Seminar/Talk

First principles theory of nonlinear long-range electron-phonon interaction

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Electron-phonon interactions are often written using the approximation of linear interaction, where one only keeps the process where one electron interacts with one phonon. This is usually sufficient to quantitatively describe material properties. However, this is no longer true in anharmonic materials with significant electron-phonon interaction, such as quantum paraelectrics and halide perovskites. Currently, the only available models for nonlinear electron-phonon interaction are model Hamiltonians, written in terms of phenomenological parameters. Here, we provide a microscopic semi-analytical expression for the long-range dipole part of the 1-electron-2-phonon matrix element, which can be interfaced with first principles techniques. We show that unlike for the long-range 1-electron-1-phonon interaction, the continuum approximation is not sufficient and that the entire phonon dispersion must be considered. We calculate an expression for the quasiparticle energies and show that they can be written in terms of a 1-electron-2-phonon spectral function. To demonstrate the method in practice, we calculate the 1-electron-2-phonon spectral function for LiF and $CsPbI_3$ from first principles, and we show that the nonlinear interaction contributes significantly to the electron mobility of $CsPbI_3$. The framework presented here bridges the gap between model Hamiltonians and first-principles calculations for the 1-electron-2-phonon interaction.

Thursday, January 29, 2026 11:00am - 12:00pm
Office Bldg West / Ground floor / Foyer seminar room

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