

Magnetic properties in BiFeO<sub>3</sub> doped with Cu and Zn First-principles investigation

Qing-Yan Rong, Wen-Zhi Xiao, Gang Xiao, Ai-Ming Hu, Ling-Ling Wang



PII: S0925-8388(16)30589-8

DOI: [10.1016/j.jallcom.2016.03.032](https://doi.org/10.1016/j.jallcom.2016.03.032)

Reference: JALCOM 36920

To appear in: *Journal of Alloys and Compounds*

Received Date: 2 November 2015

Revised Date: 1 March 2016

Accepted Date: 6 March 2016

Please cite this article as: Q.-Y. Rong, W.-Z. Xiao, G. Xiao, A.-M. Hu, L.-L. Wang, Magnetic properties in BiFeO<sub>3</sub> doped with Cu and Zn First-principles investigation, *Journal of Alloys and Compounds* (2016), doi: 10.1016/j.jallcom.2016.03.032.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

## Magnetic properties in BiFeO<sub>3</sub> doped with Cu and Zn

### First-principles investigation

Qing-Yan Rong <sup>a, b</sup>, Wen-Zhi Xiao <sup>a, b\*</sup>, Gang Xiao <sup>a, b</sup>, Ai-Ming Hu <sup>b</sup>, Ling-Ling Wang <sup>a\*</sup>

<sup>a</sup> School of Physics and Electronics, Hunan University, Changsha 410082, China

<sup>b</sup> Department of Physics and Mathematics, Hunan Institute of Engineering, Xiangtan 411104, China

**Abstract:** Based on first-principles spin-polarized density functional theory calculations, the electronic structures, and magnetic properties of Cu and Zn-doped BiFeO<sub>3</sub> are investigated. The calculated formation energies show that Cu prefers to occupy Fe site, while the Zn prefer to occupy Bi site. All the doped BiFeO<sub>3</sub> systems turn out to be favorable for G-type antiferromagnetic arrangement. The substitution of Cu and Zn for Fe produces a magnetic moment of 3.0 and 4.0  $\mu_B$  per dopant, respectively. The net magnetic moments are from the broken symmetry of the AFM spin ordering network. For the substitution of Cu and Zn for Bi, the net magnetic moment originates from Cu/Zn itself and hole introduced by Cu/Zn. Two-Cu/Zn-doped cases show various magnetic behaviors. If O vacancy is far away from dopants, the O vacancies don't affect the net magnetic moment of the substitution of Cu and Zn for Fe, but have notable effect for Bi site doping. The O vacancies result in metallicity in all doped cases. Our study demonstrates that the nonmagnetic Cu and Zn doping will lead to the diversity and complexity of magnetic properties depending on doping sites, distance between dopants, intrinsic defect, and so on, which could be responsible for the observed various magnetic behaviors in Cu/Zn-doped BiFeO<sub>3</sub> samples.

**Keywords:** electronic structure; magnetic property; perovskite BiFeO<sub>3</sub>.

\*Corresponding author: E- mail: [xiaowenzhi@hnu.edu.cn](mailto:xiaowenzhi@hnu.edu.cn); [llwang@hnu.edu.cn](mailto:llwang@hnu.edu.cn)

Download English Version:

<https://daneshyari.com/en/article/1605984>

Download Persian Version:

<https://daneshyari.com/article/1605984>

[Daneshyari.com](https://daneshyari.com)