

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First principles study of magnetostructural instabilities in magnetic perovskite oxides JUN HEE LEE, LUCIA PALOVA, KARIN M. RABE, Department of Physics and Astronomy, Rutgers University — First principles phonon dispersion relations are reported for a range of magnetic perovskite oxides in cubic high-symmetry reference structures. Materials considered include EuTiO_3 and BiFeO_3 . For each system, the dominant lattice instabilities are identified. These are frozen-in, singly and in combination, and the structures are optimized in the resulting space groups. From this, we identify distinct low-energy alternatives to the ground-state structure. We focus particularly on the dependence of the lattice instabilities and structural energetics of low-lying phases on the magnetic order, and extract key magnetostructural coupling parameters. The analysis is applied to predict possible structural and magnetic phase transitions as a function of epitaxial strain and/or of composition in low-concentration solid solutions ($A_{1-x}A'_xB\text{O}_3$, $AB_{1-x}B'_x\text{O}_3$, $A_{1-x}A'_xB_{1-y}B'_y\text{O}_3$ for small x,y).

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Date submitted: 22 Nov 2008

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