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 ($A_{1-x}A'_xBO_3$, $AB_{1-x}B'_xO_3$, $A_{1-x}A'_xB_{1-y}B'_yO_3$ for small $x,y$).