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Combined molecular and spin dynamics study of collective excitations in BCC iron[1] DILINA PERERA, DAVID P. LANDAU, Center for Simulational Physics, The University of Georgia, DON NICHOLSON, G. MALCOLM STOCKS, Oak Ridge National Laboratory — Spin dynamics simulations of classical spin systems have revealed a substantial amount of information regarding the collective excitations in magnetic materials. However, much of the previous work has been restricted to lattice-based spin models that completely disregard the effect of lattice vibrations. Combining an empirical many body potential with a spin Hamiltonian parameterized by first principles calculations, we present a compressible magnetic model for BCC iron, which treats the dynamics of translational degrees of freedom on an equal footing with the magnetic (spin) degrees of freedom. This model provides us with a unified framework for performing combined molecular and spin dynamics simulations and make simultaneous quantitative measurements of the spin wave and vibrational spectrum. Results from our simulations reveal that the presence of lattice vibrations leads to softening and damping of spin waves, as well as evidence for a novel form of longitudinal spin wave excitation coupled with the longitudinal phonon mode of the same frequency. Furthermore, we will also discuss the influence of lattice vibrations at different temperatures and the implications of using different atomistic potentials.

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Dilina Perera
Center for Simulational Physics, The University of Georgia

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