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**First-principles study of the structural and magnetic phase transition in $CdCr_2O_4$** ANIL KUMAR, KARIN RABE, Rutgers University — We use first-principles calculations to investigate the mechanism for the paramagnetic (PM) cubic to an antiferromagnetic (AFM) tetragonal structural phase transition at 7.8 K in the spinel oxide compound $CdCr_2O_4$. Because of the magnetic frustration associated with AFM interactions on the pyrochlore lattice formed by the Cr ions, we focus on the spin-lattice coupling, specifically (a) the forces on the atoms and resulting atomic displacements induced by the spin configuration and (b) the spin-phonon coupling. Using the linear response method, we determine the full phonon dispersion relations for the PM, FM and AFM orderings in cubic and tetragonal structures. We determine the strength of spin-phonon couplings using IFCs for various magnetic orderings and show that the spin-phonon couplings are large but do not lead to any unstable modes that could alone drive the structural transition at low temperatures. Instead, we find that it is the symmetry-lowering forces and stresses induced by AFM ordering that drive the cubic to tetragonal phase transition at low temperature. The results are compared with a recent experimental determination of the phonon dispersion in the in the cubic and tetragonal phases of $CdCr_2O_4$ and the implications for related compounds discussed.

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