Phase transitions and magnetostructural coupling in ZnCr$_2$O$_4$
from first principles

CARL-JOHAN EKLUND, Rutgers University, CRAIG J. FENNIE, Cornell University, KARIN M. RABE, Rutgers University — In the spinel structure oxide ZnCr$_2$O$_4$, a phase transition is observed from the high-temperature cubic phase to a low-temperature low-symmetry phase, reported as tetragonal$^1$ or orthorhombic.$^2$ Building on a previous first-principles analysis of the zone-center phonons and spin-phonon coupling,$^3$ we construct a first-principles effective Hamiltonian to investigate this transition. The local modes included are the Cr displacements, distortions of the Zn-centered tetrahedra, and the homogeneous strain. The magnetostructural coupling of these degrees of freedom to the spins of the Cr$^{3+}$ ions is included in the effective Hamiltonian parameterization and first-principles determination using a symmetry analysis. The role of the magnetostructural coupling in the phase transition will be analyzed and discussed.

2. V. N. Glazkov et al., http://arxiv.org/abs/0807.0546