIFERROIC MATERIALS (YMnO₃, BiCrO₃)

In this first principle study of electronic structure on multiferroic materials, YMnO₃ and BiCrO₃ 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 YMnO₃ was influenced by Jahn-Teller effect as the results of crystal field splitting by oxygen anions.