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A bond-selective view of electron-phonon coupling[1]

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X-ray free electron lasers (XFELs) hold promise for revealing the properties of materials on their fundamental length and time scales near and far from equilibrium. Their combination of high flux, short pulse duration x-ray pulses makes them ideally suited for time-domain x-ray scattering studies of phonons. We can reconstruct nonequilbrium interatomic forces using optical pump, x-ray probe studies. The forces are obtained by a constrained least-squares fit of a pairwise interatomic force model to the excited-state phonon dispersion relation. This bond-selective approach to measuring electron-phonon coupling is relevant to a broad range of photoinduced phase transitions and transient light-driven states. Here, we show how this approach reveals the role of short-range forces in the bonding prototypical Peierls distorted material – bismuth, and long-range forces in the gold-standard thermoelectric bismuth telluride.

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