SYTS 1: Interaction effects and correlations in twodimensional systems - New challenges for theory

Time: Wednesday 15:00–17:45 Location: H1

Invited Talk SYTS 1.1 Wed 15:00 H1

Spectra of layered semiconductors from many-body perturbation theory — Thorsten Deilmann, Peter Krüger, Philipp Marauhn, and •Michael Rohlfing — Westfälische Wilhelms-Universität Münster, Institut für Festkörpertheorie, Münster, Germany

Two-dimensional systems pose particular challenges in describing electronic correlation effects: dielectric screening becomes highly anisotropic, and spatial confinement enhances the interaction between electrons and/or holes. Such effects modify both the electronic spectrum and excitonic binding effects, both of which also depend on sample thickness, substrate, and inter-layer wave function overlap.

These mechanisms can be described by ab-initio many-body perturbation theory (MBPT), notably by the GW approximation and the Bethe-Salpeter equation (GW-BSE). Its particular merit is the consideration of non-local dielectric screening effects.

We discuss spectral shifts of transition-metal dichalcogenides depending on the environment. Compared to an isolated monolayer, excitons are shifted to lower energy with increasing number of layers or when a monolayer is deposited on a substrate [1]. In addition, we discuss the competition between intra-layer excitons (i.e. with electron and hole on the same layer) and inter-layer excitons [2].

[1] M. Drüppel et al., Nature Comm. 8, 2117 (2017); Y. Niu et al., Nanomaterials 8, 725 (2018).

[2] A. Arora et al., Nature Comm. 8, 639 (2017); Nanoscale 10, 15571 (2018).

Invited Talk SYTS 1.2 Wed 15:30 H1

Dark exciton dynamics in 2D materials — •Ermin Malic — Chalmers University of Technology, Göteborg, Sweden

Transition metal dichalcogenides (TMDs) exhibit a remarkably strong Coulomb interaction giving rise to the formation of tightly bound excitons. In addition to regular bright excitonic states, there is also a variety of dark excitons that cannot be accessed by light due to the required momentum-transfer or spin-flip.

Combining semiconductor Bloch equations and the Wannier equation, we demonstrate time- and momentum-resolved formation, thermalization, and photoemission of bright and dark intra- and interlayer excitons in TMD monolayers and heterostructures. In particular, we reveal the impact of dark exciton states on photoemission and differential absorption spectra. We present in a joint theory-experiment collaboration a direct evidence for the existence of energetically lowest momentum-dark excitons in tungsten-based TMDs. Finally, we show a possible technological application of 2D materials by predicting a novel dark-exciton-based mechanism for optical sensing of molecules and strain.

Invited Talk SYTS 1.3 Wed 16:00 H1

Excitons versus electron-hole plasma in monolayer transition metal dichalcogenide semiconductors — •Alexander Steinhoff[1], Matthias Florian[1], Malte Rösner[1,2,3], Gunnar Schönhoff[1,2], Tim O. Wehling[1,2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Germany — [3]Present address: Center for Computational Quantum Physics, Flatiron Institute, New York

When electron-hole pairs are excited in a semiconductor, it is a priori not clear if subsequent relaxation leads to a gas of bound excitons or to an interacting plasma of unbound electrons and holes. In atomically thin transition metal dichalcogenide semiconductors, excitons are particularly important even at room temperature due to strong Coulomb interaction.

I will show how many-body methods can be combined with first-principle calculations to quantify the thermodynamic fission-fusion balance of excitons and electron-hole plasma. Due to the two-dimensional nature of these materials, the exciton-plasma balance can be efficiently tuned via the dielectric environment. We observe entropy ionization of excitons at low excitation densities and a Mott transition to a fully ionized plasma at high densities. Below the Mott transition, excitonic screening plays an important role in the description of the exciton-plasma balance. We propose the observation of these effects by studying exciton satellites in photoemission spectroscopy, which is sensitive to the single-particle spectral functions.

15 min. break

Invited Talk SYTS 1.4 Wed 16:45 H1

Theory of near K-point optical properties of TMDC multilayers — •Tineke Stroucken, Lars Meckbach, Ulrich Huttner, and Stephan W. Koch — Department of Physics and Materials Sciences Center, Philipps-Universität Marburg, D-35032 Marburg, Germany

With the ability to create them as monolayers, van der Waals bonded layers have emerged as a new material class. The availability of different materials with a similar lattice structure but different band-gaps combined with recent advances in stacking technology allows for the engineering of the overall electronic and optical properties to a wide extent, making them an especially promising platform for fundamental material physics studies of two-dimensional systems as well as potential applications in optoelectronic and valleytronic devices.

From a theoretical point of view, the systematic design and engineering of the electronic and excitonic properties of TMDC systems demands a predictive microscopic theory that includes the fundamental structural properties as well as the strong Coulomb interaction effects among the electronic excitations. To this end, we developed a theoretical framework that combines density-functional theory with a dielectric model to determine the Coulomb interaction potential in a multilayer environment, the gap equations for the renormalized ground state, and the Dirac-Bloch equations for the calculation of the optical excitations. Within this framework, we determine both the Coulombic renormalization of the K- point band gap and the optical response for different multilayer configurations and excitation conditions.

Invited Talk SYTS 1.5 Wed 17:15 H1

High-throughput modeling and discovery of novel 2D materials — •Kristian Thygesen — Technical University of Denmark, Lyngby, Denmark

I will discuss how the electronic and optical properties of general 2D materials and their heterostructures can be accurately predicted by combining classical electrostatic models with many-body quantum mechanics and high-performance computing. I will give examples from our recent research focusing on 2D structures with tunable band energies, excitons, and plasmons[1]. Finally, I will present our recent efforts to establish a comprehensive database of 2D materials using an automatic high-throughput framework (http://c2db.fysik.dtu.dk) and show how it can be used to identify novel 2D materials with interesting physical properties such as ferromagnetism and non-trivial topology[2].

[1] Calculating excitons, plasmons, and quasiparticles in 2D materials and van der Waals heterostructures, K. S. Thygesen, 2D Materials 4, 022004 (2017)

[2] The Computational 2D Materials Database: High-throughput modeling and discovery of atomically thin crystals, S. Haastrup et al. 2D Materials 5, 042002 (2018)