

Bonding analysis BiFeO₃ substituted by Gd³⁺

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BiFeO₃ is very impressive due to its initial multiferroic features. Bulk BiFeO₃ with the space group $R\bar{3}c$ exhibits a G -type antiferromagnetic (AFM) order. Unfortunately, this AFM order in BiFeO₃ prevents the observation of any net magnetization and the linear magnetoelectric effect. However, some investigations show that the partial ionic substitutions of Bi by Gd³⁺ is necessary for obtaining spontaneous magnetization in BiFeO₃. In respect to this fact, we present results of DFT calculations for Bi₅GdFe₆O₁₈ in the rhombohedral $R\bar{3}c$ structure. Our calculations are performed using full-potential projector-augmented wave method, as implemented in the Vienna *ab initio* simulation package (VASP). Within LSDA+U approach it is found that the G -type AFM structure with the insulating ground state gives a minimal total energy for studied compound. The effect of Gd substitution is observed as an increase in magnetization compared to the pure BiFeO₃. The Bi₅GdFe₆O₁₈ compound has nonzero total magnetic moment, which arises from antiparallel moments on Fe sites and reduced moment on Gd. Chemical bonding of the compound is analyzed using partial density of states, electron localization function and charge density distribution.

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