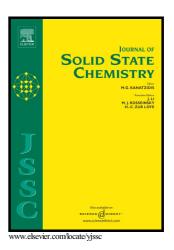
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First-principles analysis of ferroelectric transition in MnSnO₃ and MnTiO₃ perovskites

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First-principles analysis of ferroelectric transition in MnSnO₃ and MnTiO₃ 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, MnSnO₃ and MnTiO₃, in *Pnma* phase. Phase transitions to the *Pnma* phase at elevated pressures were observed. MnSnO₃, which has a lower (larger) tolerance factor (B-site cation radius), showed a higher ferroelectric mode amplitude than MnTiO₃. The distribution of the bond length of Mn-O and the mean quadratic elongation (QE) of octahedra (SnO₆ or TiO₆) were investigated for structural analysis. However, MnTiO₃ showed a larger spontaneous polarization than MnSnO₃ 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 MnSnO₃ and MnTiO₃. MnSnO₃ which has a lower tolerance factor showed a higher amplitude of ferroelectric mode (Γ_4) and larger octahedral distortions than MnTiO₃. However, MnTiO₃ showed a larger spontaneous polarization than MnSnO₃ due to high Born effective charges of titanium.

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