Abstract

In recent years, two-dimensional (2D) van der Waals crystals, such as bilayer graphene (BLG) and transition metal dichalcogenides (TMDCs), have emerged as promising platforms for exploring novel physical phenomena at the atomic scale. These materials hold significant potential for advancing quantum technologies due to their unique electronic, optical, and mechanical properties. However, the role of many-body effects—particularly in the optical response—remains not fully understood. This dissertation develops and extends the theoretical framework for modeling electron–electron interactions in 2D crystals, focusing on the formation and evolution of neutral and charged excitonic complexes in 2D electron gases in these materials.

We investigate the optical properties of gated BLG quantum dots (QDs), where electrical gating opens an energy gap, transforming BLG into an electrically tunable semiconductor, with both electrons and holes confined by lateral gates. The BLG QDs are modeled using an atomistic tight-binding (TB) approach, enabling the calculation of confined electron and hole states in structures containing over a million atoms. Coulomb matrix elements and self-energies are computed to capture many-body effects, and the Bethe-Salpeter equation (BSE) is solved for both neutral and charged excitons. The resulting emission and absorption spectra provide insight into the optical response. Our results show that excitons in BLG QDs differ from those in conventional semiconductor QDs, with their energy tunable by voltage across a broad range, from terahertz (THz) to far infrared. The conservation of spin, valley, and orbital angular momentum leads to a fine structure in the excitons, characterized by a band of dark low-energy states. We also explore negatively charged excitons (trions), which, unlike in conventional QDs, exhibit a rich fine structure. Furthermore, we predict the existence of bright low-energy emission states and propose that temperature-dependent emission spectra could be used to extract the fine structure of the trion.

The research also explores the behavior of excitonic complexes in TMDC monolayers in high magnetic fields, focusing on how charge density and magnetic field strength influence the formation and properties of magnetoexcitons. Single layers of TMDCs, with their unique electronic and optical characteristics driven by strong spin-orbit coupling (SOC), broken inversion symmetry, and direct band gaps in the visible spectrum, provide a versatile platform for investigating many-body effects. A high magnetic field alters the energy spectrum of TMDC monolayers, leading to the formation of quantized Landau levels, along with spin and valley Zeeman splittings. These phenomena significantly enhance light-matter interactions and the optical response of the material. The electronic structure is first obtained through *ab initio* calculations, which are then used to parameterize a material-specific model incorporating both SOC and magnetic field effects. To study the optical response, the BSE is solved for magnetoexcitons—bound electron-hole pairs that form under the influence of the magnetic field. Special emphasis is placed on the impact of charge density and magnetic field strength on the excitonic spectrum, allowing for a detailed analysis of many-body effects and the resulting optical transitions.

The electronic properties of $MoSe_2/WSe_2$ heterostructures are also studied, with a focus on the effects of vertical electric fields on interlayer coupling and band alignment. *Ab initio* calculations reveal a type-II band alignment, with conduction band minima at the K and Q points in the Brillouin zone and valence band maxima at the K and Γ points. Analyzing the Kohn-Sham wave functions reveals the

contributions from layer, spin, and orbital degrees of freedom. A TB model based on these results is then constructed to provide a deeper understanding of interlayer interactions. The effect of a vertical electric field is explored, showing that vertical gating allows control over the valleys' extrema and their occupancy. Additionally, the study investigates laterally gated quantum dots within the heterostructure, analyzing how a perpendicular electric field influences their energy spectrum. The results demonstrate that tuning the electric field enables selective control over the valley character of the quantum dot states, localizing them in either the K or Q valleys, as evidenced by characteristic degeneracies and wave functions. This approach reveals the tunability of confined quantum dot states, offering new strategies for controlling optical transitions in 2D material heterostructures.

Ultimately, this dissertation advances the understanding of the optical properties of 2D materials by providing a comprehensive theoretical description of many-body effects in excitons and trions. The insights gained into the control and manipulation of excitonic states—under the influence of electric and magnetic fields, interlayer coupling, and valley-dependent interactions—offer new perspectives for tuning optical responses at the nanoscale. These findings lay the groundwork for the development of next-generation optoelectronic and quantum devices, including exciton-based transistors, high-efficiency light emitters, and scalable quantum information platforms. By deepening our knowledge of correlated states in low-dimensional materials, this work contributes both to fundamental science and to the design of novel quantum materials and photonic technologies.