



Seminarankündigung

**Dienstag, 17. Januar 2017
16:00 Uhr**

WSI, Seminarraum S 101

“Microscopic theory of optical properties and excited-carrier dynamics of transition metal dichalcogenides”

Atomically thin layers of transition metal dichalcogenides (TMD) have emerged in the wake of graphene as new class of optically active materials. New and exciting optical properties are the result of the two-dimensional carrier confinement and a particularly strong Coulomb interaction due to strongly reduced dielectric screening. Many theoretical investigations were concerned with band structure and ground-state absorption properties in the framework of ab-initio calculations. Accessing the emission properties in the presence of excited carriers requires to go beyond these methods. Our approach combines ab-initio models for the calculation of electronic properties with semiconductor many-body theory to describe the dynamics of excited carriers and their influence on optical properties.

Under photoexcitation of carrier densities up to 10^{13} cm^{-2} , absorption spectra reveal a redshift and mild bleaching of the excitonic ground state resonance, whereas higher excitonic lines are found to disappear successively due to Coulomb-induced band-gap shrinkage of more than 500 meV and binding-energy reduction. Results for different TMD materials are compared and discussed.

Complementary information about the system is obtained from photoluminescence spectra, which are calculated in the same spirit of combining an accurate ground-state description with systematic many-particle theory. We show that the presence of several band-structure valleys in close energetic vicinity manifests itself in a strongly carrier-density- and strain-dependent emission intensity yield.

Although excitonic signatures appear in the optical absorption and emission spectra the properties of incoherent exciton populations are difficult to determine and are still an open question. We will present first results about the ionization equilibrium between excitons and the electron-hole plasma in monolayer TMDs.

For investigations of the carrier dynamics we present results of a quantum-kinetic theory for the carrier scattering. Ultrafast relaxation of initial nonequilibrium carrier distributions due to optical excitation are demonstrated. Large excess energies of 400meV can be dissipated within a few ten fs due to efficient carrier scattering, also observed in recent experiments.

Besides excitonic features, signatures of trions appear in optical spectra if one carrier species (electrons or holes) is injected into the material, for example via chemical doping by a substrate, or if electrons and holes are excited simultaneously. Linear absorption spectra including trionic effects are presented and the doping dependence of trion oscillator strength and binding energies is discussed.

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