First-Principles Study of Magnetic Phase of $Bi_xCa_{1-x}MnO_3$

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Manganese oxide $Bi_xCa_{1-x}MnO_3$ has a perovskite structure and shows quite variable physical properties. Depending on the alloy ratio x of bismuth and calcium, $Bi_xCa_{1-x}MnO_3$ has been reported to show different electric, magnetic, and other physical characteristics. So far, most of pre-existing studies on $Bi_xCa_{1-x}MnO_3$ were conducted experimentally, and theoretical investigation has been done only for limited range of bismuth/calcium content. The purpose of this study is to identify the stable magnetic phase of $Bi_xCa_{1-x}MnO_3$ through the first-principles electronic structure calculations for whole range of its bismuth/calcium content x.

We performed the first-principles calculations based on density functional theory for $Bi_xCa_{1-x}MnO_3$ of x = 1, 0.875, 0.75, 0.5, 0.25, 0.125, and 0. For the $Bi_xCa_{1-x}MnO_3$ having each of these seven compositions, we compared stabilities of ferromagnetic phase and three anti-ferromagnetic phases; G-type, A-type, and C-type (Fig. 1). Local spin density approximation with on-site Coulomb interaction scheme was taken and the projection augmented wave pseudopotentials were used. Each supercell was consisted of eight manganese atoms, eight bismuth/calcium atoms, and twenty four oxygen atoms, so that various magnetic phase stability could be compared.

Based on our calculations, it is found that $Bi_xCa_{1-x}MnO_3$ is ferromagnetic for x larger than 0.5 and antiferromagnetic for x smaller than 0.25. Two calculated electronic density of states for x = 1 or 0.5 are illustrated in Fig. 2. The calculated magnetic moments of manganese ions for each compositions are given in Fig. 3.

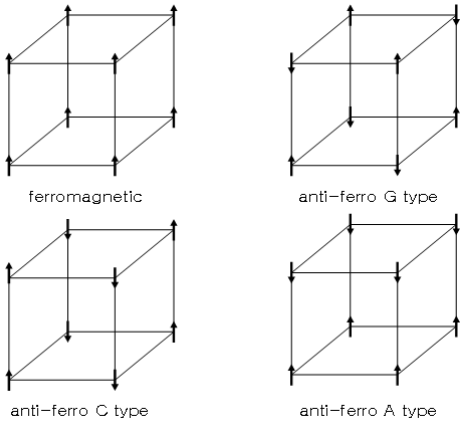

Fig. 1. Schematic illustrations for magnetic phases

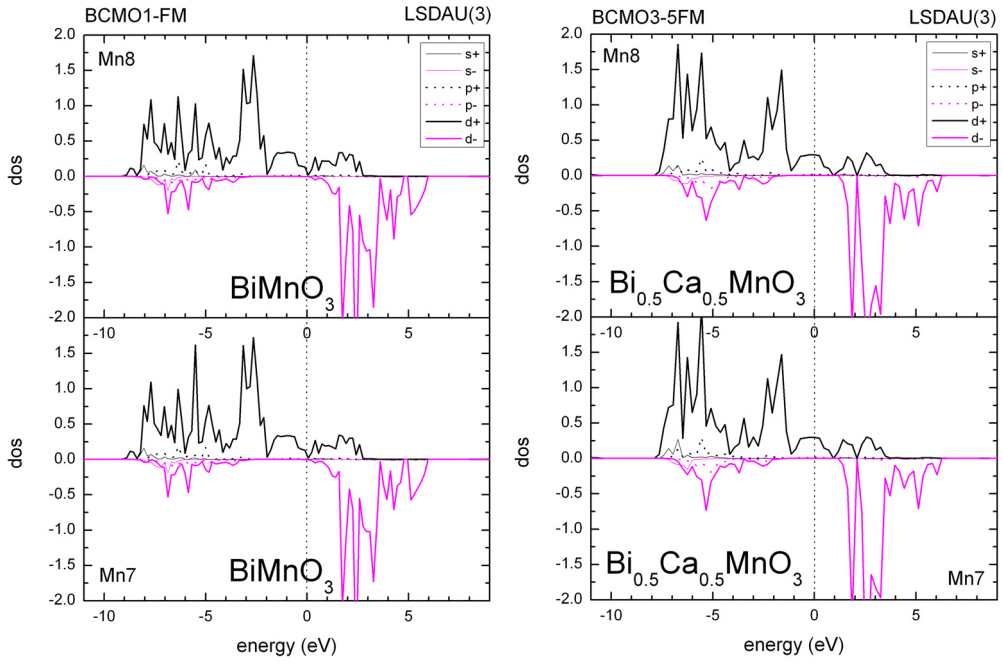

Fig. 2. Density of electronic states of $Bi_xCa_{1-x}MnO_3$ for x=1 and 0.5. LSDA+U calculation predicts ferromagnetic states for both compositions.

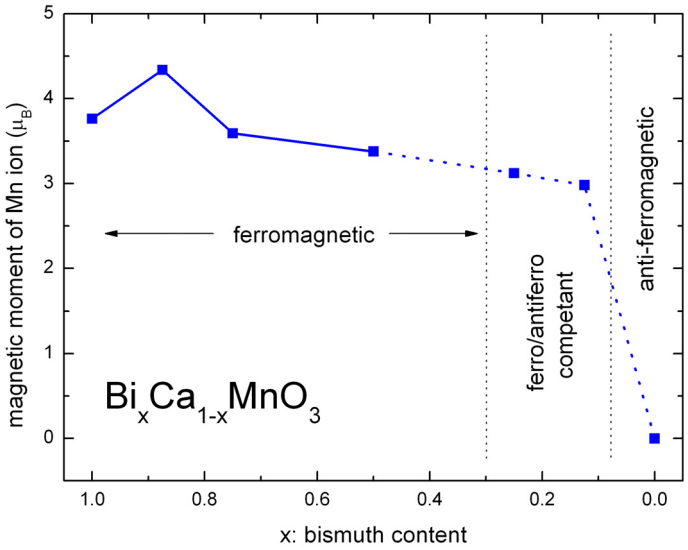

Fig. 3. Calculated magnetic moments of $Bi_xCa_{1-x}MnO_3$ in this study.