A Material Design on New Ferroelectric of $ATiO_2C$ Perovskite

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Abstract

Ferroelectric $BaTiO_3$ is widely used as non-volatile memory. The ferroelectric property at room temperature is caused by tetragonality.[1] In this study, we have proposed $ATiO_2C$ perovskite (A=divalent counter cations such as Sr^{+2}, Ba^{2+} etc) as the next-generation new ferroelectric. Hybrid density functional theory (DFT) calculations have been performed to clarify the ferroelectric mechanism of $ATiO_2C$ perovskite. As Ti-C-Ti covalent bonding is formed in carbon-doped perovskite [2-3], the detailed chemical bonding analysis has been performed by the use of Onishi chemical bonding rule.

References

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