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First-principles analysis of ferroelectric transition in MnSnO_3 and MnTiO_3 perovskitesSung Gu Kang^{*}*School of Chemical Engineering, University of Ulsan, 93, Daehak-ro, Nam-gu, Ulsan 44610,**Republic of Korea*

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Abstract

The ferroelectric instabilities of an artificially adopted *Pnma* structure in low tolerance perovskites have been explored [Int. J. Quantum Chem., **117**, e25420 (2017)], where an unstable A-site environment was reported to be the major driving source for the low tolerance perovskites to exhibit ferroelectric instability. This study examined the ferroelectric transition of two magnetic perovskite materials, MnSnO_3 and MnTiO_3 , in *Pnma* phase. Phase transitions to the *Pnma* phase at elevated pressures were observed. MnSnO_3 , which has a lower (larger) tolerance factor (B-site cation radius), showed a higher ferroelectric mode amplitude than MnTiO_3 . The distribution of the bond length of Mn-O and the mean quadratic elongation (QE) of octahedra (SnO_6 or TiO_6) were investigated for structural analysis. However, MnTiO_3 showed a larger spontaneous polarization than MnSnO_3 due to high Born effective charges of titanium. This study is useful because it provides a valuable pathway to the design of promising multiferroic materials.

Graphical abstract

First-principles study demonstrates how ferroelectric transitions occur in high pressure phase of *Pnma* MnSnO_3 and MnTiO_3 . MnSnO_3 which has a lower tolerance factor showed a higher amplitude of ferroelectric mode (Γ_4^-) and larger octahedral distortions than MnTiO_3 . However, MnTiO_3 showed a larger spontaneous polarization than MnSnO_3 due to high Born effective charges of titanium.

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