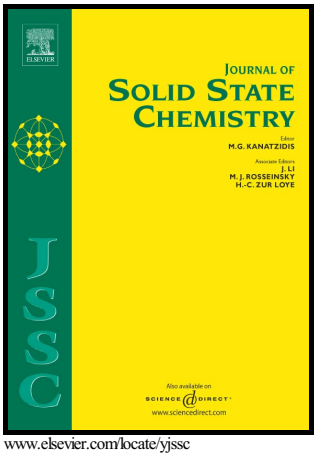

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First-principles analysis of ferroelectric transition in $MnSnO_3$ and $MnTiO_3$ perovskites

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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.