

Large phonon anharmonicity in complex oxide and thermoelectrics

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Harmonic and quasi-harmonic models of lattice dynamics are widely successful in explaining thermodynamic properties of materials. However, in some cases, strong anharmonicity can critically affect physical properties, therefore it is important to consider the anharmonic effect in the lattice dynamics models. In this talk, we present the results of *ab initio* molecular dynamics studies of strong anharmonicity in long-standing debated VO₂ and record-high thermoelectrics SnSe. Our first-principles simulations provide good agreement with our measurements of phonon dispersions. We established that the entropy driving the metal-insulator transition in VO₂ is dominated by soft, anharmonic phonons of the metallic phase [1]. We revealed that the origin of strong anharmonicity is responsible for the unique properties of SnSe [2]. This understanding of the role of anharmonicity in lattice provides a critical component for developing more complete physical models of functional materials and energy materials.

[1] J. D. Budai*, J. Hong*, M. E. Manley, E. D. Specht, C. W. Li, J. Z. Tischler, D. L. Abernathy, A. H. Said, B. M. Leu, L. A. Boatner, R. J. McQueeney and O. Delaire, Metallization of vanadium dioxide driven by large phonon entropy. *Nature*, 515, 535–539 (2014)

[2] C.W. Li,* J. Hong,* A.F. May, D. Bansal, S. Chi, G. Ehlers and O. Delaire, submitted to *Nature Physics*.

Theoretical calculations were performed using the NERSC at LBNL and OLCF at ORNL. Modeling of neutron data was performed in CAMM, measurements were funded by the US DOE, BES, Materials Science and Engineering Division.