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Effect of Electromechanical Properties in Mn-doped BaTiO₃¹ HIROYUKI TAKENAKA, Carnegie Inst of Washington, R.E. COHEN, Carnegie Inst of Washington and Department of Earth and Environmental Sciences, Ludwig Maximilians University Munich, Germany — Experimental studies reported that Mn doping in BaTiO₃ could improve their electromechanical properties. In addition, ageing process gives rise to a significant reversible strain effect. Performing density functional theory (DFT) calculations, we find that Mn dopant with oxygen vacancy induces local electric field of 20 MV/m in 2x2x2 (39 atom) supercell. In order to understand effects of the electromechanical properties from phenomenological point of view, we optimize electric enthalpies in Landau-Devonshire model, parametrized from DFT results, under applying electric fields. We show dielectric constant and piezoelectric coefficients from the optimized polarization paths.

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