Ab Initio Approach to Spin-Phonon Coupling in Transition Metal Insulators

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Within the framework of numerical des Cloiseaux effective Hamiltonians, we introduce a method to compute generic spin-phonon couplings in transition metal insulators. By incorporating lattice degree of freedom and treating phonon as genuine dynamical variable within the low energy space, we compute arbitrary multipole-phonon couplings with full q-dependence. One key advantage of this approach is its ability to provide a comprehensive estimation of spin-phonon coupling, including "Raman" coupling that is required for the evaluation of phonon Hall effect [1], at a relatively modest computational expense. We benchmark this method for MnPSe3, a layered honeycomb material, to reproduce temperature-dependent damping of phonon Raman lineshapes[2].

[1] L. Sheng, D. Sheng, and C. Ting, Phys. Rev. Lett. **96**, 155901 (2006)
[2] T. T. Mai, K. F. Garrity, A. McCreary, J. Argo, J. R. Simpson, V. Doan-Nguyen, R. V. Aguilar, and A. R. H.Walker, Sci. Adv. **7**, eabj3106 (2021)