Effects of Fe substitution by Nb on physical properties of BaFeO3: A DFT + U study

Imène Cherair, Nadia Iles, Lyacine RABAHI, Abdelhafid Kellou

Abstract: The structural, electronic, magnetic and thermal properties of BaFe$_{1-x}$Nb$_x$O$_3$ perovskites oxides are investigated using the Density Functional Theory (DFT). The Generalized Gradient Approximation (GGA) and on-site Hubbard potential corrections (GGA + U) are considered. According to the formation energies and phonon spectra, the stoichiometric BaFeO$_3$ and BaNbO$_3$ oxides have a stable cubic phase. The GGA+ U calculations show a half metallic behavior of BaFeO$_3$ with a large exchange splitting, in agreement with previous experimental and theoretical works. The Fe substitution by Nb for $x = 0.5$ leads to a surprising insulating ground state. The values of the band gap is 0.40 eV and 1.84 eV using GGA and GGA + U, respectively. For $x = 0.875$ and $x = 1$, the corresponding alloys are metallic and non-magnetic, while for $x = 0.5$ and $x = 0.625$ the antiferromagnetic ground state is found using GGA + U. For the remaining Nb compositions a half metallic character is noticed with a ferromagnetic state. The quasi-harmonic Debye model is successfully applied to study the temperature evolution of lattice parameters and bulk moduli for different Nb compositions.

Keywords: BaFe$_{1-x}$Nb$_x$O$_3$ perovskites, Structural properties, Magnetic moments, Density Functional Theory, GGA + U, Quasi-harmonic Debye model