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Phase transitions and magnetostructural coupling in ZnCr_2O_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_2O_4 , a phase transition is observed from the high-temperature cubic phase to a low-temperature low-symmetry phase, reported as tetragonal¹ 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.

1. S. H. Lee et al., J. Phys. Cond. Matt. 19, 145259 (2007)
2. V. N. Glazkov et al., <http://arxiv.org/abs/0807.0546>
3. C. J. Fennie and K. M. Rabe, Phys. Rev. Lett. 96, 205505 (2006)

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