

**FIRST PRINCIPLE DFT+U STUDY ON THE STRUCTURAL,
DYNAMICAL, AND ELECTRONIC PROPERTIES OF
MULTIFERROIC BiFeO₃**

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ABSTRACT

First principle DFT+U study in the structural and electronic properties of multiferroic BFO (Bismuth Ferrite)

The structural and electronic properties of BiFeO_3 (BFO) were investigated employing the first principles within LSDA+U method. In this work the orthorhombic perovskite structure is used. The value correlation U is varied at 0eV, 3eV and 6eV which found that 6eV calculated band gap is more closed to the experimental one. For geometry optimization the volume is found to be underestimation when it is compared to experimental data. The band gap of BFO was found to be 2.0eV by the electronic structure calculation. Analysis of the density of states indicated that the valence band was consisted with Fe-d and O-p states, and the conduction band was composed of Fe-d and Bi-p states.

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND STUDY

Multiferroic materials are very promising nowadays since they can exhibit more than one good characteristics and properties. Multiferroic is a material that can exhibit more than one ferroic group for example ferroelectric and ferromagnetic. The multiferroic is being proposed in 2003, when the large polarization in epitaxially grown thin film of bismuth ferrite and also magnetic and electric coupling by orthorhombic TbMnO_3 are being discovered. For material that can consider as ferroelectric, it must be able to switch between these states with an applied electric field, which changes the relative energy of the states through the coupling of the field to the polarization.

The presence of both magnetic and ferroelectric above room temperature with potential coupling between the two order parameters makes BFO a good candidate for with have immense potential for technological device applications and at the same time they pose very interesting and fundamental physics problems.