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**Structural instabilities in Aurivillius compound $Bi_4Mn_3O_{12}$ from First Principles** SILVIA TINTE, INTEC, Univ. Nac. del Litoral, Santa Fe, Argentina, MARCELO STACHIOTTI, IFIR, Univ. Nac. de Rosario, Rosario, Argentina, RUBEN WEHT, CNEA, Buenos Aires, Argentina — Layered perovskite oxide materials are good candidates for the potential synthesis of natural multiferroic materials. One approach is to choose a ferroelectric host and to incorporate a magnetically active species. The Aurivillius layered perovskites are chosen because most are ferroelectric. Described by the formula $[Bi_2O_2][A_{n-1}B_nO_{3n+1}]$, they are formed by stacking $Bi_2O_2$ slabs with $n$ perovkitelike blocks. A ferroelectric prototype compound is $Bi_4Ti_3O_{12}$ (BIT), where bismuth also occupies the $A$ sites. Using first-principles calculations, we investigate here the three-layer Aurivillius $Bi_4Mn_3O_{12}$ (BIM) that results of substituting all $Ti^{4+}$ B-site cations in the BIT lattice by $Mn^{4+}$ cations. We report the structural instabilities in the high-symmetry tetragonal structure (space group symmetry $I4/mmm$). We find an unstable $E_u$ phonon mode, which mainly involves movements of the Bi ions in the perovskite $A$ sites with respect to the $TiO_6$ octahedra. This instability, also observed in non-magnetic BIT and associated to the in-plane electronic polarization, suggests the presence of ferroelectricity in BIM. We also explore different collinear spin orderings of the magnetic Mn atoms and its effect on the structural instabilities.

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