

Abstract Submitted
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Effects of Manganese Addition on Ferroelectric Properties of BaTiO₃ : Ab initio Study IVAN NAUMOV, R.E. COHEN, Carnegie Institution of Washington — As it is well known, Mn is intensively used to improve the electromechanical properties of perovskite oxides like BaTiO₃, PbTiO₃ or PbZr_xTi_{1-x}O₃. Despite the interest in Mn as a dopant, it is currently poorly understood from the fundamental point of view. Here, we present the results of our ab initio study aimed to elucidate the role of Mn defects and associated with them vacancies on the electronic, atomic and ferroelectric properties of BaTiO₃. Namely, we discuss the equilibrium geometry and electronic properties of the Mn ions occupying A or B sites and their valence or oxidation states in the presence or absence of an compensated oxygen vacancy. A special attention is given to the formation of dipole moments \mathbf{P}_d associated with the dopants and to the interaction between \mathbf{P}_d and spontaneous polarization \mathbf{P}_s . This work is supported by the US Office of Naval Research.

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