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Study of anomalous vibrational dynamics in tetrahedrite thermoelectrics by integrated computational and experimental methods

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Tetrahedrites with the general compostion of $Cu_{12-x}M_xSb_4S_{13}$ recently have emerged as promising thermoelectrics with earth-abundant and environment-friendly elements. While it has been shown that they possess favorable electronic properties and low lattice thermal conductivity (<1 W m-1 K-1 for a wide temperature range), the vibrational dynamics in this family of materials is not well-understood. In this talk, we will present some of our integrated computational and experimental efforts to study anomalous vibrational dynamics in tetrahedrites. We will first show computational results on the electron density, heat capacity, elastic moduli, and EXAFS spectra that agree with experiments. We will then focus on the role of lone-pair electrons of Sb on the vibrational dynamics, anomalous "phonon softening upon cooling", and quasi-localized vibration modes that lead to low lattice thermal conductivity.

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