Multiferroic behavior of Aurivillius $Bi_4Mn_3O_{12}$ from first-principles

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Multiferroic materials, exhibiting both ferroelectricity and magnetic order in the same phase, are of particular interest for their potential technological applications. One of the current trends in the searching of new multiferroic compound is, starting from a ferroelectric host, to incorporate magnetically active species and check whether it is (anti)ferromagnetic and insulating.

In this work, on the basis of density functional calculations we investigate the multiferroic behavior of the hypothetical three-layer Aurivillius compound $Bi_4Mn_3O_{12}$ which results of substituting the three B-site Ti^{+4} ions by magnetically active Mn^{+4} in the lattice of the prototypical ferroelectric $Bi_4Ti_3O_{12}$. We find that the tetragonal paraelectric phase of $Bi_4Mn_3O_{12}$ is ferromagnetic, showing ferroelectric and antiferrodistortive instabilities similar to the ones observed in its ferroelectric parent compound $Bi_4Ti_3O_{12}$. Our results indicate however that the presence of Mn^{+4} ions shrinks the cell volume and consequently the unstable polar mode, associated to the ferroelectric polarization, is overcame by an antiferrodistortive distortion. In this way, $Bi_4Mn_3O_{12}$ exhibits incipient ferroelectricity at its equilibrium volume. Finally we investigate the possibility to favor the ferroelectric distortion by strain and chemical engineering.