Streszczenie w języku angielskim

This dissertation is devoted to the investigation of the optical properties of excitonic complexes in monolayers of transition metal dichalcogenide alloys, particularly $MoWSe_2$ and WSSe. TMD alloys constitute a particularly attractive class of two-dimensional materials due to the possibility of nearly continuous tuning of their electronic and optical properties through variations in chemical composition. This enables the design of materials with tailored characteristics, making them promising candidates for applications in optoelectronics and valleytronics.

The main objective of this work was to identify and investigate the optical properties of excitonic complexes observed in low-temperature photoluminescence spectra of hBN-encapsulated TMD alloy monolayers. An important aspect of this study was also the investigation of the evolution of these complexes under an external magnetic field applied both perpendicular and parallel to the monolayer plane.

For WSSe monolayer encapsulated in hBN, photoluminescence spectra as a function of sample temperature and low-temperature photoluminescence spectra as a function of excitation power were investigated. Based on these measurements, the resonances associated with the neutral exciton and trion were identified. Measurements performed under an external magnetic field applied parallel to the monolayer plane enabled the identification of an optically forbidden excitonic ground state. Measurements under a magnetic field applied perpendicular to the monolayer plane enabled the determination of the g-factors of the observed resonances from their Zeeman splitting. Analysis of the obtained g-factor values allowed an unambiguous identification of excitonic complexes observed in low-temperature photoluminescence spectra of hBN-encapsulated WSSe monolayers.

For hBN-encapsulated $Mo_xW_{1-x}Se_2$ monolayers with different Mo/W ratios of 85/15, 68/32, 49/51, 46/54, and 23/77, the evolution of photoluminescence spectra as a function of sample temperature and low-temperature photoluminescence spectra as a function of excitation laser power were investigated. Based on these measurements, resonances corresponding to the neutral exciton and trion were identified. Photoluminescence measurements under a magnetic field applied perpendicular to the monolayer plane were performed. The obtained Zeeman splitting enabled the determination of the g-factors of neutral excitons and trions. A nonlinear dependence of the neutral exciton g-factor on alloy composition was observed. DFT band structure calculations were performed to explain this effect. The calculated values of the conduction-band, valence-band, and effective neutral exciton g-factors enabled interpretation of the experimental results. Large values of the neutral exciton g-factor were attributed to the mixing of conduction-band states originating from the K and Q valleys, leading to changes in the orbital character of the conduction band.

The influence of an in-plane magnetic field on the optical properties of hBN-encapsulated $Mo_xW_{1-x}Se_2$ monolayers was investigated. The dark neutral exciton emission became increasingly pronounced with increasing in-plane magnetic field. The lower energy of this resonance relative to the bright neutral exciton indicates an optically forbidden excitonic ground state. The dark excitonic ground state was confirmed by DFT calculations including GW corrections, which enabled determination of the spin ordering of the conduction and valence bands. Based on the experimental and theoretical results, $Mo_{0,49}W_{0,51}Se_2$, $Mo_{0,46}W_{0,54}Se_2$, and $Mo_{0.68}W_{0.32}Se_2$ monolayers were identified as materials with an optically forbidden excitonic ground state. The energy splitting between bright and dark neutral excitons was also determined for these monolayers. Additionally, for $Mo_{0.68}W_{0.32}Se_2$, the in-plane g-factor associated with the mixing of bright and dark neutral exciton states was determined. A decrease in the bright exciton emission intensity with increasing in-plane magnetic field was also observed. This effect has not previously been reported for TMD monolayers. A theoretical model explaining the observed effect and its relation to the in-plane g-factor was proposed.

The obtained results provide an important contribution to the understanding of the optical properties of transition metal dichalcogenide alloy monolayers and provide the information essential for the design of future optoelectronic and valleytronic devices based on two-dimensional materials.

This dissertation is divided into eight chapters and supplementary materials.

- **Chapter 1** provides a literature review on two-dimensional materials, semiconducting transition metal dichalcogenides, and excitonic complexes. The influence of temperature and excitation power on the photoluminescence spectra of TMD monolayers, as well as the properties of dark excitons, the Zeeman effect, and the optical properties of transition metal dichalcogenide alloys, are discussed.
- **Chapter 2** is devoted to sample preparation methods, including bulk crystal growth and determination of alloy composition using SEM-EDX techniques. Mechanical exfoliation, methods for monolayer selection and identification, as well as deterministic transfer techniques used for hBN encapsulation of alloy monolayers are also described.
- In **Chapter 3** presents the experimental techniques applied in this work, including photoluminescence and Raman scattering measurements.
- **Chapter 4** describes the experimental setups used in this work, including low-temperature photoluminescence measurements, experiments performed under an external magnetic field, and Raman spectroscopy measurements.
- **Chapter 5** focuses on the optical properties of hBN-encapsulated WS_xSe_{1-x} monolayers and the influence of temperature, excitation power, and external magnetic fields on the observed excitonic complexes.
- **Chapter 6** presents studies of hBN-encapsulated $Mo_xW_{1-x}Se_2$ monolayers under an external magnetic field applied perpendicular to the monolayer plane and an analysis of the dependence of g-factor values on alloy composition. DFT band structure calculations and theoretical values of the neutral exciton g-factor used to interpret the experimental results are also presented.
- **Chapter 7** is devoted to studies of the influence of an in-plane magnetic field on the optical properties of $Mo_xW_{1-x}Se_2$ monolayers. The analysis includes dark exciton brightening and bright exciton darkening effects. Band structure calculations confirming the dark nature of the excitonic ground state are also presented. In addition, a theoretical model explaining the observed decrease in bright exciton emission intensity and its relation to the in-plane g-factor is discussed.
- **Chapter 8** summarizes the main results of the dissertation and presents the scientific achievements of the Author.

Supplementary materials include three appendices containing additional theoretical calculations and an analysis of measurement uncertainties related to the determination of g-factor values.