

# In-situ Oxygen-driven Growth Regulation and Defect Passivation in Chemical Vapor Deposited MoS<sub>2</sub> Monolayers

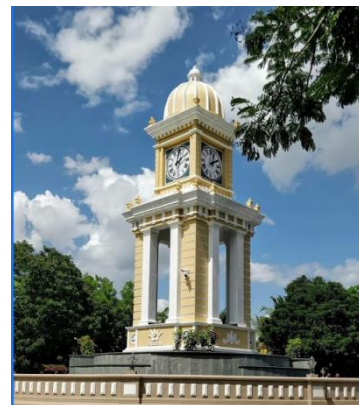
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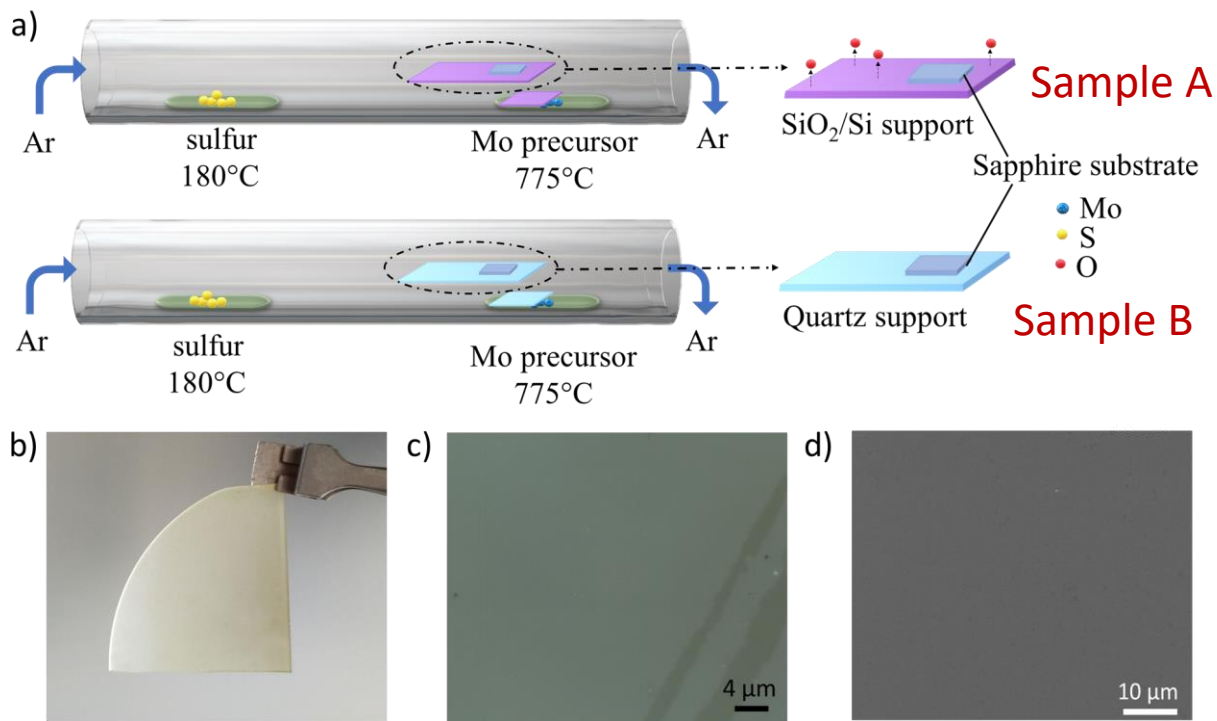
by

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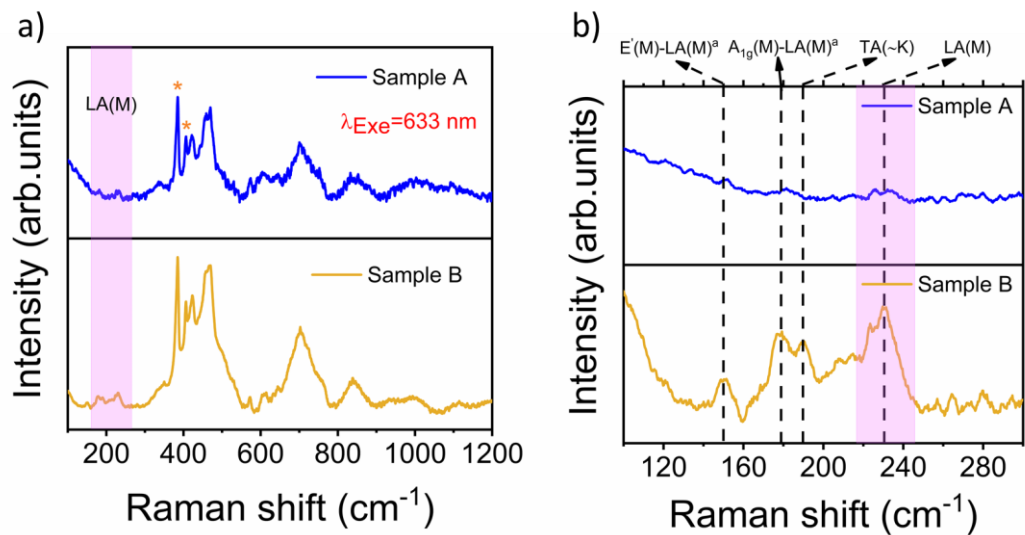
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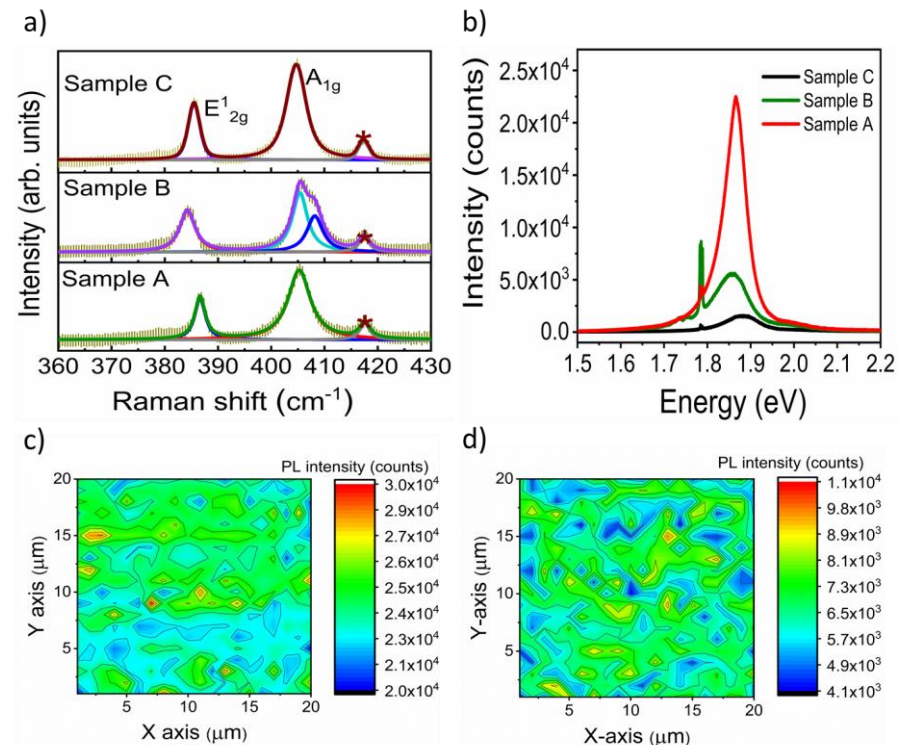




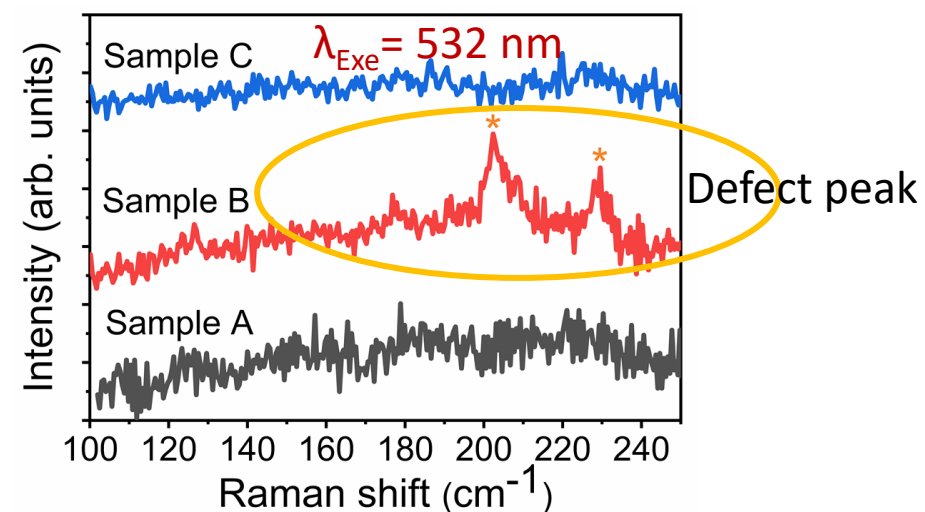
(a) Schematic diagram of the experimental setup used for growth of MoS<sub>2</sub> (b) photograph of the grown MoS<sub>2</sub> on sapphire substrate (c,d) Optical microscope and HRSEM image of MoS<sub>2</sub>



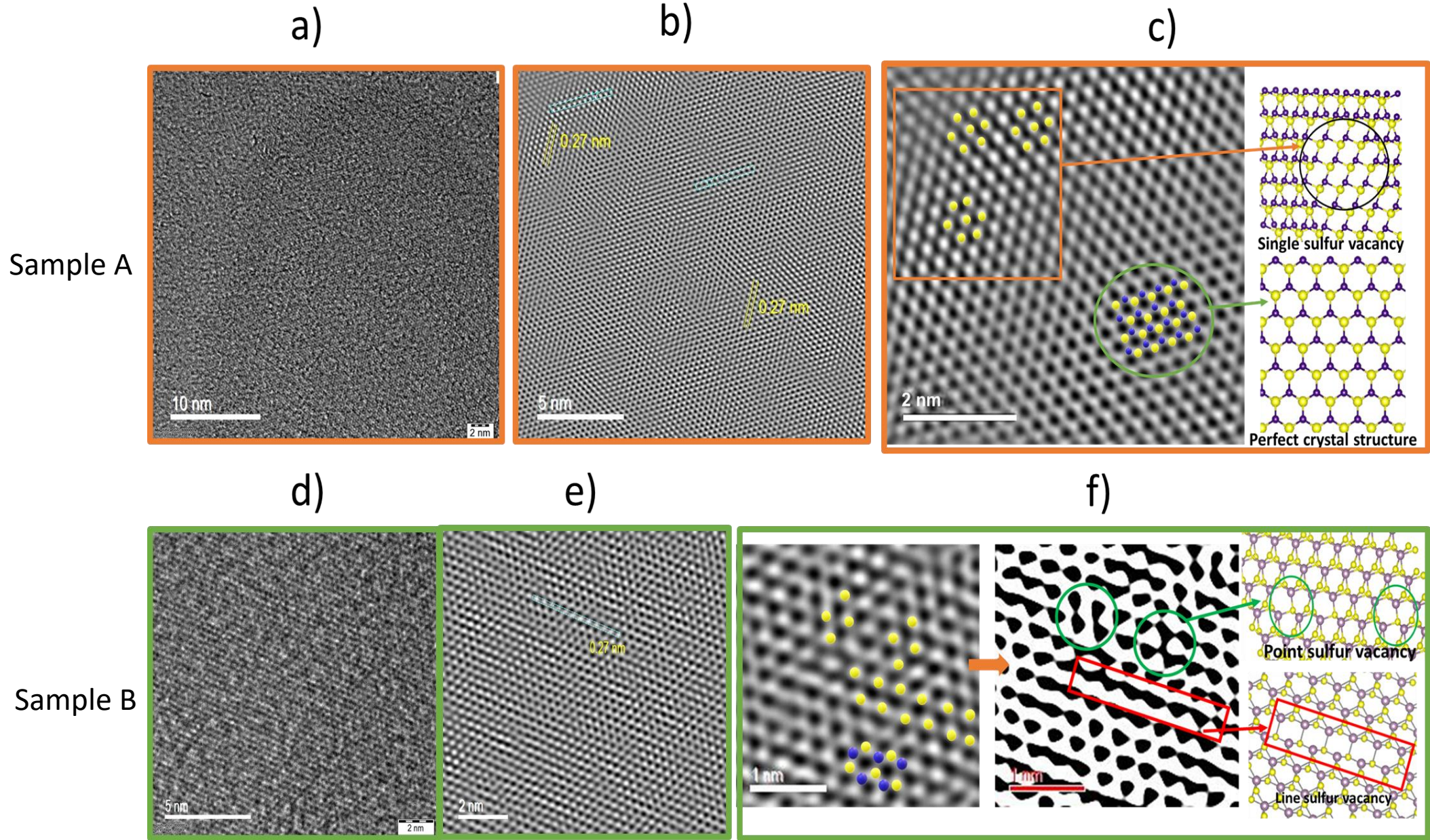
(a, b) Resonance Raman spectra of sample A and sample B



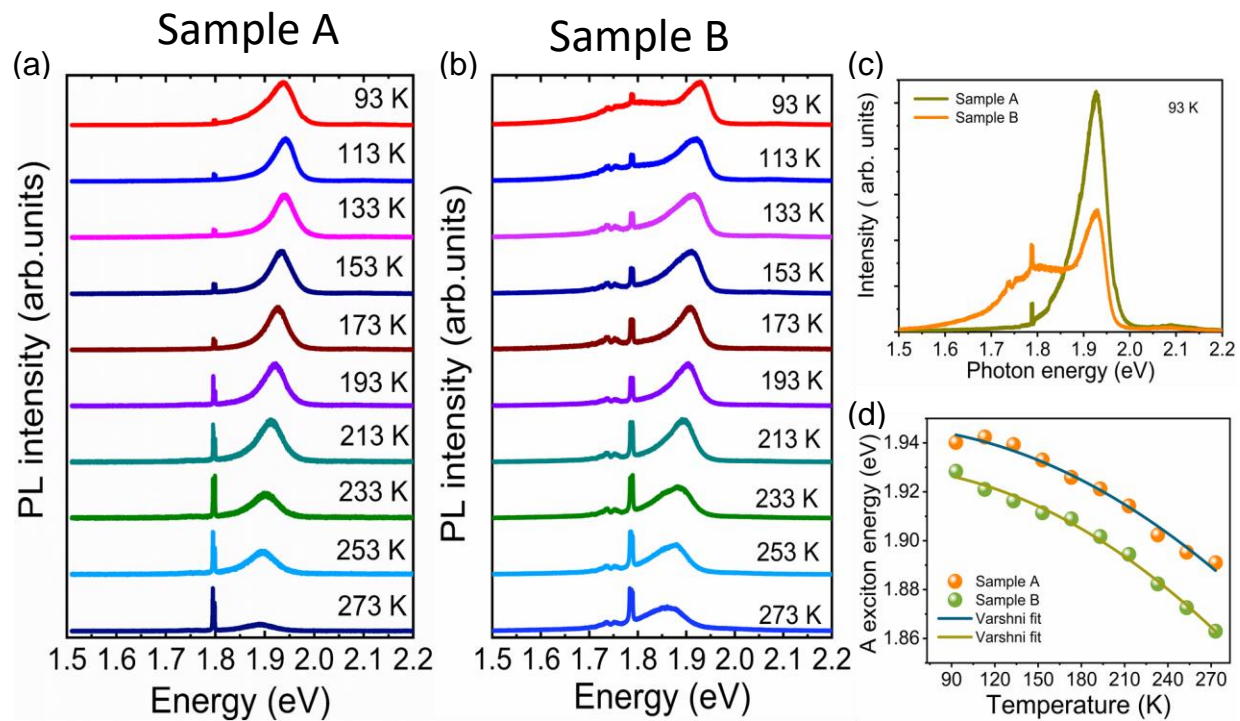
(a) Raman spectra of sample A (SiO<sub>2</sub> support), sample B (quartz support) and sample C (Gas phase) CVD (b) μ-PL spectra of sample A, B and C (c,d) PL intensity maps of sample A and B



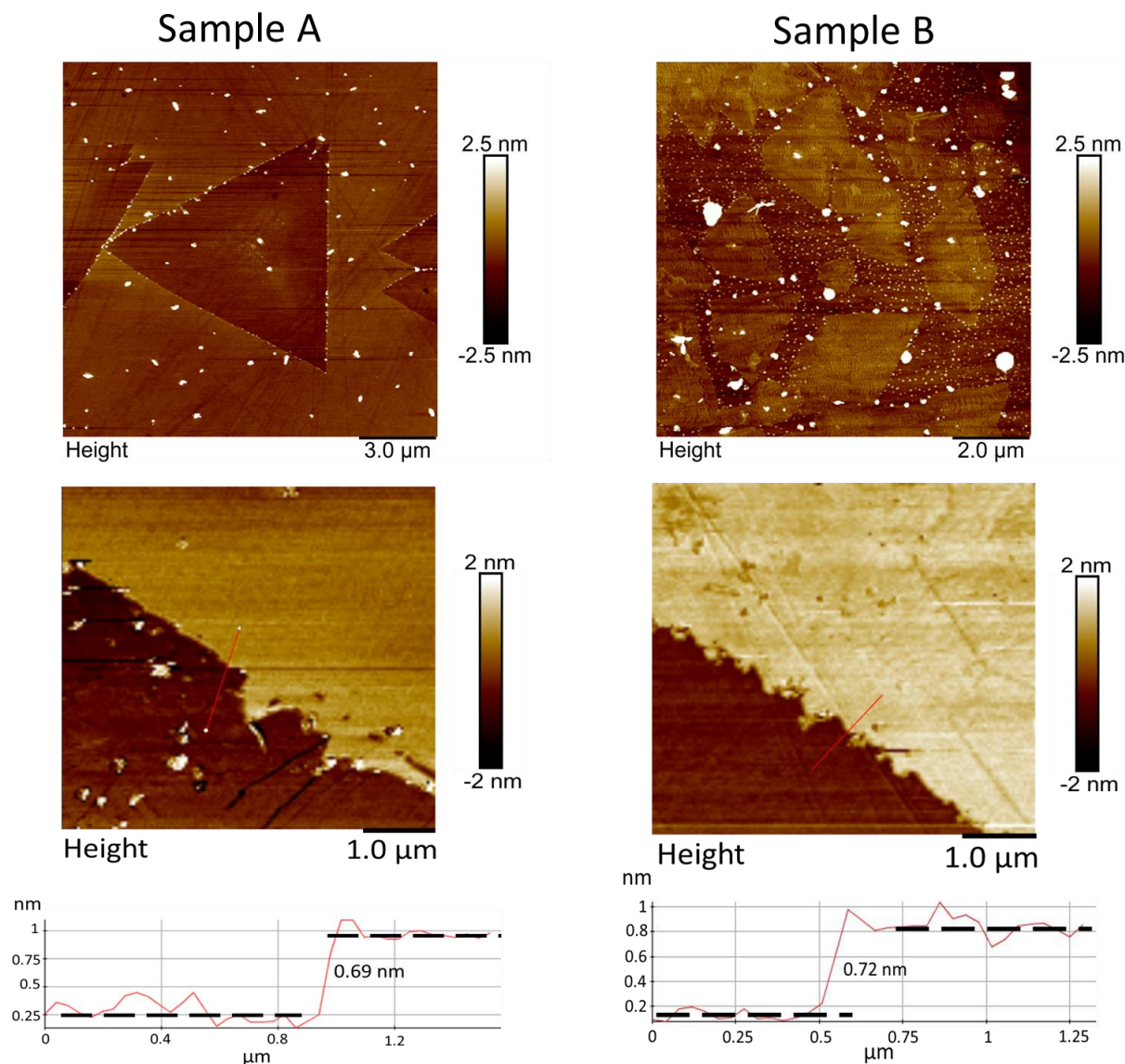
Raman spectra of MoS<sub>2</sub> samples in the frequency range from 100-250 cm<sup>-1</sup>



HRTEM analysis of the grown MoS<sub>2</sub> films. Figure (a) shows the raw image and (b) and (c) are the inverse FFT images of sample A. The raw and inverse FFT images of sample B are shown in (d) and (e-f), respectively.



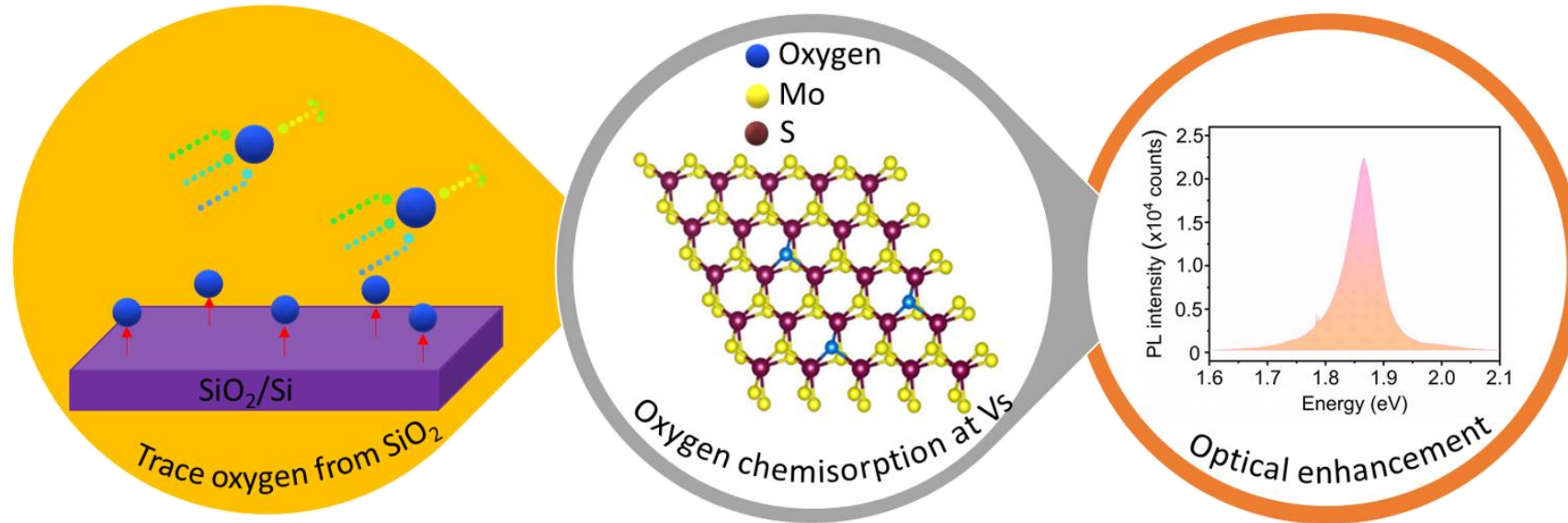
Temperature-dependent  $\mu$ -PL spectra of MoS<sub>2</sub> for (a) sample A and (b) sample B. (c) Comparison of the PL spectrum recorded at 93 K. (d) Variation in the A exciton energy with temperature. The solid lines are Varshni fit to the experimental data.



AFM topography images of MoS<sub>2</sub> domains and continuous film of sample A and sample B



# Conclusion



- ❑ An effective method for passivating the  $V_S$  *in situ* by using an oxide substrate in the vapor phase CVD
- ❑ The chemisorbed oxygen is found to have a strong impact on the defect sites such that it transforms the localized trap states to electronically benevolent sites, which exhibited very strong band edge photoluminescence
- ❑ In the absence of oxygen, the growth of MoS<sub>2</sub> and its structure is greatly altered. The present findings also provided new insights into the phonon behavior in highly defective monolayer MoS<sub>2</sub>

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