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First-principle Approaches to Exciton-Exciton and Exciton-Phonon Interactions in Two-Dimensional Semiconductors

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Marrying the predictive power of ab initio calculations with many-body effects of ever increasing complexity remains a challenging task. For the extensively studied class of semiconducting van der Waals materials, exciton-exciton and exciton-phonon interactions are key to understanding (non)linear optical and transport phenomena. In this talk, I will present recent developments in the first-principle description of these interaction mechanims.

Exciton-exciton interactions are particularly important in certain van der Waals heterobilayers, which host layer-separated, Coulomb-correlated electron-hole pairs forming interlayer excitons with binding energies of more than 100 meV and lifetimes that are often drastically increased in comparison to excitons within a single layer. Our combined theory-experiment study of excitonic many-body effects in hBN-encapsulated $MoSe_2$/WSe_2 heterobilayers is based on first-principle band structures and Coulomb interaction matrix elements. Key to our approach is the explicit treatment of the fermionic substructure of excitons and dynamical screening effects for density-induced energy renormalization. We demonstrate that dipolar blueshifts are almost perfectly compensated by many-body effects, mainly by screening-induced self-energy corrections. Moreover, we identify a crossover between attractive and repulsive behavior at elevated exciton densities. Our results revise the established picture of dipolar repulsion dominating exciton-exciton interactions in van der Waals heterostructures.

As a complementary development, understanding carrier-phonon interaction from first principles is a field of growing interest. Here, I will introduce a many-body theory for coupled free-carrier, exciton, phonon and photon dynamics based on consistent carrier-carrier and carrier-phonon interaction matrix elements. Numerical simulations demonstrate the impact of carrier-two-phonon scattering processes on optical spectra and coupled nonequilibrium carrier-phonon kinetics in monolayer $MoSe_2$. Our studies open a perspective to advance the material-realistic description of nonequilibrium physics in two-dimensional nanostructures to new many-body levels.

Für diese Zeit steht eine Kinderbetreuung nach vorheriger Anmeldung zur Verfügung.

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