# Anharmonic phonons near lattice instabilities: beyond harmonic quasiparticles

Olivier Delaire, Duke University

A detailed understanding of atomic vibrations in solids is needed to refine microscopic theories of thermal transport and thermodynamics, and is of practical interest for the design of future materials. In particular, quasiparticle interactions arising from phonon-phonon, electron-phonon, or spin-phonon couplings are key to rationalize numerous functional properties, ranging from multiferroics for information processing and superionics for solid-state batteries, to thermoelectrics for waste-heat harvesting, or metal-insulator transitions for ultrafast transistors. Near phase transitions associated with phonon instabilities, one needs to properly account for the effect of strong anharmonicity, which disrupts the quasiharmonic phonon gas model through large phonon-phonon coupling terms. Large phonon amplitudes can also amplify the electron-phonon interaction and lead to renormalization of a material's electronic structure. These interactions, often neglected in textbooks, remain insufficiently understood but could open the door to new and improved material functionalities.

State-of-the-art inelastic x-ray scattering techniques are key to probe atomic dynamics in small samples and complement more traditional neutron scattering approaches. By mapping phonon spectral functions across reciprocal space, and comparing with theoretical models, phonon anharmonicity and couplings to other degrees of freedom are revealed in great detail. Our investigations bring direct insights into phonon scattering mechanisms, including anharmonicity, electron-phonon coupling, spin-phonon coupling, or scattering by defects and nanostructures. Our first-principles simulations enable the quantitative rationalization of these effects, for example with ab-initio molecular dynamics simulations and anharmonic renormalization at finite-temperature. This presentation will highlight results from our investigations of atomic dynamics in several classes of materials impacted by lattice instabilities, such as halide perovskite photovoltaics [1], ferroelectrics and multiferroics [2], thermoelectrics [4,5], superionic conductors [6,7], and $VO_2$ across its metal insulator transition [8,9].

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