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

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Abstract: The structural, electronic, magnetic and thermal properties of BaFe1 xNbxO3 perovskites oxides are investigatedusing the Density Functional Theory (DFT). The Generalized Gradient Approximation (GGA) andon-site Hubbard potential corrections (GGA + U) are considered. According to the formation energiesand phonon spectra, the stoichiometric BaFeO3 and BaNbO3 oxides have a stable cubic phase. The GGA+ U calculations show a half metallic behavior of BaFeO3 with a large exchange splitting, in agreementwith previous experimental and theoretical works. The Fe substitution by Nb for x = 0.5 leads to a surprisinginsulating 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 forx = 0.5 and x = 0.625 the antiferromagnetic ground state is found using GGA + U. For the remaining Nbcompositions a half metallic character is noticed with a ferromagnetic state. The quasi-harmonicDebye model is successfully applied to study the temperature evolution of lattice parameters and bulkmoduli for different Nb compositions.

Keywords : BaFe1-xNbxO3 perovskites, Structural properties, Magnetic moments, Density Functional Theory, GGA + U, Quasi-harmonic Debye model