Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Phonon anisotropy in $ZnCr_2O_4$ from first principles CRAIG J. FENNIE, RutgersUniversity, KARIN M. RABE — The geometrically frustrated spinel $ZnCr_2O_4$ undergoes a cubic-to-tetragonal structural transition simultaneously as it enters a Neel state at T_c=12.5K. A recent experiment[1] using infrared spectroscopy measured a large splitting of an optical phonon frequency at T_c; it was argued that this splitting was due to a direct spin-phonon coupling. Here, we describe a first-principles study of the zone-center optical phonons in metrically cubic $ZnCr_2O_4$, with the LSDA+U as implemented in VASP. For selected collinear magnetically ordered structures, the influence of magnetic order on the phonon frequencies is identified, confirming the recent experimental results. The origin of this large phonon anisotropy will be discussed.

[1]A.B. Sushkov et al., Phys. Rev. Letters 94 (2005) 137202.

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Date submitted: 30 Nov 2005 Electronic form version 1.4