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What controls the sign of exchange-induced phonon splitting in ACr_2O_4 spinels? ALEKSANDER WYSOCKI, TURAN BIROL, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — The interplay of spin and lattice degrees of freedom can lead to a variety of fundamentally and technologically interesting phenomena. In ACr_2O_4 spinels, it has been well established that antiferromagnetic order alone can lower the symmetry of a crystal resulting in a splitting of degenerate phonon frequencies without any structural distortion. A simple model based on nearest neighbor exchange striction has been proposed and confirmed by a novel first-principles approach. Recently however it has been suggested that magnetically induced phonon splitting is universally controlled by the nondominant exchange interaction. In this talk we present our recent first principles study of magnetically induced phonon anisotropy in ACr_2O_4 (A=Mg, Zn, Cd, Hg) spinels. We demonstrate that the different spin ordering patterns observed in the different spinel compounds can lead to an opposite sign of phonon splitting. This naturally explains the difference in sign experimentally observed for $ZnCr_2O_4$ compared with $CdCr_2O_4$, which have very different magnetic ground states. Additionally, we show that the *ab initio* values for the phonon frequencies can be very well fitted to the previously proposed spin-phonon coupling model including only the nearest neighbor exchange interaction.

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