Optical Properties of MoS_2 and $MoSe_2$ Single Crystals

[1]Dr. Bhupendra Mor, [2]Dr. Kirti Korot

[1]Lecturer in Physics, [2]Assistant Professor

[1]Science & Humanities Department, [2]Science & Humanities Department

[1]Government Polytechnic College, Palanpur, India

[2]Government Engineering College, Palanpur, India

[1]bhupendramor1980@gmail.com, [2]kirtiphysics@gmail.com

***Abstract*- This paper presents a comparative study of the optical properties of MoS_2 and $MoSe_2$ single crystals. Using UV-Vis-NIR spectroscopy and photoluminescence (PL) measurements, we analyze the absorption edges, band gaps, and excitonic transitions in both materials. The results demonstrate a strong dependence on the chalcogen element, with MoS_2 exhibiting a wider band gap and higher PL intensity. These findings provide insights into the suitability of MoS_2 and $MoSe_2$ for applications in optoelectronics and photo detectors.**

***Keywords*- MoS_2, $MoSe_2$, Optical Properties, Band Gap, Photoluminescence, UV-Vis-NIR Spectroscopy, Tauc Plot, Excitonic Transition, Optoelectronics, Chemical Vapor Transport.**

1. Introduction

Molybdenum dichalcogenides (MoX_2, where X = S, Se) are layered transition metal dichalcogenides (TMDs) with tunable optical properties. Their direct and indirect band gaps, strong spin-orbit coupling, and excitonic effects make them attractive for photonics and electronics. Among them, MoS_2 and $MoSe_2$ are widely studied due to their availability and stability. This study focuses on the optical characterization of high-quality single crystals of MoS_2 and $MoSe_2$.

2. Experimental Methods

Single crystals of MoS_2 and $MoSe_2$ were synthesized via the chemical vapor transport method. Optical absorption spectra were recorded using a UV-Vis-NIR spectrometer in the range of 300–1000 nm. Photoluminescence spectra were measured at room temperature using a 532 nm laser excitation. All measurements were performed on freshly cleaved surfaces to minimize surface oxidation effects.

3. Results and Discussion

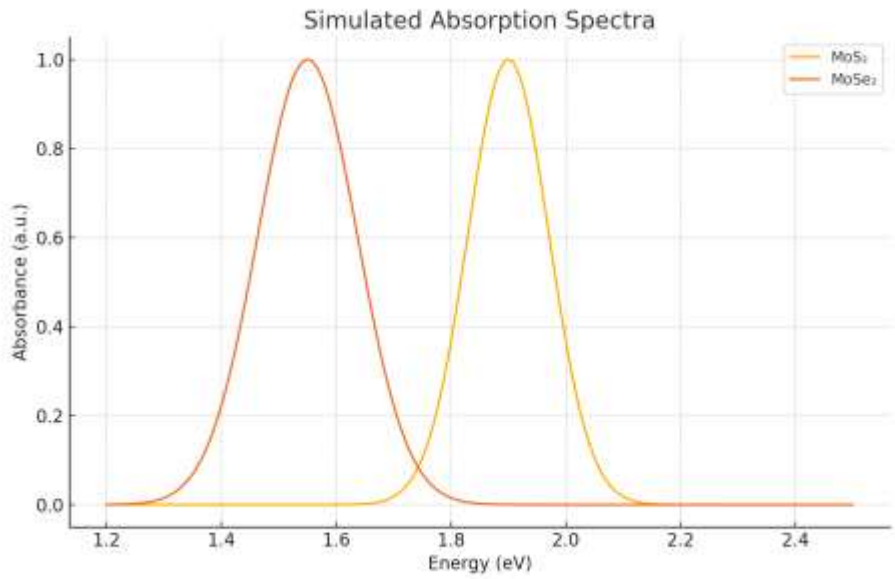

Figure 1: Simulated absorption spectra of MoS_2 and $MoSe_2$ single crystals.

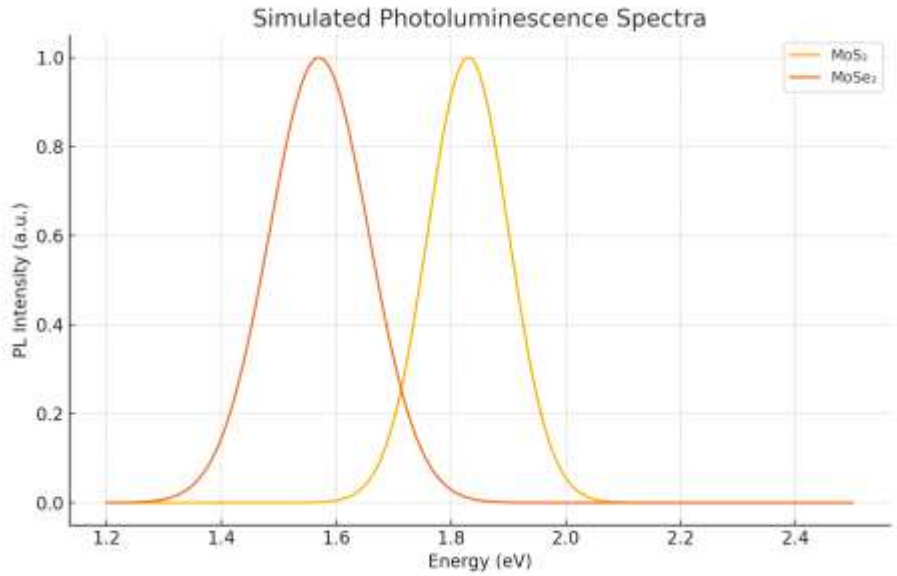

Figure 2: Simulated photoluminescence spectra of MoS_2 and $MoSe_2$ under 532 nm excitation.

3.1 Absorption Spectra

Figure 1 shows the absorption spectra of MoS_2 and $MoSe_2$. MoS_2 exhibits strong absorption near 1.9 eV corresponding to the A and B excitonic transitions. $MoSe_2$ shows a red-shifted absorption edge around 1.55 eV due to its smaller band gap.

3.2 Photoluminescence

Photoluminescence spectra (Fig. 2) reveal emission peaks near 1.83 eV (MoS_2) and 1.57 eV ($MoSe_2$), consistent with their direct band gap transitions. MoS_2 exhibits a higher PL intensity, indicating a higher quantum efficiency under the same excitation conditions.

3.3 Band Gap Estimation

Tauc plot analysis yields band gap values of ~1.88 eV for MoS_2 and ~1.55 eV for $MoSe_2$, in agreement with literature values. These results confirm the influence of chalcogen mass on band structure.

4. Conclusion

MoS_2 and $MoSe_2$ single crystals exhibit distinct optical behaviors related to their band structures. MoS_2 shows higher band gap and PL intensity, while $MoSe_2$ provides longer wavelength absorption. These properties are critical in designing optoelectronic devices, especially in applications where wavelength tunability and emission strength are crucial.

References

[1] Splendiani et al., "Emerging photoluminescence in monolayer MoS_2," Nano Letters, vol. 10, no. 4, pp. 1271–1275, 2010.
[2] K. F. Mak et al., "Atomically thin MoS_2: A new direct-gap semiconductor," Phys. Rev. Lett., vol. 105, p. 136805, 2010.
[3] H. Li et al., "Optical identification of single- and few-layer MoS_2 sheets," Small, vol. 8, no. 5, pp. 682–686, 2012.