A Comparative Evaluation of Hydrothermal & Liquid Phase Exfoliation Techniques for high quality $MoSe_2$ Production

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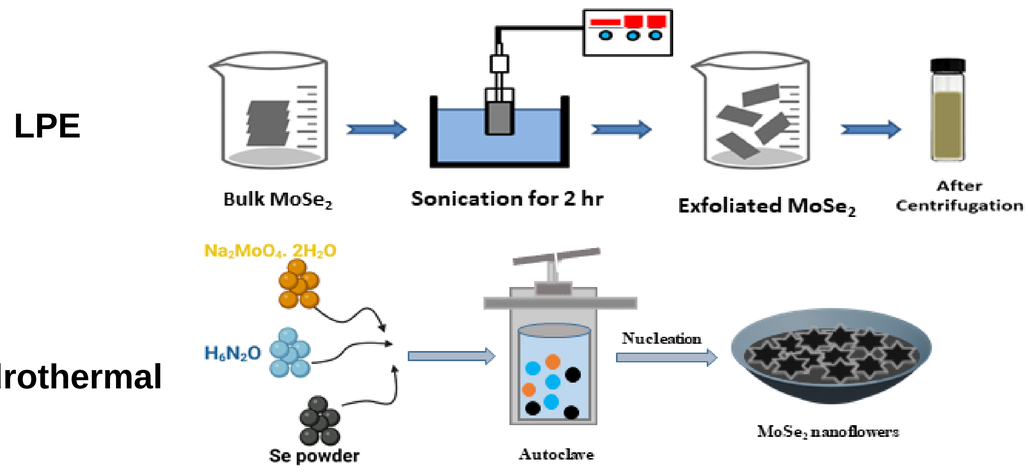
Abstract

Two-dimensional material possesses several extraordinary advantages, including large surface to-volume ratio, atomic thickness and having outstanding mechanical, electrical & optical properties. Among various 2D materials, Transitional metal dichalcogenides (TMDs) that includes MoS_2, WS_2, $MoSe_2$ etc. are layered materials that exhibit electronics, optoelectronics, photocatalysis & energy storage applications. Various synthesis routes can be employed for synthesizing these 2-D material each having their advantages for as desired application. In this discussion, we have focused on two different techniques, Hydrothermal and Liquid Phase Exfoliation (LPE) for synthesizing 2D $MoSe_2$ to study their advantages and disadvantages over each other such as the control over morphology hydrothermal technique provide over LPE and the control of layers provided by LPE over hydrothermal synthesis route. Both methods are cost effective, facile, scalable, and eco-friendly methods and gives different morphology, size and surface area. The synthesis material has been characterized using various characterization techniques viz, XRD, Raman, UV, SEM and TEM to study their structural, chemical and optical properties and discussing. The characterized result can be applied to the desired applications. A

Schematic of Synthesis of $MoSe_2$

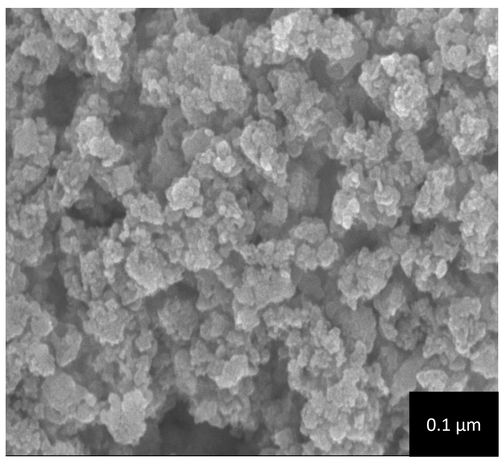


Introduction

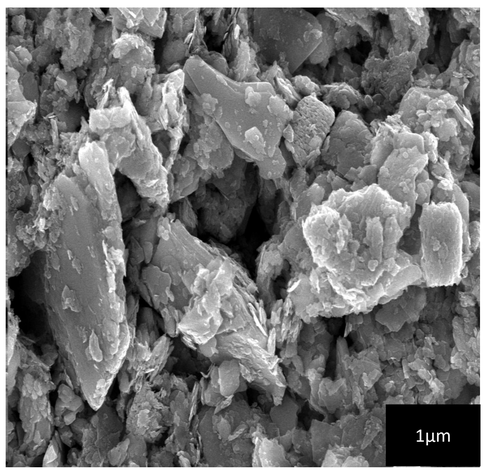
- Molybdenum diselenide ($MoSe_2$) is a two-dimensional (2D) transition metal dichalcogenide (TMD) with exceptional electronic, optical, and catalytic properties.
- It has gained significant attention for applications in energy storage, catalysis, and optoelectronic devices.
- Its layered structure enables easy exfoliation, making it a promising material for applications in energy storage, optoelectronics, and catalysis.
- In this study, we explore two effective synthesis techniques for $MoSe_2$: Liquid Phase Exfoliation (LPE) and the Hydrothermal Method. LPE is a scalable approach to obtaining high-quality $MoSe_2$ nanosheets in solution, while the hydrothermal method provides controlled growth of $MoSe_2$ with tunable morphology.

Characterizations

SEM Data



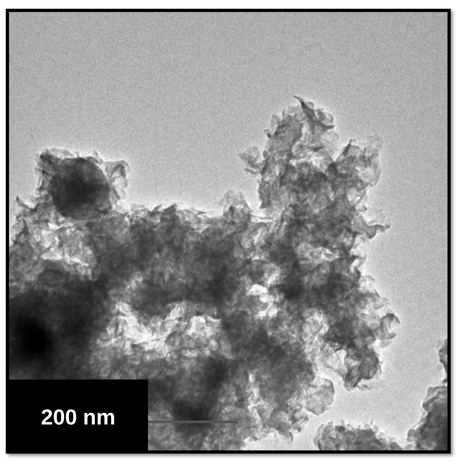
SEM Image of $MoSe_2$ by Hydrothermal method



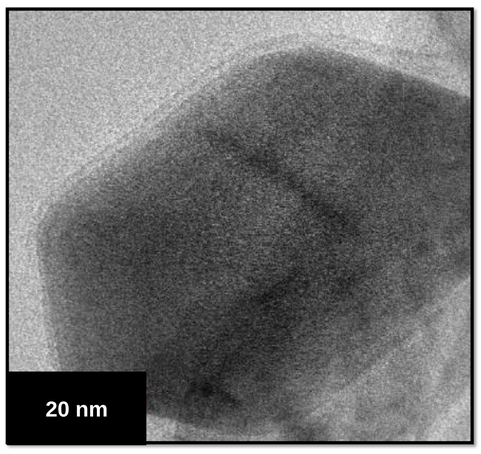
SEM image of $MoSe_2$ by LPE Method

- By Hydrothermal method , we get flower-like or stacked structures due to controlled crystal growth.
- By LPE, we get some thin, nanosheets like structure with fewer layers due to the exfoliation process.

TEM Data

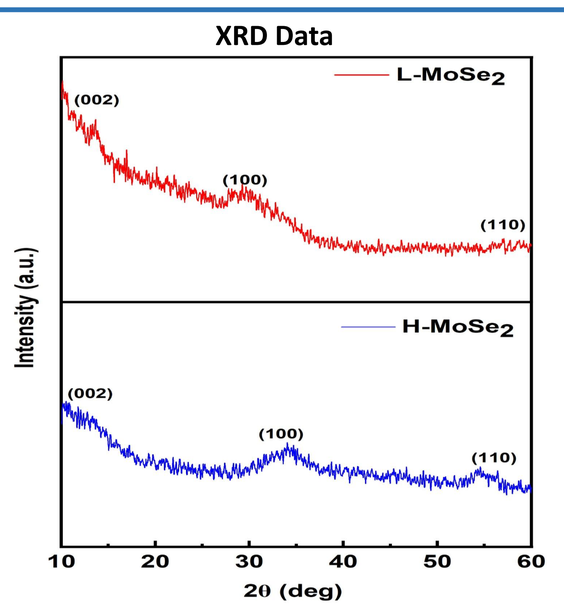


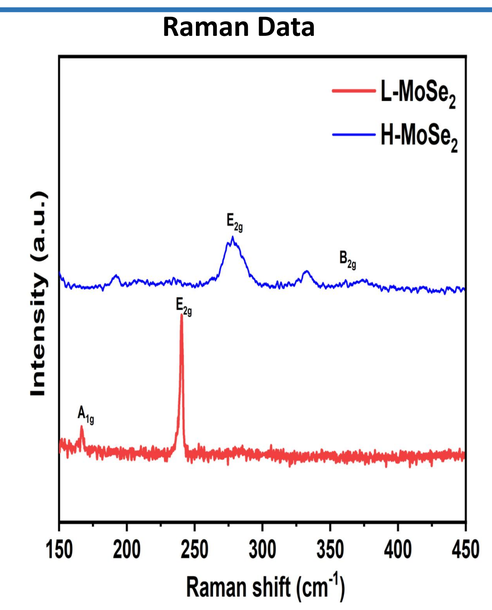
TEM image of $MoSe_2$ by Hydrothermal Method

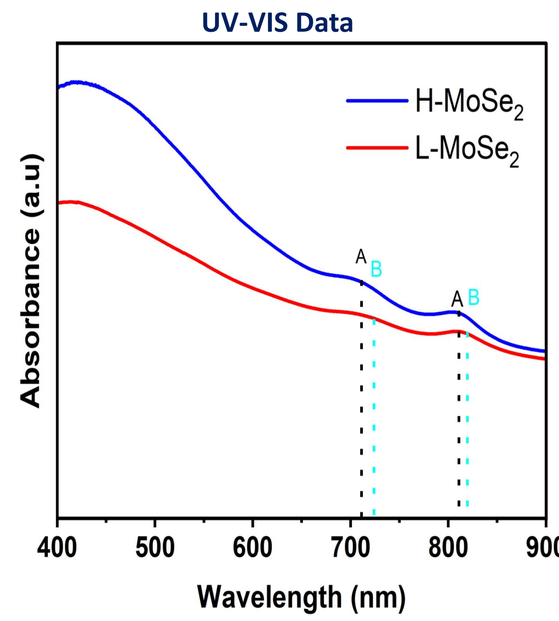


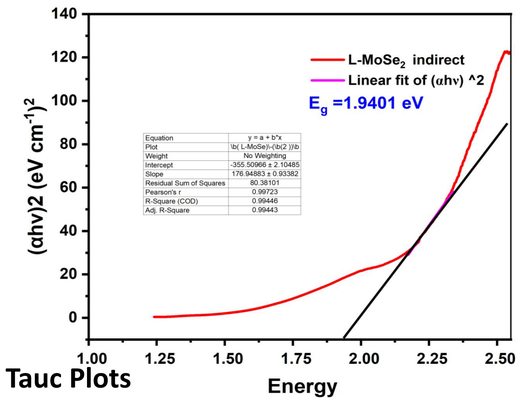
TEM image of $MoSe_2$ by LPE method

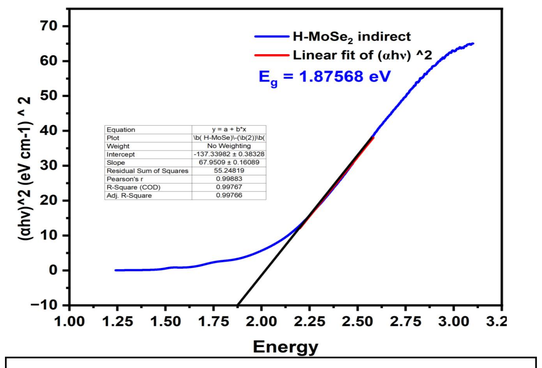
Results











XRD Spectrum :-

- A strong 002 peak at 13.3° which indicates the layer stacking information.
- A (100) and (110) peak at 36° and 56° respectively indicates the in- plane crystallinity & lattice distortion/strain.

Raman Spectrum :-

- In $MoSe_2$ the two major peaks A_{1g} (167 cm^{-1}) & E_{2g} (241 cm^{-1}) are observed in LPE method. A_{1g} is due to out-of-plane vibration of Mo and Se atoms which indicates few layer of $MoSe_2$ & E_{2g} indicates better crystallinity.
- In Hydrothermal method E_{2g} (278 cm^{-1}) indicates more disorder and defects & B_{2g} (361 cm^{-1}) peak indicates more structural distortions, stacking, or thicker layers.

UV-Vis Data (Band Gap Energy) :-
LPE Method – 1.9401 eV
Hydrothermal method – 1.8756 eV

- A higher band gap (LPE method) indicates fewer layers or monolayer form, it is more suitable for Optoelectronics applications.
- A lower band gap (hydrothermal method) suggests a thicker structure or defects, which may affect charge transport properties but it is suitable for applications requiring better catalytic or electrochemical performance.

Conclusion

For high-quality, few-layer $MoSe_2$ with superior electronic and optical properties, the LPE method is the better choice due to its higher band gap and better exfoliation. However, for catalytic and electrochemical applications, the Hydrothermal method may be more suitable due to its slightly lower band gap and possible defect-induced activity and suitable for applications requiring better cataytic or electrochemical performance.

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