

Abstract Submitted
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Ab initio study of renormalized phonon modes in magnetic materials¹ MATTHEW HEINE, Boston College, OLLE HELLMAN, Linköping University, Sweden, NINA SHULUMBA, California Institute of Technology, DAVID BROIDO, Boston College — Understanding the temperature dependent vibrational properties of magnetic materials in the presence of disordered local moments is a challenging problem. In such materials, the spin-spin interactions between neighboring magnetic atoms augment the usual electrostatic interactions thereby modifying the phonon spectra. To investigate such behavior, we apply a theoretical approach based on the Temperature Dependent Effective Potential (TDEP) method [1] to study the interdependence between the atomic and magnetic degrees of freedom in magnetic materials. In the framework of density functional theory we calculate the renormalized phonon dispersions at different temperatures, using the TDEP approach, sampling the appropriate thermally-relevant phase space. Results for several magnetic materials will be presented and compared to available measured data. [1] Olle Hellman, Peter Steneteg, I. A. Abrikosov, and S. I. Simak, Phys. Rev. B 87, 104111 (2013).

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Matthew Heine
Boston College

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