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Title
Ultrafast dynamics of coupled electrons, phonons and excitons from first principles

Abstract
Combining density functional theory and related methods with kinetic equations has enabled remarkable advances in computing the ultrafast dynamics of materials from first principles. After reviewing this framework and discussing early *ab initio* calculations of electron scattering rates and ultrafast dynamics, we will focus on recent developments. The talk will present a numerical approach to evolve in time the coupled Boltzmann transport equations (BTEs) of electrons and phonons, using *ab initio* electron-phonon and phonon-phonon interactions together with a parallel algorithm to explicitly time step the BTEs. Our approach can simulate the coupled electron and phonon dynamics up to tens of picoseconds (with a femtosecond time resolution) and its quantitative accuracy can be validated by computing transport properties. Using graphene as a case study, we will demonstrate calculations of coupled ultrafast carrier and phonon dynamics, time-resolved transient absorption, structural snapshots, and diffuse X-ray scattering. Extensions to include excitons will also be discussed, focusing on calculations of exciton-phonon interactions and real-time exciton dynamics in two-dimensional materials. We will outline code development efforts, open problems and future directions.