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Electron-phonon coupling phenomena in metals: A computational perspective

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The interaction of electrons and lattice vibrations lies at the heart of many physical phenomena like electrical and heat conductivity, phonon-mediated superconductivity, dynamics of excited electrons and holes, and various temperature-dependent properties. Detailed knowledge of the electron-phonon interaction is therefore of basic interest for many phenomena in condensed matter physics. Modern DFT based techniques nowadays provide powerful tools to analyze and predict electron-phonon interaction on a microscopic level including its full momentum structure.

I will demonstrate the usefulness of this computational approach for several examples focusing on metallic systems. First the characterization of quantum size effects on electron and phonon quasiparticles as well as on superconductivity in ultrathin Pb films will be discussed. Then I will address the stability of topological surface states of Bi2Se3 against phonon-induced many-body interactions, and finally discuss the role of the electron-phonon interaction in driving charge-density wave transitions in layered transition-metal dichalcogenides.

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