

Abstract Submitted
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Non- d^0 Mn-driven ferroelectricity in antiferromagnetic BaMnO₃
JAMES RONDINELLI, NICOLA SPALDIN, UC Santa Barbara — Using first-principles density functional theory calculations we predict a ferroelectric ground state structure – driven by off-centering of the magnetic Mn ion – for perovskite-structure BaMnO₃. Our finding is surprising, since the competition between energy-lowering covalent bond formation, and energy-raising Coulombic repulsions (the 2nd order Jahn-Teller effect) usually only favors off-centering for non-magnetic d^0 ions. It is consistent, however, with the recent observation [S. Bhattacharjee, E. Bousquet and P. Ghosez, Arxiv e-prints **811**, 0811.2344 (2008)], that large lattice constants can stabilize polar off-centering of magnetic ions, by lowering the short-range Coulomb repulsions that favor the centrosymmetric phase. We calculate the Born effective charges for the compound, and find anomalously large values for Mn and O, consistent with the large calculated ferroelectric polarization of 30 $\mu\text{C}/\text{cm}^2$. We also describe the changes that occur in the electronic structure when the system transitions from a centrosymmetric to polar state. Finally, we suggest possible routes by which the cubic perovskite phase can be stabilized over the usual hexagonal phase.

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