Probing Excitonic Transitions at Atomic-Scale Defects in Chemical Vapor Deposition-Grown MoS_2 and WSe_2

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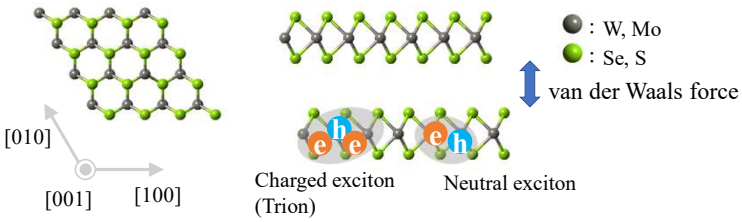
Abstract

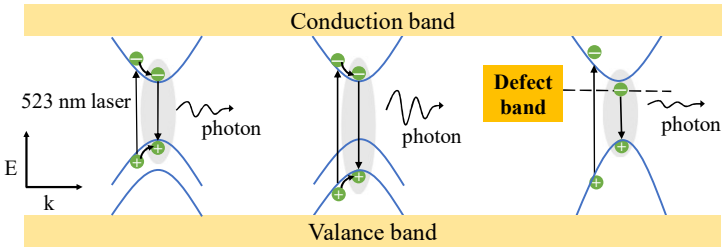
Transition metal dichalcogenides (TMDs), such as MoS_2 and WSe_2, have attracted considerable attention due to their distinctive excitonic properties and promising applications in optoelectronic devices. In this work, we investigate the optical transitions and defect-related excitonic states in chemical vapor deposition (CVD)-grown MoS_2 and WSe_2, where the defect density is controlled by the gas flow rate during growth. Low-temperature photoluminescence (PL) and differential reflectance (DR) spectroscopy are employed to accurately identify various band-to-band optical transitions, including neutral excitons, trions, and defect bound excitons. The energy separations between defect-related emissions and free excitons exhibit similar trends in both materials, indicating analogous defect origins. These findings offer critical insights into defect engineering, bandgap modulation, and essential parameters for optimizing crystal growth in two-dimensional semiconductors.

Key words：transition metal dichalcogenide, defect-bound exciton, bandgap modulation, photoluminescence, dielectric screening

Transition Metal Dichalcogenides (TMDs)



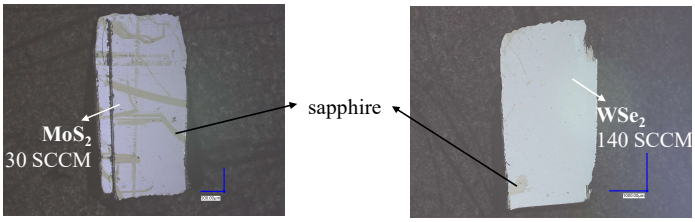
Excitons



Method

TMDs Grown by Chemical Vapor Deposition (CVD)

controled by the gas flow rate during growth



4K Optical Measurement

•Photoluminescence (PL)

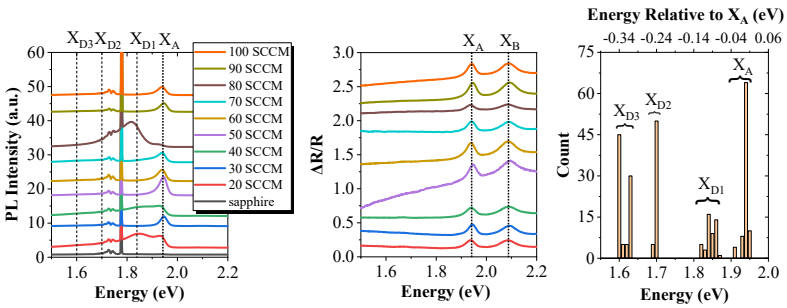
•Differential reflectometry (DR)

MoS_2 or WSe_2 with different gas flow rate

sapphire

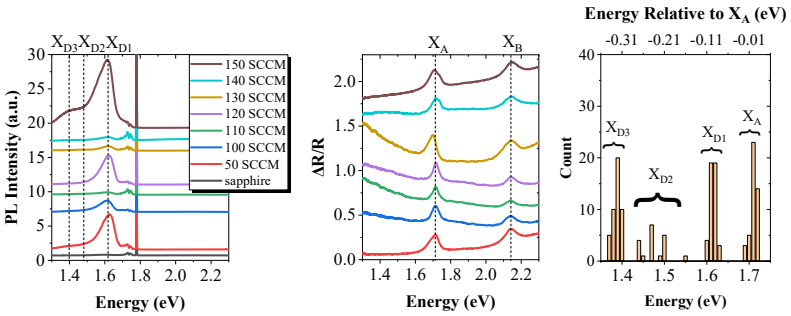
Result & Discussion

- **Exciton Properties of MoS_2 at Different Gas Flow Rates**



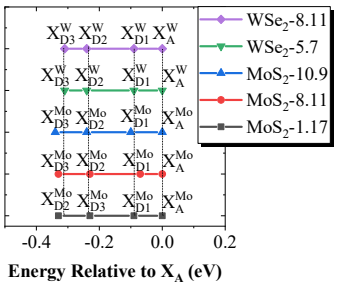
The quality ranks as：50 ≈ 60 ≈ 30 ≈ 90 ≈ 100 > 70 > 20 ≈ 40 > 80 SCCM

- **Exciton Properties of WSe_2 at Different Gas Flow Rates**



The quality ranks as：150 > 50 ≈ 120 > 100 > 130 ≈ 140 > 110 SCCM

- **Comparison between MoS_2 and WSe_2**



1. Nearly identical redshift relative to the A exciton.
2. Indicates a similar defect-induced binding potential.
3. Suggests similar defect structures.

Conclusion

1. PL spectra reveals A, B, and three defect-bound excitons in both CVD-grown MoS_2 and WSe_2.
2. Spectral analysis shows comparable energy offsets of defect-bound excitons from the A exciton, suggesting similar defect origins and atomic strctures.

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