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Phonon induced magnetism in ionic materials OSCAR D. RESTREPO, NIKOLAS ANTOLIN, Materials Science and Engineering, The Ohio State University, Columbus OH 43210, HYUNGYU JIN, Mechanical and Aerospace Engineering, The Ohio State University, JOSEPH P. HEREMANS, Mechanical and Aerospace Engineering, Physics,The Ohio State University, WOLFGANG WINDL, Materials Science and Engineering, The Ohio State University — Thermoelectric phenomena in magnetic materials create exciting possibilities in future spin caloritronic devices by manipulating spin information using heat. An accurate understanding of the spin-lattice interactions, i.e. the coupling between magnetic excitations (magnons) and lattice vibrations (phonons), holds the key to unraveling their underlying physics. We report ab initio frozen-phonon calculations of CsI that result in non-zero magnetization when the degeneracy between spin-up and spin-down electronic density of states is lifted for certain phonon displacement patterns. For those, the magnetization as a function of atomic displacement shows a sharp resonance due to the electronic states on the displaced Cs atoms, while the electrons on indium form a continuous background magnetization. We relate this resonance to the generation of a two-level system in the spin-polarized Cs partial density of states as a function of displacement, which we propose to be described by a simple resonant-susceptibility model. Current work extends these investigations to semiconductors such as InSb. ODR and WW are supported by the Center for Emergent Materials, an NSF MRSEC at OSU (Grant DMR-0820414).HJ and JPH are supported by AFOSR MURI Cryogenic Peltier Cooling, Contract #FA9550-10-1-0533.

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