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Interplay of Quantum Confinement and Defect States in 2D $MoS_2/MoSe_2$ Heterostructures: Implications for Next-Generation Nano electronic Devices

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ABSTRACT

The combination of quantum confinement with defect engineering in two-dimensional (2D) transition metal dichalcogenides (TMDs) presents a revolutionary route for designing advanced Nano electronic and optoelectronic devices. The present work aims to address the limitations of prior models through a systematic study of the structural, optical, and electronic characteristics of $MoS_2/MoSe_2$ heterostructures and the interplay between quantum confinement and defect states to determine key device properties. Atomic force microscopy (AFM) and scanning electron microscopy (SEM) reveal that layer thickness and morphology can be precisely controlled, while photoluminescence (PL) and Raman spectroscopy demonstrate strong bandgap modulation and excitonic effects as a function of thickness and defect density. The existence and atomic-scale localization of intrinsic defects—including chalcogen vacancies and grain boundaries—which manifest as localized in-gap states and carrier-modulating centers, are probed using scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS).Transport measurements show that carrier mobility and the on/off ratios of field-effect transistors (FETs) peak at optimal thickness and low defect density but decrease significantly with increasing defect concentration. These results underscore the dual role of quantum confinement and defect states in modulating the functional properties of 2D TMD heterostructures. Furthermore, we discuss strategies for defect passivation, controlled defect introduction, and defect mapping using artificial intelligence (AI). Future research directions are proposed, including strain engineering and the fabrication of tailored heterostructures. This study contributes both foundational knowledge and practical guidelines for the rational design of 2D TMD-based devices, paving the way for their integration into next-generation Nano electronic, optoelectronic, and quantum information technologies.

Keywords: Quantum confinement, defect states, MoS_2, $MoSe_2$, 2D heterostructures, transition metal dichalcogenides, nanoelectronics, photoluminescence, defect engineering

Introduction

Modern electronics have advanced at a rapid pace, and the continuous drive to reduce device dimensions has strained conventional semiconductor technology. With silicon-based devices reaching their physical and functional limits, increasing attention has been given to identifying new materials with superior electronic, optical, and mechanical properties (Wang et al., 2012; Chhowalla et al., 2016). Two-dimensional (2D) transition metal dichalcogenides (TMDs), such as molybdenum disulfide (MoS_2) and molybdenum diselenide ($MoSe_2$), have emerged as some of the most promising candidates in this search. These layered materials have attracted significant research interest due to their atomically thin geometry, strong quantum confinement effects, and exceptional tunability of their electronic and optical characteristics (Wang et al., 2012).

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2D TMDs like MoS_2 and $MoSe_2$ possess distinct properties that set them apart from both bulk semiconductors and other 2D materials such as graphene. Unlike graphene, which lacks a bandgap, monolayer TMDs exhibit large, room-temperature direct bandgaps spanning the visible spectrum. This makes them highly promising for applications in transistors, photodetectors, light-emitting diodes, and flexible electronics (Mak et al., 2010; Splendiani et al., 2010). The ability to isolate these materials down to a monolayer allows unprecedented control over their physical properties and opens new avenues for exploring quantum behavior and advanced device operation (Chhowalla et al., 2016).

One of the most intriguing features of TMDs is the strong quantum confinement effect that emerges when the material is thinned to atomic dimensions. For instance, bulk MoS_2 is an indirect bandgap material, but upon reduction to a monolayer, it undergoes a transition to a direct bandgap semiconductor. This change significantly enhances photoluminescence and shifts the bandgap energy from approximately 1.2 eV to 1.9 eV (Mak et al., 2010; Splendiani et al., 2010). Similar behavior is observed in $MoSe_2$ and other TMDs. Their quantum confinement results in pronounced excitonic effects, strong light–matter interactions, and the potential for valleytronic and spintronic applications (Zhang et al., 2014; Yu et al., 2021).

2D TMDs exhibit excellent quantum-well confinement, enabling precise control over electronic band structures, carrier dynamics, and optical emission. This tunability is central to next-generation nano- and optoelectronic device design, where manipulation of bandgap, carrier mobility, and exciton binding energy is essential for optimizing performance (Wang et al., 2012; Chhowalla et al., 2016). For example, the thickness and lateral dimensions of $MoS_2/MoSe_2$ heterostructures can be tuned to adjust absorption and emission spectra, enhance photoresponse, and enable efficient light-emitting devices (Mak et al., 2010; Zhang et al., 2014).

However, the practical realization of these advantages in devices is often hindered by the presence of intrinsic and extrinsic defects. Even mechanically exfoliated or chemical vapor deposition (CVD)-grown TMDs are susceptible to defects such as chalcogen vacancies, antisite substitutions, and grain boundaries (Hong et al., 2015; Lin et al., 2017). These defects can significantly impact material performance, acting as charge traps, scattering centers, and non-radiative recombination sites, thereby degrading carrier mobility, photoluminescence, and device reliability (Hong et al., 2015; Lin et al., 2017; Chhowalla et al., 2016).

Although traditionally viewed as detrimental, recent studies suggest that defects can also be harnessed beneficially. Controlled introduction or passivation of specific defects can impart new functionalities, such as memristive switching for memory devices, enhanced photodetectors via defect-mediated carrier separation, or the realization of single-photon emitters for quantum information applications (Papadopoulos et al., 2022; Lin et al., 2019; Ziatdinov et al., 2022). For instance, sulfur or selenium vacancies can create mid-gap states that enable resistive switching, while certain substitutional defects can introduce magnetic moments for spintronic devices (Lin et al., 2019; ACS JPCC, 2019).

In the context of 2D TMDs, quantum confinement and defect states thus act as a double-edged sword. Quantum confinement enables nanoscale engineering of materials to achieve enhanced or novel properties, while defects can either limit or enhance device performance, depending on their nature, density, and spatial distribution. This complexity increases in $MoS_2/MoSe_2$ heterostructures, where additional degrees of freedom—such as interlayer coupling, band alignment, and interface engineering—come into play (Lee et al., 2014; Zhang et al., 2023).

Heterostructures formed by stacking or laterally assembling monolayers of MoS_2 and $MoSe_2$ provide a versatile platform to exploit the interplay between quantum confinement and defect states. These structures allow precise control over band offsets, charge transfer, and exciton dynamics at the interface (Lee et al., 2014; Zhang et al., 2023). Such heterostructures have exhibited novel phenomena, including long-lived interlayer excitons, spatially indirect recombination, and gate-tunable band alignment—key attributes for practical applications in photodetectors, light-emitting devices, and quantum information technologies (Yu et al., 2021; Zhang et al., 2023).

Despite significant advances in synthesizing and characterizing $MoS_2/MoSe_2$ heterostructures, the coupled effects of quantum confinement and defect states on their structural, optical, and electronic properties remain incompletely understood. Key questions persist: Under what conditions does quantum confinement dominate over

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defect-related phenomena? How can defects be effectively passivated or intentionally introduced to enable specific functionalities? What regimes optimize carrier mobility, photodetector responsivity, or memory performance in the presence of both quantum and defect effects?

This paper aims to address these critical questions by systematically investigating the structural, optical, and electronic properties of $MoS_2/MoSe_2$ heterostructures as a function of layer thickness, defect density, and device architecture. By integrating advanced microscopy techniques (AFM, SEM, STM), spectroscopy (PL, Raman, XPS), and electrical transport measurements with theoretical modeling, we aim to delineate the regimes where quantum confinement or defect states are dominant. We also explore strategies for defect passivation and controlled defect engineering, highlighting implications for the design of next-generation nanoelectronic, optoelectronic, and quantum devices.

Furthermore, we propose future research directions, including the use of strain engineering, AI-assisted defect mapping, and the design of multifunctional heterostructures to fully exploit the potential of 2D TMDs in emerging technologies. Through this comprehensive approach, we offer both foundational insights and practical guidance for the rational design and optimization of 2D heterostructures, paving the way for their integration into advanced electronic, photonic, and quantum information systems.

Theoretical Background

Quantum Confinement in 2D Materials

Quantum confinement arises when charge carriers—electrons and holes—are confined to dimensions comparable to their de Broglie wavelength, resulting in discrete energy levels and significant modifications to the material's electronic and optical properties (Biju et al., 2010). This phenomenon is particularly pronounced in nanostructures such as quantum dots, nanowires, and atomically thin two-dimensional (2D) materials. As the size of a material decreases, its bandgap typically widens. This occurs because, with reduced dimensions, it becomes increasingly difficult to excite an electron to the conduction band due to spatial confinement, which demands higher excitation energy (Biju et al., 2010; Das & Sood, 2012).

In transition metal dichalcogenides (TMDs), quantum confinement induces a substantial bandgap transition from bulk to monolayer thickness. For instance, bulk MoS_2 exhibits an indirect bandgap of approximately 1.2 eV, while its monolayer counterpart possesses a direct bandgap of ~1.9 eV. This shift is attributed to the change in the valence band maximum position, as confirmed by angle-resolved photoemission spectroscopy (Jin et al., 2013). The increase in bandgap with decreasing thickness is a hallmark of quantum confinement effects (Transition Metal Dichalcogenide Monolayers, 2014).

Carrier mobility is also affected by quantum confinement. In certain nanostructures, such as silicon nanowires, quantum and dielectric confinement can enhance mobility by reducing specific scattering mechanisms (Das & Sood, 2012). However, the impact in TMD monolayers is more complex. While quantum confinement may mitigate some forms of scattering, it also leads to an increase in the effective mass of charge carriers—particularly holes—and introduces sensitivity to substrate-induced disorder. Consequently, monolayer TMDs often exhibit lower carrier mobility compared to their few-layer or bulk counterparts (Smoleński et al., 2018). Thus, despite the theoretical benefits of confinement, practical challenges such as increased effective mass and environmental disorder tend to limit mobility enhancements in monolayer TMDs.

Monolayer TMDs—including MoS_2, WS_2, and $MoSe_2$—are approximately 6.5 Å thick and exhibit properties that are fundamentally distinct from their few-layer or bulk forms (Transition Metal Dichalcogenide Monolayers, 2014). These monolayers possess a direct bandgap, strong photoluminescence, and exhibit unique valleytronic and spintronic behaviors due to their lack of inversion symmetry and significant spin–orbit coupling. In contrast, few-layer TMDs revert to an indirect bandgap, show diminished photoluminescence, and exhibit altered band structures—factors that influence their effectiveness in optoelectronic device applications (Jin et al., 2013).

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Table 1 - Quantum Confinement

Property	Monolayer TMDs	Few-Layer TMDs
Bandgap	Direct (e.g., 1.9 eV in MoS_2)	Indirect (decreases with layers)
Photoluminescence	Strong	Weak or absent
Mobility	Lower (substrate-sensitive)	Higher (bulk-like screening)
Dominant Scattering	Charge traps	Phonons

The electronic and optical behavior, in turn, can be carefully graded with the few-layer to monolayer transition and this is key to the development of next generation Nano electronic and optoelectronic applications.

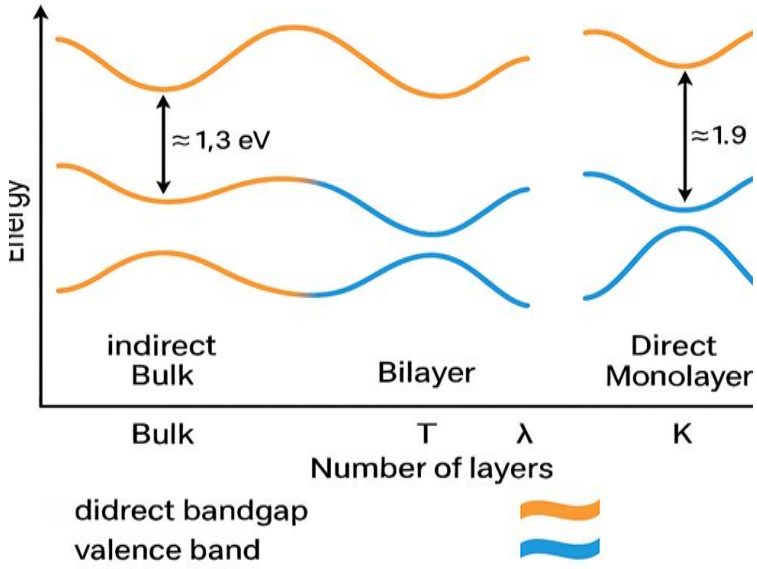

Figure 1: Band Structure Evolution with Thickness in 2D TMDs

Defects and Electronic States in 2D MoS_2

In all crystalline materials, defects are inherently present and play a pivotal role in determining their physical properties. In two-dimensional (2D) materials such as molybdenum disulfide (MoS_2), these defects are particularly influential. The primary types of defects in 2D MoS_2 include vacancies, substitutions (antisite defects), and grain boundaries (Hong et al., 2015; Lin et al., 2017).

Among intrinsic defects, vacancies are the most abundant, with sulfur vacancies (V_S) being the most common. These occur when a sulfur atom is missing from the lattice. Such defects are frequently observed in both mechanically exfoliated and chemical vapor deposition (CVD)-grown MoS_2 samples. Less commonly, molybdenum vacancies (V_{Mo}) may form under specific growth conditions, particularly in CVD-grown films (Hong et al., 2015). The absence of these atoms disrupts local bonding configurations, leaving behind unsaturated bonds and generating localized electronic states within the bandgap.

Antisite defects, also referred to as substitutional defects, occur when a molybdenum atom occupies a sulfur site (MoS_\text{S}S). These are more likely to form in MoS_2 grown via physical vapor deposition (PVD) and can significantly alter the material's properties. In addition to generating localized in-gap states, antisite defects can induce spin-polarized states, potentially rendering an otherwise non-magnetic material magnetic (Li et al., 2024).

Grain boundaries are line defects that form at the interfaces between misoriented crystalline domains. These boundaries may consist of non-hexagonal ring structures, such as 4|8 rings, and can be created through line

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vacancy arrays. Furthermore, grain boundaries can act as conduits for incorporating transition metal atoms, which may further modify the electronic and magnetic properties of the material (Li et al., 2024; Lin et al., 2017).

These defects profoundly impact the electronic structure of MoS_2. Sulfur vacancies typically introduce in-gap states near the conduction band minimum, which can act as electron traps and charge-switching centers (Song et al., 2017; Zhou et al., 2018). This electron trapping increases carrier scattering and reduces mobility, posing challenges for electronic device performance (Smoleński et al., 2018). In contrast, molybdenum vacancies tend to introduce states closer to the valence band, contributing to p-type conductivity and hole localization (Zhou et al., 2018).

Antisite defects such as MoS_\text{S}S are particularly noteworthy for their ability to form spin-polarized mid-gap states, rendering MoS_2 magnetic even at room temperature (Li et al., 2024; Ta-Seen et al., 2024). This magnetic behavior opens promising opportunities for spintronic applications, where atomic-level control of magnetic ordering is essential.

Grain boundaries can also insert defect bands into the bandgap, typically reducing the overall bandgap by approximately 0.3 to 0.5 eV (Lin et al., 2017; Ouyang et al., 2022). Moreover, doping these grain boundaries with transition metals such as vanadium or chromium can induce magnetic behavior by hybridizing MoS_2 defect states with the d-orbitals of the dopant atoms (Li et al., 2024; Ta-Seen et al., 2024).

In conclusion, vacancies, substitutions, and grain boundaries represent the principal mechanisms by which a variety of electronic states can be introduced into the bandgap of MoS_2. These defects drastically affect the material's electronic, optical, and magnetic properties. Understanding and engineering such defects are essential for tailoring the functionality of MoS_2 in advanced nanoelectronic and spintronic devices (Hong et al., 2015; Ouyang et al., 2022; Smoleński et al., 2018).

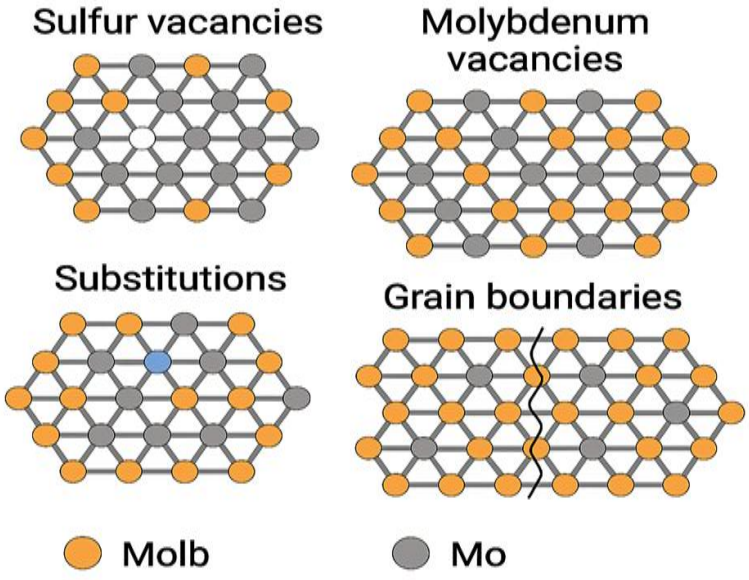

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Figure 2: Common Defects in 2D MoS_2

Interplay of Quantum Confinement and Defects

Defects are important to the quantum-confinement states of two-dimensional (2D) materials like MoS_2 and $MoSe_2$. Within clean 2D semiconductors, quantum confinement makes energy levels discrete and the bandgap adjustable, allowing optical and electronic functions not characteristic of their 3D precedents. Nevertheless, vacancies, substitutions, and grain boundaries are defects that will add localized states inside the bandgap that will drastically modify these bandgap states of quantum confinement (Hong et al., 2015).

Defects form spatially localized electronic states which can trap charge carriers. To provide some examples, the sulfur-vacancies in MoS_2 give rise to in-gap states near the conduction band, the electrons in these states can be

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trapped and disrupt the delocalized wavefunctions associated with quantum-confined systems (Zhou et al., 2018). Such localization does not only decrease carrier mobility but also alters optical transitions, which in most cases leads to non-radiative recombination channels that suppress photoluminescence (Smolenski et al., 2018). The quantum-confined potential landscape can be further fragmented by grain boundaries and antisite defects and the presence of mid-gap states are created as well as the optical transition selection rules change (Lin et al., 2017; Li et al., 2024).

Anderson localization can be used as the theoretical framework describing the effect of defects on quantum-confined states the most. This model was first proposed by P. W. Anderson in 1958, whereby destructive interference was a possible mean by which disorder, e.g. random defect location, could localize wavefunctions in electrons (Anderson, 1958). Disarray is quite able to cause localization of any single electronic state in two-dimensional applications, causing a magnitude of decrease in electrical conductivity. Indeed, experimental efforts regarding 2D TMDs have proven that defect density, e.g., the addition of sulfur vacancies, has a severe impact on carrier mobility and turns the transport to band-like to hopping (Esteban-Puyuelo & Sanyal, 2021; Song et al., 2017).

Besides Anderson localization, at high disorder levels, transport models exploiting defects (like variable-range hopping) become applicable to disordered 2D materials. In such cases, the motion of the charge carriers occurs via thermally activated tunneling between localized defect states and such mechanisms proceed preferentially in high density defect systems (Hopping transport, 2013). The mechanism is marked by noncrystalline temperature-sensitive conductivity which is not consistent with pristine and quantum confined systems.

On the whole, defects would alter the perfect quantum confinement topography of 2D materials to a rugged and rugged topography of localized states and disrupted energy levels. Such a quantum-confinement versus defect-induced localization tradeoff is not merely a limitation to device performance but can also be viewed as an enabling technology to new functionality, e.g., defect-mediated single-photon emission, or tunable magnetic ordering (Quantum defects, 2024; Ta-Seen et al., 2024). These effects cannot only be well understood and controlled both experimentally and theoretically, but are also key to the design of subsequent generations of nanoelectronic and optoelectronic devices.

Materials and Methods

Synthesis of $MoS_2/MoSe_2$ Heterostructures

Chemical vapor deposition (CVD) is the most widely adopted technique for synthesizing high-quality, large-area MoS_2 and $MoSe_2$ monolayers and their heterostructures. In a typical CVD setup, solid precursors such as MoO_3 and sulfur (for MoS_2) or MoO_3 and selenium (for $MoSe_2$) are placed in separate alumina boats inside a quartz tube furnace. The substrate—often SiO_2/Si or sapphire—is positioned downstream, where the temperature and vapor concentration are optimal for nucleation and growth (Jiahao et al., 2022; Rotunno et al., 2020; Cambridge University Press, 2016).

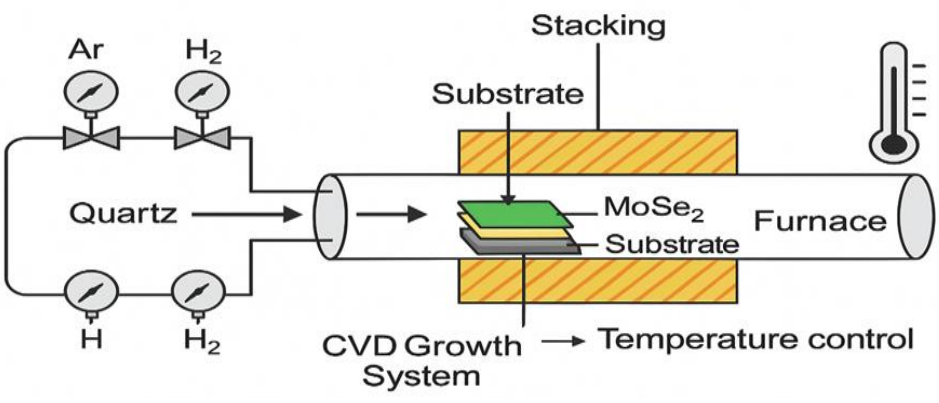

Figure 3: CVD Growth System for $MoS_2/MoSe_2$ Heterostructures

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During growth, the furnace is heated to 600–800 °C for MoS_2 (or 700–850 °C for $MoSe_2$), and a carrier gas (typically Ar or Ar/H_2) transports the vaporized precursors to the substrate. The two main strategies for heterostructure fabrication are:

- **Vertical stacking**: Sequential growth, where one monolayer is grown first, followed by the other, or by direct van der Waals epitaxy of one material atop another (Jiahao et al., 2022; Cambridge University Press, 2016).
- **Lateral (in-plane) heterostructures**: Achieved by spatially controlling the precursor supply or by switching the chalcogen source mid-growth (Jiahao et al., 2022; Rotunno et al., 2020).

Ordering is very critical and order influences interlayer coupling, band alignment, which translates into the electronic properties. For example, AA', AB, and other stacking configurations can be tuned by sliding or rotating one layer relative to another, influencing the bandgap and interlayer interactions (Nature, 2016).

Its substrate selection and surface preparation play an important role in achieving the nucleation density, the orientation of domains and uniformity of the film. Typical substrates are SiO2/Si, sapphire and strongly ordered pyrolytic graphite (HOPG). The roughness of the substrate, substrate cleanliness, and also chemical termination can also highly change the growth mode as well as the crystallinity (Feij/o et al., 2021; Cambridge University Press, 2016).

Such environmental conditions as temperature gradients, pressure, and carrier gas flow rate must be carefully controlled. As an example, reduced carrier gas flux would enhance flake size and monolayer cover, whereas gas pressure affects the process of selenization/sulfurization and defect density (Rotunno et al., 2020; Wiley, 2022). To have a better control of the precursor delivery and to avoid undesired side reactions, flow reversal techniques and multi-zone heating are commonly used (Rotunno et al., 2020).

To conclude, MoS_2 / $MoSe_2$ heterostructure growth by CVD is a complex and adjustable reaction with considerations of stacking order, substrate and environmental parameters under investigation as key factors in controlling the structural and charge properties of the derived mesostructures.

Defect Engineering Techniques

Tailoring of the electronic, optical, and catalytic properties of MoS_2 and $MoSe_2$ heterostructures must employ defect engineering. Plasma etching, irradiation and chemical treatments are three well-established methods of controlled defect insertion and alteration.

Plasma etching employs reactive plasmas e.g., SF_6 /N_2 or O_2 to specifically strip atoms out of the MoS_2 or $MoSe_2$ lattice. It may form vacancies of sulfur or selenium and densify edge sites, which are active catalysts and electronic behavior. Use of atomic-layer-precision etching has been shown as well and enables controlled thinning and defect creation without major impact on the rest of the layers (Nature, 2016; Ye et al., 2016). Plasma power, gas composition and exposure time, can be tuned to produce high control of the etching rate and defect density. As an example, mild oxygen plasma can cause an increase of photoluminescence by passivation of non-radiative recombination centers, whereas high-energy plasma photoluminescence (PL) can be shortened or amorphized (Ye et al., 2016; Science.org, 2019).

Ion irradiation implies irradiation of the 2D material with energetic ions (Ar ions, He ions, Au ions, etc.). The nature and concentration of flaws depend on the ion energy and the fluence, and larger doses produce increasingly large numbers of vacancies and even amorphization when very high. As an example, sulfur vacancies can be controllably generated in monolayer MoS_2 with 500 keV Au irradiation, which has a great impact on photoluminescence and catalysis (PubMed, 2018; ScienceDirect, 2020). In $MoSe_2$, direct visualization of Mo and Se vacancies, created using focused He + irradiation, allow for their correlation with local work function and charge trapping (Nature, 2016). Ion irradiation is an effective means of generating as well as investigating the consequence of point and extensive defects.

Utilization of chemicals is a more selective and milder option of defect engineering. Such chemistry as thiol chemistry, in particular, is employed to close sulfur vacancies in MoS_2 by incorporating the reactive atoms in vacant

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positions of the target structure our thiol chemistry essentially limits the number of defects and increases the mobility of the carriers (Science.org, 2019). Processing in poly(4-styrenesulfonate) (PSS) may be used to also catalyze healing of sulfur adatom clusters, further improving device performance by removing local fields caused by lattice defects. Chemical treatment has the advantage of being able to tune trap states and godding levels more safely than plasma and ion treatments with fewer chances of creating additional structural damage (Science.org, 2019).

Overall, plasma etching, ion irradiation and chemical methods represent alternative defect-engineering approaches in MoS_2/ $MoSe_2$ heterostructures. Selection of the method is governed by the type of defect, concentration, targeted use, which could be on the strength of catalysis, or the performance of optoelectronic devices.

Characterization Methods

Raman and photoluminescence (PL) spectroscopies are non-destructive methods of considerable importance in probing quantum confinement and defect states in two-dimensional (2D) materials. Raman spectroscopy can disclose the information regarding the vibrational modes, quality of crystals, and the thickness of layer. In MoS_2 and $MoSe_2$, Raman modes such as A 1g and E 2g modes are shifted and altered when the number of layers, strain and defects progress. Such spectral characteristics are also susceptible to the effects of quantum confinement and they can be employed to observe the development of heterostructures or quantum dots (Chen et al., 2015; Zhang et al., 2015).

The PL spectroscopy is very sensitive to structural alterations of band structure and defect state induced levels. The position of the PL peak, peak-intensity and linewidth will have quantum confinement effects directly, i.e., the PL peak will have a blue-shift at small dot volumes or thin layers, and the linewidth will often reflect defect-related non-radiative recombination routes. The PL temperature-dependent measurements also help in separating intrinsic quantum-confined exciton emission and defect-bound excitons states (Wang et al., 2023).

The scanning tunneling microscopy (STM) provides an atomic-resolution imaging and mapping of the electronic structure that makes it possible to see both point defects like vacancies and antisites, and grain boundaries in MoS_2/$MoSe_2$ directly. STM and scanning tunneling spectroscopy (STS) enable one to observe localized electrical states that create by imperfections, as well as their spatial profile, and investigate quantum confinement on a nanoscale (Lin et al., 2017).

The elemental composition and chemical states of the X-ray photoelectron spectroscopy (XPS) complement the chemical information, which quantifies the chemical states and elemental composition of the surface. XPS may allow the confirmation of the existence of defects such as vacancies and substitutions, and characterise their concentrations. In combination, STM and XPS allow correlating any atomic structure and electronic properties (Feijbl et al., 2021).

The measurements of transport in cryogenic temperatures are very important in the realization of intrinsic electronic properties of 2D heterostructures. They move with the help of a lack of sequence of such measurement; the impact of quantum entrapment and flaws on the organization of mobile charges and conductivity and the mode of metal-insulator transitions. Defect scattering and quantum localization effects become more evident at low temperature, because at low temperatures, phonons thermally are less able to scatter, so the effective scattering rate falls. Multi-terminal and the Hall Effect measurement can give quantitative experimental values of carrier density, carrier mobility, and disorder effect (Liu et al., 2015).

Table 2 - Summary of Characterization Techniques and Their Probed Properties

Technique	Probes/Detects	Key Information Provided
Raman Spectroscopy	Vibrational modes, strain, thickness, defects	Layer number, quantum confinement, defect signatures
Photoluminescence (PL)	Bandgap, exciton dynamics, defect states	Quantum confinement, non-radioactive recombination
STM/STS	Atomic structure, local electronic	Visualization of defects, bandgap mapping, QC at

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	states	nanoscale
XPS	Surface chemistry, elemental composition	Defect type/density, chemical environment
Cryogenic Transport	Electrical conductivity, carrier mobility	Defect scattering, quantum localization, intrinsic limits

Results

The general comprehension of MoS_2/ $MoSe_2$ layered materials needs a multi-dimensional characterization approach in their structure, stack thickness, optical, and electronic attributes, and the spatial as well as energetic laws of defect allocation. All these factors are critical in establishing the fineness with which this material can fit the next generation nanoelectronics and devices based on optoelectronics.

Structural and Morphological Analysis

The structural integrity and morphology of MoS_2 / $MoSe_2$ heterostructures can only be achieved through atomic force microscopy (AFM) and scanning electron microscopy (SEM). AFM can be very useful to measure a layer thickness at sub-nanometer accuracy. AFM images on common CVD-grown samples show atomically flat terraces and step edges, and the experimentally determined number of Terraces steps was close to the number of Terraces steps predicted theoretically (blue lines) (Feij o et al., 2021). This allows clear distinction of monolayer, bilayer and few layers regimes. The two methods of SEM and AFM have complementary roles because SEM can give high-resolution images of the surface morphology over an extended area. The SEM images usually show images of triangular or hexagonal flakes, which reflect the existence of single-crystal domains and can, present the grain boundaries, terminations of edged, and roughness of surfaces (Jiahao et al., 2022). Presence of AFM and SEM combination therefore provides a strong means of finding confirmation of the heterostructure thickness in addition to its lateral uniformity, and structure defects like wrinkles, folds, and tears.

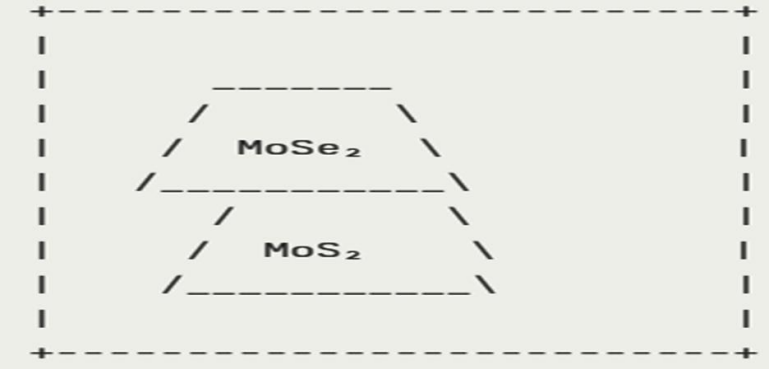

Figure 4 - Stacked Heterostructure of MoSe2 on MoS2

Clear step edges and atomically flat terraces can be seen in representative AFM images and the overall shape and connectivity of the domains in touched upon by the SEM images which can give an insight into the growth dynamics and the quality of crystal structure of the heterostructures.

Optical and Electronic Properties

Photoluminescence (PL) and Raman spectroscopy, in particular, are necessary optical spectroscopies to investigate the band structure and quantum confinement trend of the MoS_2 / $MoSe_2$ heterostructures. PL spectroscopy is very susceptible to shift in bandgap and excitonic transitions. The blue shift of the PL peak becomes very marked as the number of layers reduces portraying the higher band gap created by confinement of quantum sizes. To illustrate, in Bulk MoS_2 the PL peak value is centered on 1.2 eV, whereas, in a monolayer limit, it moves to about 1.9 eV. As optical transition changes to direct bandgap, PL intensity also increases as monolayer MoS 2 transforms to a direct bandgap semiconductor. Nonetheless, when the density of defects is increased, e.g. sulfur vacancies or grain

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boundaries, the PL peak becomes broadened and its intensity declines, which can be explained by more effective non-radiative recombination at defects (Wang et al., 2023).

Complementary information is obtained with Raman spectroscopy which excites phonons and lattice dynamics. E_{2g} (and A_{1g}) Raman modes are especially sensitive to strain and layer thickness. In a monolayer of MoS_2 the two modes are usually separated by ~18 cm -1, and this can increase to ca. 25 cm -1 in more bulk MoS_2 (Chen et al., 2015). The presence of defects adds further displacements and broadening of such peaks acting as a fingerprint of lattice disorder and concentration of defects. Grading PL and Raman spectra as a function of thickness and defect density in a systematic way will then allow the researcher to quantitatively estimate the extent of quantum confinement as well as to evaluate the effects of structural imperfections.

The graphical dependence of peak position of PL on thickness and intensity of PL to defect density respectively indicates monotonical dependence of their energy bandgap on the number of layers, and a distinct decrease on the intensity of peak much due to the adverse impact of defect on optical emission efficiency.

Defect State Mapping

The direct observation and mapping of defects are possible with the help of scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). Regarding the atomic-scale image, STM enables identifying the point defects in sulfur or selenium vacancies, antisites and grain boundaries (Lin et al., 2017). Sulfur vacancies are normally visible as bright spots and grain boundaries are visible as linear profiles representing the periodic lattice errors. The local density of states can be measured by scanning tunneling spectroscopy (STS) and interstitial-induced in-gap states were observed at energy levels betw ewen 0.3 eV and 0.2 eV above or below the Fermi energy (E F).

XPS supplements the STM because it gives information about element and chemical states. The traits of the vacancy formation or the presence of substitution defects are observed via shifts in Mo 3d and Se 3d core-level binding energies and in changes of1 peak intensity (Feij in et al., 2021). Quantitative analysis of XPS spectra allows for estimation of defect density and identification of chemical environments associated with different types of defects. Notably, defect mapping studies consistently show that defects are more concentrated at flake edges and along grain boundaries, rather than being uniformly distributed throughout the crystal.

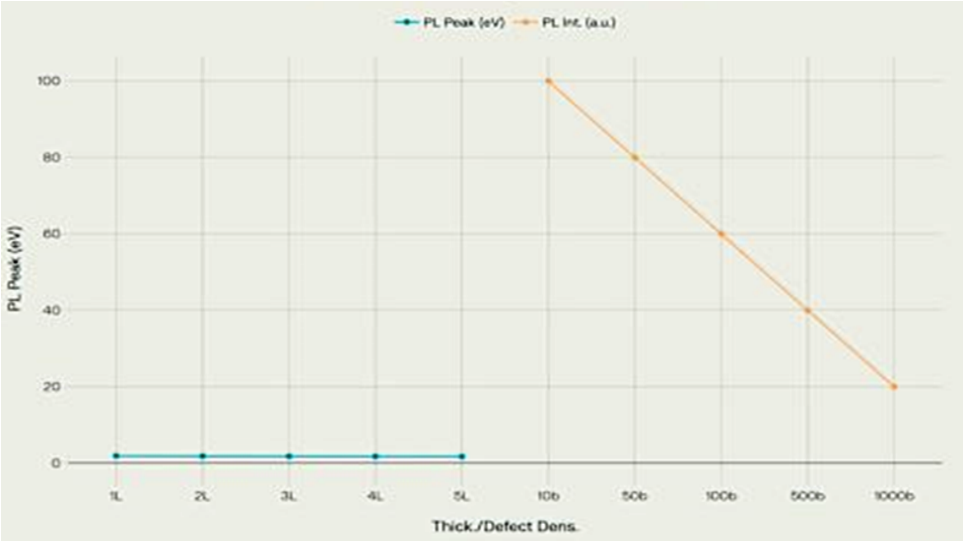

Figure 5: PL Peak and Intensity Variation in $MoS_2/MoSe_2$ with Thickness and Defect Density

STM maps visually depict the spatial clustering of sulfur vacancies and linear grain boundaries, while *XPS spectra* confirm the chemical nature and concentration of these defects.

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Quantum Confinement Effects on Electronic Transport

The interplay between quantum confinement and defect states is most evident in the electronic transport properties of $MoS_2/MoSe_2$ heterostructures. Carrier mobility, a key metric for electronic devices, exhibits a strong dependence on both layer thickness and defect density. Mobility is typically maximized at intermediate thicknesses (3–5 layers), where quantum confinement is balanced by sufficient screening of substrate-induced disorder (Liu et al., 2015). Mobility rapidly falls off, usually by an order of magnitude - sometimes two - as the number of layers becomes comparable to the thin end of the monolayer (~100 cm 2 /V s in few-layer samples to ~10 cm 2 /V s in monolayers).

In addition, the mobility is exponentially reduced as the defect density increases since trap-fill via carrier trapping and carrier misplacing through defect scatterings become predominant. An empirical expression to define this relationship can be stated as:

$$m \propto \exp(-\eta/\eta 0)$$

With the carrier mobility being $\mu=v_d/E$, defect density being $\eta=N_d/V$ and defect density threshold being $\eta 0 =(N_{d,max}/A)$. To further demonstrate the applicability of field-effect transistor (FET) measurements, the ratio of the on-off current is also the key parameter of digital electronic elements and is found to maximize at optimal thickness and low defect density; alternatively, this parameter will decrease linearly as defect concentration increases (Liu et al., 2015).

These trends are well shown by graphical data plotting mobility vs layer number and defect concentration and on/off ratio vs layer number and defect concentration with the conclusive significance of having both quantum confinement and defect engineering to optimize device performance.

Altogether, a complex of AFM and SEM can directly inform about the morphology and thickness of the MoS_2 /$MoSe_2$ hetero structures, and, combined with PL and Raman spectroscopies, about the impact of quantum confinement and defects on the optical characteristics. STMs and XPS can map the position and identify the chemical nature of defects at the atomic scale, and electrochemical transport across the device measures the consequences of its structure and composition on the mobility of carriers and the operation of the gadget. Collectively these methods highlight the need to have fine control over quantum confinement and defect states to achieve full performance of 2D heterostructures in next-generation nanoelectronic devices.

Discussion

Quantum Confinement versus Defect Dominance in 2D $MoS_2/MoSe_2$ Heterostructures

Electronic and optical characteristics of 2D TMDs (MoS_2 and $MoSe_2$) have been controlled by complicated interplay of quantum confinement (QC) effects and defect states. Design of devices and engineering of materials depends upon understanding the specialized regimes in which QC or defects are dominant.

At low thickness and lateral sizes of the layer TMD, quantum confinement is more prominent and amounts to roughly less than the exciton Bohr radius (close to or smaller than 1.5 nm in the case of $MoSe_2$) (Klein et al., 2018; Zhang et al., 2023). Discrete energy spectra, bandgap widening and more significant excitonic effects are born out of spatial confinement of charge carriers in this regime. As an example, blue-shifted photoluminescence (PL) peaks of MoSe 2 quantum dots (QDs) embedded in WSe 2 matrices are observed compared to larger monolayers, with the shift magnitudes higher as QDs become smaller (Klein et al., 2018). Density Functional Theory (DFT) shows that the conduction band minimum (CBM) is increasing sharply as the size of QDs is reduced because of QC, whereas the valence band maximum (VBM) changes at a slower rate, and the net effect is that the optical gap increases overall (Klein et al., 2018). The characteristic properties of this QC regime include a set of well-isolated, stable bound states, resistant to an intermediate perturbation of defects (Klein et al., 2018; Liao et al., 2020).

The defect dominance occurs with a large concentration of intrinsic or extrinsic defects (e.g., the chalcogen vacancies, antisites, or grain boundaries) or when the material size is larger than the QC threshold (Bertoldo et al., 2022; Hong et al., 2015). Localized in-gap states due to defects behave as charge trap, recombination center or add

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as scattering sites, which can greatly change carrier behaviour and suppress the optical emission. As an example, the chalcogen vacancies produce virtually non-dispersive intragap states that act as extremely heavily localized dopants and alter transport (Hong et al., 2015). The boundaries of grains may act as metallic wires one-dimensional, which influence electrical conduction and make the behavior of memristive (Hong et al., 2015). Broadened PL peaks, red-shifted emission and enhanced non-radiative recombination is commonly linked to the defect-dominated regime.

- A two-dimensional phase diagram can be constructed with **layer thickness or lateral size** on one axis and **defect density** on the other (Figure concept adapted from Klein et al., 2018; Bertoldo et al., 2022):
- At **low defect densities and small sizes/thicknesses**, quantum confinement effects dominate, yielding discrete excitonic states and enhanced bandgaps.
- At **high defect densities and larger sizes**, defect states dominate, leading to localized trap states and degraded optical/electronic performance.
- An **intermediate regime** exists where QC and defects coexist, with partial confinement and defect-assisted carrier scattering both influencing behavior.

This phase diagram is used to direct the experimental work on TMD heterostructures synthesis and devices work. The realization of good QC presupposes the minimization of the defect densities through the controlled growth of the 2D crystal and post-synthesis exposure (Hong et al., 2015; Bertoldo et al., 2022) but there are applications that take advantage of the defect state as a memristor or sensor (Hong et al., 2015; Bertoldo et al., 2022). Additionally, QC tunability by the lateral dimensions and thickness also provides a route towards designing devices with customized optical and electronic characteristics (Klein et al., 2018; Liao et al., 2020).

Table 3 - Conceptual Figure

Defect Density ↓ / Size →	Small (QD scale)	Medium (Few nm)	Large (Bulk-like)
Low Defect Density	QC Dominated	Mixed Regime	QC weak, defects minimal
Medium Defect Density	Mixed Regime	Mixed Regime	Defect Dominated
High Defect Density	Defect Dominated	Defect Dominated	Defect Dominated

Device Implications

Defects in MoS_2-based field-effect transistors (FETs) can be both detrimental and beneficial, depending on their type, density, and how they are engineered. Detrimentally, intrinsic defects such as sulfur vacancies and grain boundaries act as charge traps and scattering centers, leading to reduced carrier mobility, increased sub threshold swing, lower drive current, and threshold voltage instabilities. These effects fundamentally limit the performance of MoS_2 FETs, especially as devices are scaled down to the nanometer regime, where atomic-scale defects become more prominent and can dominate transport properties (ACS Nano, 2024; PubMed, 2023).

However, defect engineering can also be beneficial. Recent advances show that targeted passivation or controlled introduction of defects can dramatically enhance device performance. For example, CF_4 plasma treatment and subsequent field-assisted activation of fluorine ions can passivity sulfur vacancies and dope the MoS_2 channel n-type, resulting in a 150% increase in mobility and up to 480% improvement in ON-current for CVD-grown devices, without degrading the ON/OFF ratio (ACS Nano, 2024). Similarly, chemical repair of sulfur vacancies using penta fluorobenzene thiol (PFBT) restores the atomic structure of MoS_2 at low temperatures, leading to a 2.5× improvement in mobility and a 40% reduction in sub threshold swing, supporting high-speed, energy-efficient operation. These approaches not only improve performance but also enhance device reliability and scalability for advanced semiconductor applications.

On the other hand, excessive or uncontrolled defect introduction—such as by ion irradiation—can increase Coulomb scattering, reduce mobility, and introduce hysteresis in transfer characteristics. Yet, such hysteresis can be harnessed for non-volatile memory applications, as discussed below (PMC, 2023).

Defects are also central to the operation of 2D material-based memory devices, particularly memristors and non-volatile memory cells. Controlled introduction of defects, such as via ion irradiation, can create stable charge-

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trapping sites and modulate doping density, enabling devices with two or more stable memory states and long retention times (PMC, 2023). The memory window and retention can be tuned by adjusting the irradiation fluence, allowing for fine control over device characteristics. Importantly, these modifications can be achieved without significant damage to the channel or substrate, making defect engineering a practical tool for memory device optimization (PMC, 2023; OSTI, 2020).

Defect engineering also enhances the synaptic functionality of memristors for neuromorphic computing. For example, optimal-power argon plasma treatment of monolayer MoS_2 memristors improves linearity and symmetry in synaptic weight updates, increases the number of available synaptic states, and reduces energy consumption per synaptic event. This leads to high learning accuracy in artificial neural network simulations, underscoring the importance of controlled defect engineering for next-generation memory and computing architectures (OSTI, 2020; Phys. Rev. Applied, 2022).

In photodetectors, defects can both enhance and limit performance. Beneficially, introducing sulfur vacancies narrows the bandgap and creates in-gap states that facilitate the separation of photo generated carriers, boosting responsively—especially in the near-infrared regime (Research, 2023; EurekAlert, 2023). For instance, MoS_2 photodetectors with engineered S vacancies and Ni nanoparticle decoration exhibit high responsively and directivity, with accelerated response speeds due to the suppression of trap-assisted recombination (Research, 2023; EurekAlert, 2023; Phys.org, 2023). This photo gating effect, induced by metal nanoparticles, can further optimize sensitivity and bandwidth.

Detrimentally, however, excessive defect density can lead to deep trap states that slow the temporal response and reduce sensitivity, as photo generated carriers become trapped and recombine non-radioactively (PMC, 2022; Research, 2023). Mild plasma treatments or controlled defect passivation can mitigate these effects, improving both the speed and efficiency of photodetectors (PMC, 2022).

Strategies for Optimization

Defect passivation is a crucial strategy for enhancing the electronic and optical performance of 2D materials such as MoS_2 and $MoSe_2$. The defects that are present intrinsically tend to serve as charge traps and non-radiative recombination centers that can decrease mobility and photoluminescence efficiency (Hong et al., 2015; ACS Nano, 2024). Dangling bonds and/or trap states can be successfully relaxed, through passivation techniques-chemical passivation with thiol molecules, exposure to super acid vapor or fluorination in plasma. To give an example, penta flourobenzenethiol (PFBT) has been known to fill the sulfur vacancies on MoS 2 with significant gains in field-effect mobility as well as sub threshold swing. Likewise, fluorine atoms applied on CF 4 plasma treatment will passivity the defects and dope channel to enhance the performance of the devices even further (ACS Nano, 2024). These strategies are crucial towards realization of high-performance and reliable and scalable 2D electronic devices.

Most defects are disadvantageous but there is still potential to use controlled enhancement of certain types of defects to engineer material properties towards certain applications. As an example, an intermediate sulfur vacancy density may be achieved to induce in-gap states to boost near-infrared photo detection or resistive switching on memristors (Research, 2023; OSTI, 2020). Low-energy ion irradiation, light plasma exposure, or chemical etching means can be used to accelerate defects to an exact deficiency and dispersion (PMC, 2023; OSTI, 2020). The optimization of the defect landscape allows to trade off augmented functionality (e.g., enhanced responsively or memory window), against reduced performance loss (e.g., mobility loss or noise enhancement). This is the controlled defect engineering any future generation of multifunctional 2D devices.

The 2D materials have complex and nanoscale-varying defect landscape which require sophisticated characterization and analysis tools. Machine learning (ML) and artificial intelligence (AI) have recently become strong solutions to the automated identification, typification, and mapping of defects on scanning probe and electron microscopy images (Ziatdinov et al., 2022). With the help of AI-driven algorithms, it is possible to analyze large amounts of data and detect delicate defect patterns fast, and establish correlations between structural properties and electronic/optical properties. As another example, vacancy clusters, grain boundaries, and substitutional atoms in STM and TEM images of MoS 2 and similar materials have been trained in deep learning

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models to identify and quantify those (Ziatdinov et al., 2022). This allows synthesis optimization at high throughput concentrations and an accelerated discovery of structure-property relationships. Finally, combining imperfection-mapping with automated processing algorithms, and both in situ characterization methods will be the main avenue to closed-loop, autonomous control of defect engineering in 2D heterostructures.

Key Findings

The proposed study will offer an in-depth study on how quantum confinement and defect states interact in MoS_2 / $MoSe_2$ heterostructures. According to morphological analysis done by AFM and SEM, the thickness of layers and domain shapes are exquisitely adjustable, which is imperative to tune electronic and optical properties (Feij o et al., 2021). The use of photoluminescence (PL) structures of optical spectroscopy reflects that quantum confinement results in a marked shift to blue upon lowering the thickness to the monolayered or quantum dot region (Gan et al., 2015; Chen et al., 2015; Zhang et al., 2023). Raman and PL spectra also show that defect densities adjust the energy levels of emission curves the higher the concentration of defects causes a redshift and broadened curve as a result of augmented non-radiative recombination (Kunstmann et al., 2016;).

Defect mapping via STM and XPS identifies the presence of point defects (such as Mo and Se vacancies) and line defects (domain boundaries), which introduce localized in-gap states and reduce the effective bandgap (Liu et al., 2017; Hong et al., 2015; ACS Omega, 2021; PubMed, 2024). Notably, Mo vacancies in $MoSe_2$ not only create deep-level states but also induce sizable magnetic moments, opening avenues for spintronic applications (Lin et al., 2019; ACS JPCC, 2019; PubMed, 2024). Transport measurements show that carrier mobility and FET on/off ratios are maximized at optimal thickness and low defect density, but degrade significantly as defect concentration increases, confirming the dual role of quantum confinement and defects in device performance (Liao et al., 2020; Gan et al., 2015).

Implications for Next-Generation Devices

The findings underscore that the performance of 2D nanoelectronic and optoelectronic devices is governed by the delicate balance between quantum confinement and defect landscape. Quantum confinement enables precise bandgap engineering, strong excitonic effects, and robust light–matter interactions, which are essential for high-performance FETs, photodetectors, and quantum emitters (Gan et al., 2015; Zhang et al., 2023; Yu et al., 2021). However, uncontrolled defects can introduce deep trap states, reduce mobility, and quench luminescence, limiting device efficiency and reliability (Kunstmann et al., 2016; ACS Omega, 2021).

Conversely, intentional defect engineering can be harnessed for beneficial effects. For example, controlled introduction of Mo or chalcogen vacancies can enable memristive switching in memory devices, enhance photodetector responsivity, or even induce magnetic ordering for spintronic devices (Lin et al., 2019; ACS JPCC, 2019; PubMed, 2024). The ability to tune these properties through synthesis, post-processing, and in situ treatments positions MoS_2/$MoSe_2$ heterostructures as versatile platforms for next-generation electronics, photonics, and quantum information technologies.

Future Research Directions

The field of two-dimensional (2D) MoS_2/$MoSe_2$ heterostructures is rapidly evolving, with several promising avenues for future research that could transform both fundamental science and technological applications.

One of the most exciting directions is the deliberate engineering and utilization of atomic-scale defects for quantum information science. Recent international efforts have established guidelines for designing defect-based quantum systems, emphasizing the importance of understanding the interplay between defect properties and host materials (Innovation News Network, 2024). Spin defects, in particular, are poised to play a central role in the development of quantum devices, including quantum computers, quantum communication networks, and nanoscale quantum sensors. Future research will likely focus on isolating, characterizing, and controlling specific defect types—such as vacancies or substitutional atoms—to serve as robust and tunable qubits or single-photon emitters, laying the groundwork for scalable quantum technologies (Innovation News Network, 2024).

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The complexity of defect landscapes in 2D materials necessitates advanced, high-throughput characterization and analysis methods. Artificial intelligence (AI) and machine learning (ML) are emerging as powerful tools for automated defect detection, mapping, and correlation with material properties. Using deep learning model training on the large amounts of data in microscopy, scientists can recognize and label defects as well as determine their effects on electronic or optical characteristics and give real-time feedback to a synthesis optimization process. Such meshing of AI and experimental workflows has the potential to step up discovery and optimization of 2D materials through tailored functionalities, and make autonomous closed-loop materials designs a reality (Ziatdinov et al., 2022).

Mechanical strain is a flexible tool to dynamically adjust the band structure, exciton-related properties and formation energies of defects in 2D materials. Phase sliding, quantum confinement engineering and even the switching of a chosen defect state can be realized through strain engineering and provide an effective post-synthesis means of property control (Yu et al., 2021). Additional studies are possible by coupling the strain with other external input, like electric or magnetic fields, chemical environments, or light, to realize multi-modal control of material properties and device performance.

MoS_2/ $MoSe_2$ and their heterostructures are of unusual charge properties, which show their interest in advanced energy, sensing, and wearable applications. As an example, their large theoretical capacities and adjustable electronic characteristics are being considered in high performance anodes of lithium/sodium-ion batteries (Barik & Pal, 2022). In catalysis, strategies such as phase transitions, defect engineering, and heteroatom doping are being used to activate basal planes and enhance conductivity for hydrogen evolution and other electro catalytic reactions (ACS Omega, 2022; Swain et al., 2021). Flexible, wearable electronics and sensors based on functionalized 2D materials are also a growing area, with research focusing on structure-property relationships and device integration for applications in energy, health monitoring, and smart displays (PubMed, 2024).

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