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Magnetic properties in $BiFeO_3$ doped with Cu and Zn
First-principles investigation

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Abstract: Based on first-principles spin-polarized density functional theory calculations, the electronic structures, and magnetic properties of Cu and Zn-doped $BiFeO_3$ 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 $BiFeO_3$ 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 μ_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 behaves. 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 $BiFeO_3$ samples.

Keywords: electronic structure; magnetic property; perovskite $BiFeO_3$.

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