

Wannier-Function-Based Approach to Coupled Exciton-Phonon-Photon Dynamics in Two-Dimensional Semiconductors

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Abstract

Understanding exciton-phonon interaction in two-dimensional materials from first principles is a field of growing interest. Here, we present a many-body theory for coupled free-carrier, exciton, phonon and photon dynamics based on carrier-carrier and carrier-phonon interaction matrix elements obtained via projection on Wannier orbitals. The framework is applied to study the impact of carrier-phonon correlations on optical spectra and coupled nonequilibrium carrier-phonon kinetics in monolayer MoSe₂. We find that non-Markovian effects and dynamical buildup of quasi-particles are only properly described if correlations at least on the two-phonon level are included. Our studies open a perspective to advance the material-realistic description of nonequilibrium physics in 2d nanostructures to new many-body realms.