

Abstract Submitted
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First Principle Studies of Electromechanical Properties in Mn-Doped BaTiO₃¹ HIROYUKI TAKENAKA, Carnegie Institution for Science, Washington, DC, USA, R.E. COHEN, Carnegie Institution of Washington, Washington, DC, US, Department für Geo-und Umweltwissenschaften, Ludwig-Maximilians-Universitaet, Munich, Germany — We are performing density functional calculations to elucidate the electromechanical properties for Mn-doped BaTiO₃ with an oxygen vacancy, applying electric field perpendicular to polarization directions. We find that local dipole switching and lattice changes take place at 3MV/m. Spontaneous polarization along x is 0.251 C/m² and *c/a* ratio changes from 1.021 to 1.000. This indicates that coercive field of Mn-doped BaTiO₃ increases as were experimentally reported since our results for pure BaTiO₃ exhibit onset of the switching and changes at 0.8 MV/m. We report our computational dielectric constant and strain as a function of electric field for Mn-doped BaTiO₃.

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