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Phonon Scattering in Thermoelectrics: Thermal Transport, Strong Anharmonicity, and Emergent Quasiparticles[1]

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Modern neutron and x-ray spectrometers can map phonon dispersions and scattering rates throughout reciprocal space, providing unique insights into microscopic scattering mechanisms, including anharmonicity, electron-phonon coupling, or scattering by defects and nanostructures. In addition, first-principles simulations enable the rationalization of extensive experimental datasets. In particular, ab-initio molecular dynamics simulations can capture striking effects of anharmonicity near lattice instabilities. A number of high-performance thermoelectric materials are found in the vicinity of lattice instabilities, including Pb chalcogenides PbX, SnSe, Cu2Se, among others. The large phonon anharmonicity found in such compounds suppresses the lattice thermal conductivity, enhancing their thermoelectric efficiency. In this presentation, I will present results from our investigations of phonons in these materials [1-4] using neutron and x-ray scattering combined with first-principles simulations, focusing on anharmonic effects near lattice instabilities. I will show how strong anharmonicity can lead to emergent quasiparticles qualitatively different from harmonic phonons, which we probe in our measurements and simulations of the phonon self-energy. Commonalities between systems will be highlighted, including connections between strong anharmonicity and the electronic structure. [1] O. Delaire, J. Ma, K. Marty, A. F. May, M. A. McGuire, M.-H. Du, D. J. Singh, A. Podlesnyak, G. Ehlers, M. Lumsden, B. C. Sales, Nature Materials 10, 614 (2011). [2] J. Ma*, O. Delaire*, A. F. May, C. E. Carlton, M. A. McGuire, L. H. VanBebber, D. L. Abernathy, G. Ehlers, Tao Hong, A. Huq, Wei Tian, V. M. Keppens, Y. Shao-Horn, and B. C. Sales, Nature Nanotechnology 8, 445 (2013). [3] C.W. Li, O. Hellman, J. Ma, A.F. May, H.B. Cao, X. Chen, A.D. Christianson, G. Ehlers, D.J. Singh, B.C. Sales, and O. Delaire, Physical Review Letters (2014). [4] C.W. Li,* J. Hong,* A.F. May, D. Bansal, S. Chi, T. Hong, G. Ehlers and O. Delaire, Nature Physics 11, 1063 (2015). [5] D. Bansal, J. Hong, C.W. Li, A.F. May, W. Porter, M.Y. Hu, D.L. Abernathy, and O. Delaire, Phys. Rev. B 94, 054307 (2016)

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