

## Supplementary Information

### Horizontally and Vertically Aligned Growth of Strained MoS<sub>2</sub> Layers with Dissimilar Wetting and Catalytic Behavior

Pawan Kumar and B. Viswanath\*

School of Engineering, Indian Institute of Technology Mandi, Kamand, Himachal Pradesh-175005.

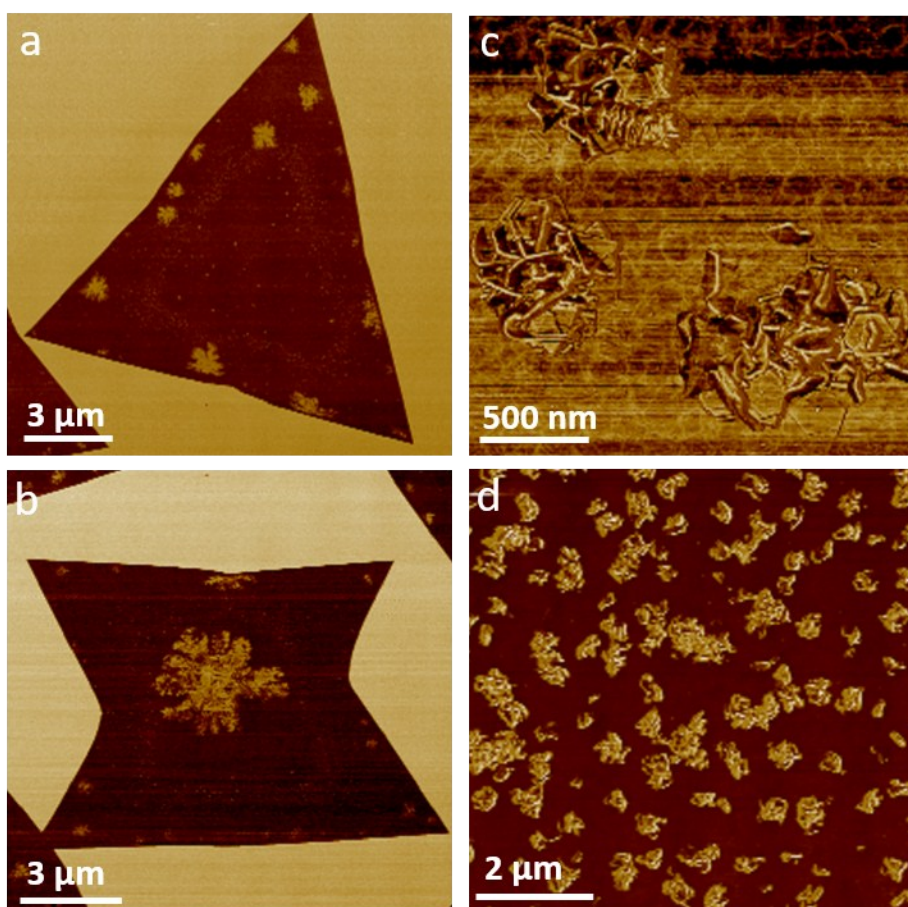


Figure S1: AFM phase imaging of horizontally aligned (a, b) and (c, d) vertically aligned MoS<sub>2</sub> nanostructure. Formation of new seed layer on top of horizontally grown MoS<sub>2</sub> flake is evident from (b). As grown vertical standing MoS<sub>2</sub> on top of horizontally aligned MoS<sub>2</sub> nanostructures are shown in (c).

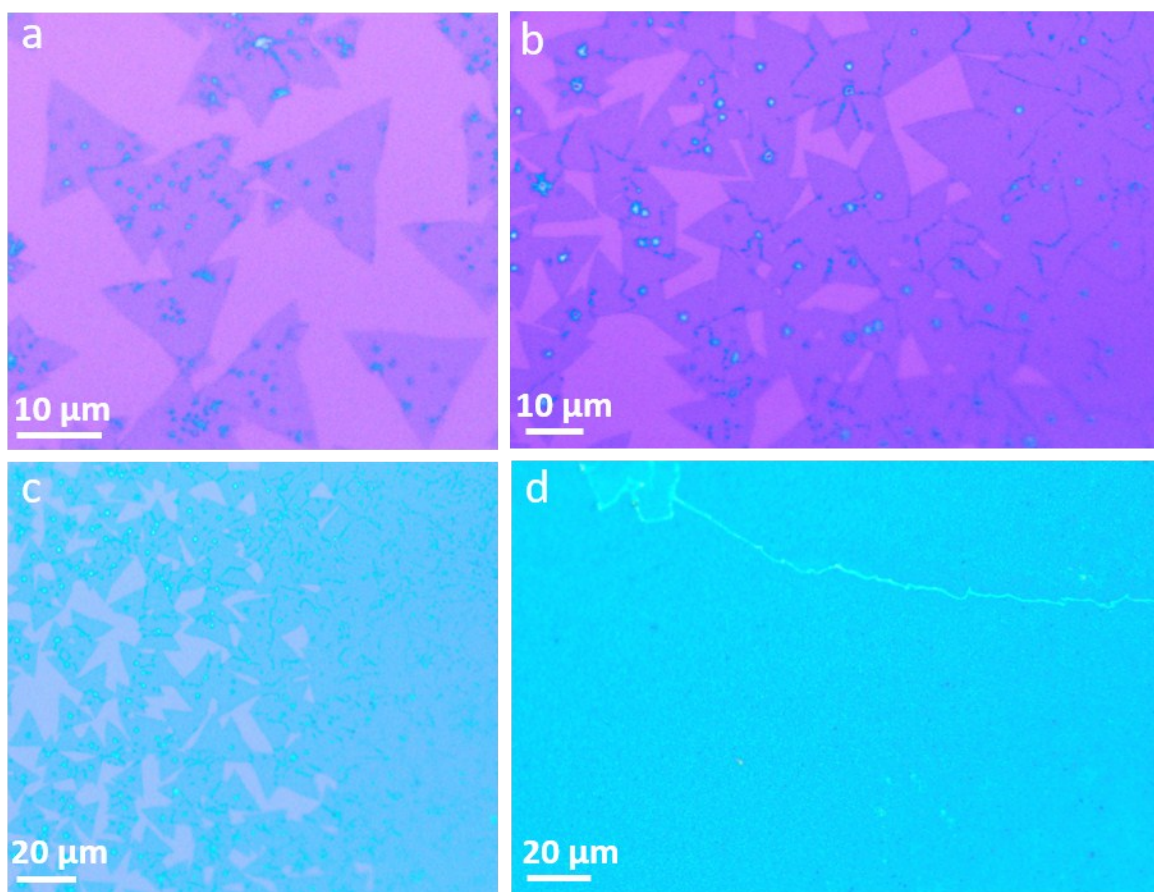


Figure S2: Visible light microscope (VLM) imaging carried out at different location showing individual as well as interconnected MoS<sub>2</sub> flakes with different coverage. (a, b) Monolayer MoS<sub>2</sub> flakes with lateral dimension of  $\sim 15 \mu\text{m}$  undergoing coalescence and forms interconnected structure. Formation of continuous film consisting of interconnected MoS<sub>2</sub> flakes with full coverage of  $1 \times 1 \text{ cm}^2$  on SiO<sub>2</sub>/Si substrate are shown in (c, d).

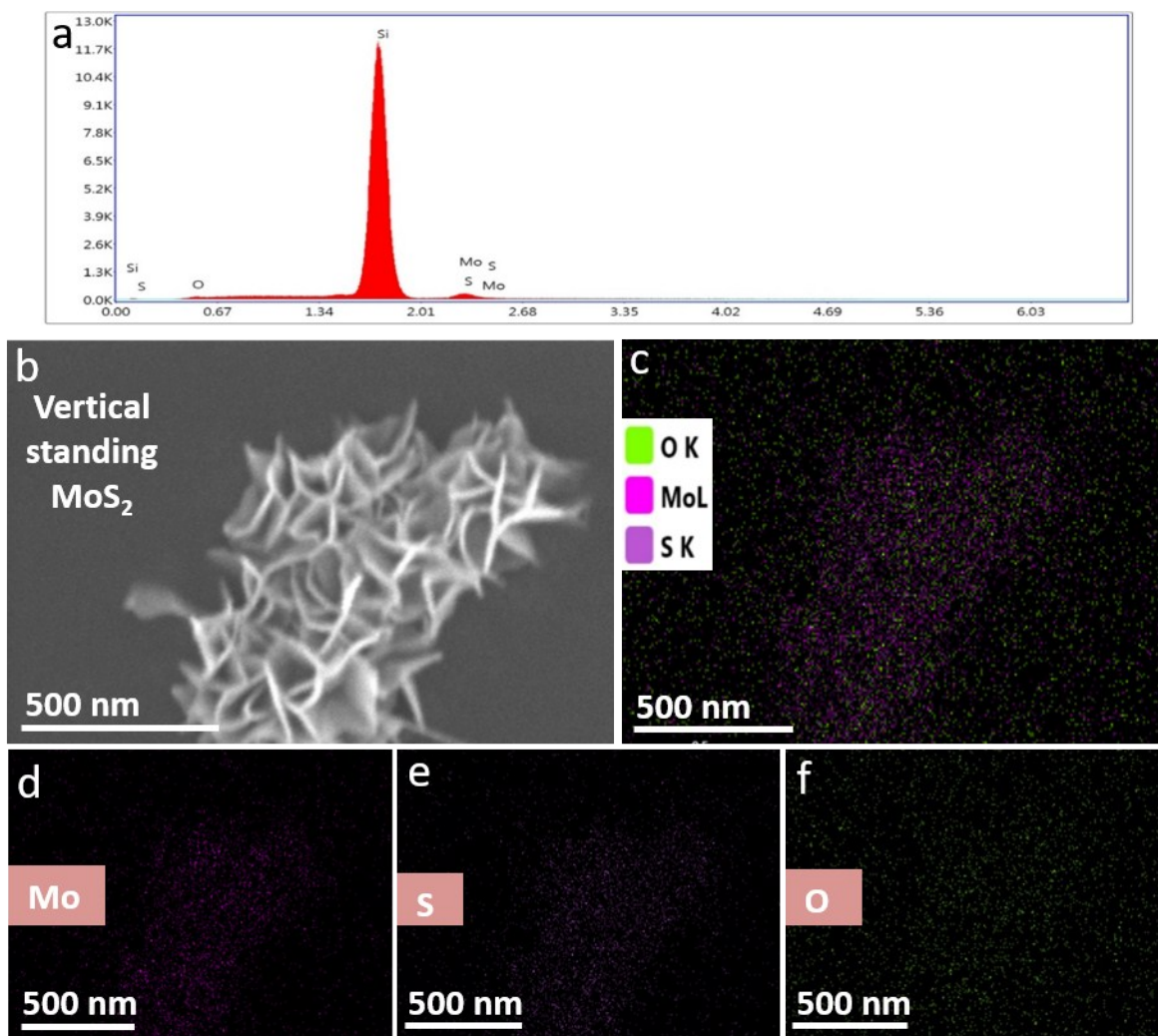


Figure S3: Elemental mapping of vertically aligned  $\text{MoS}_2$  using EDS-FESEM system; Spectrum shown in (a) has clear elemental analysis for presence of  $\text{MoS}_2$  on Si substrate. FESEM micrograph of vertically grown  $\text{MoS}_2$  nanostructure and the corresponding elemental mapping are shown in (b) and (c). Images depicting individual elements (Mo, S & O) are shown in (d) Molybdenum (e) Sulfur and (f) Oxygen.

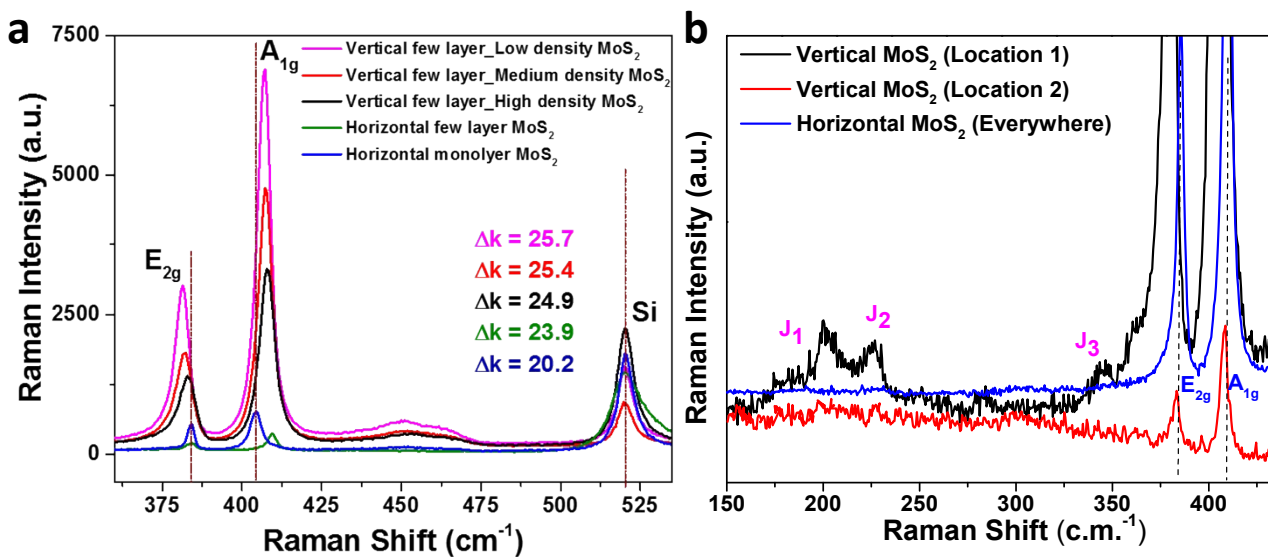
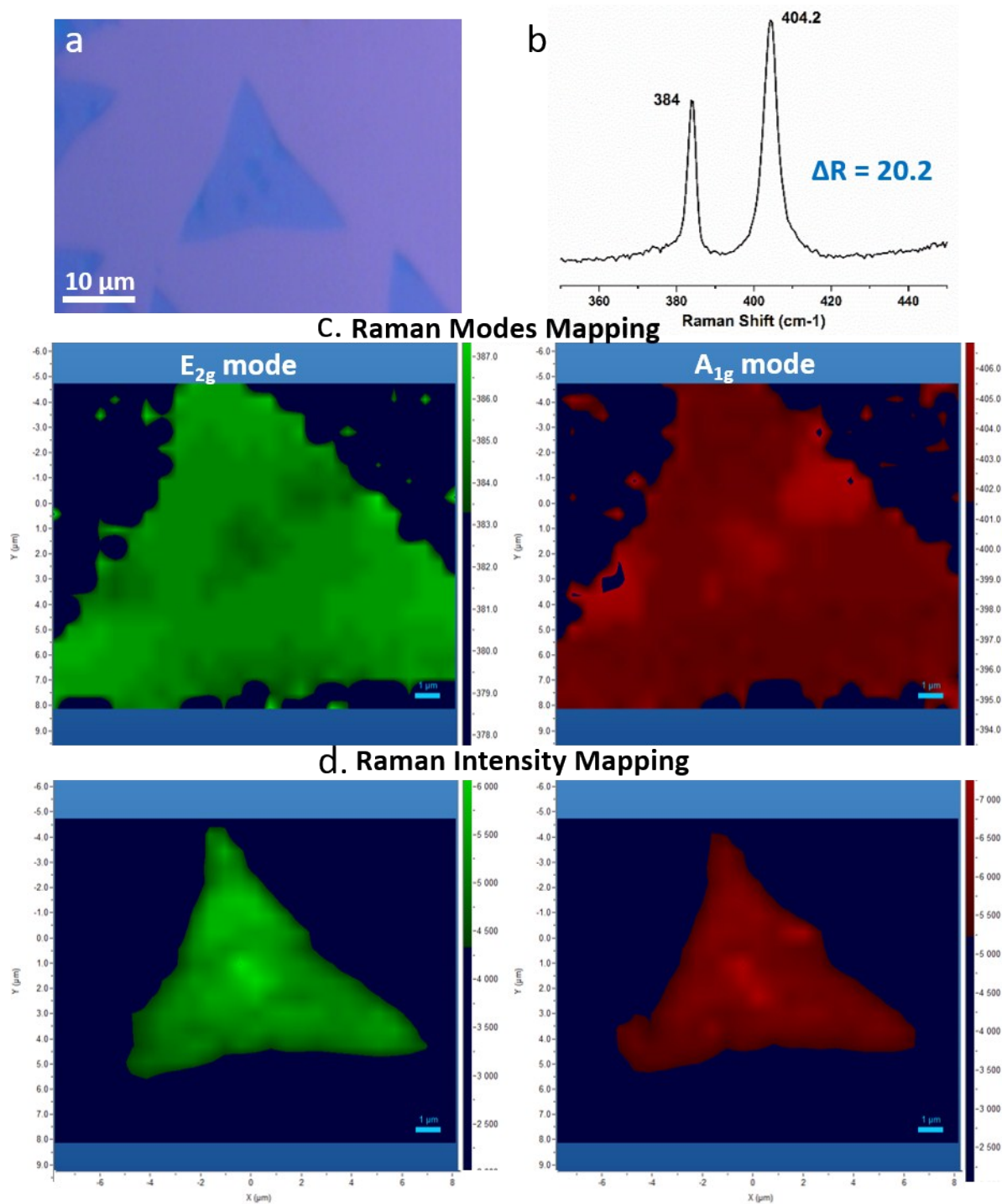


Figure S4: (a) Raman modes observed for different anisotropic aligned MoS<sub>2</sub> nanostructures with varying density. Raman shift and intensity variation influenced by the observed density variation in vertically aligned MoS<sub>2</sub>. (b) Presence of 2H and 1T phase in vertically aligned MoS<sub>2</sub> measured at different locations whereas only 2H phase significantly present in horizontally aligned MoS<sub>2</sub>.

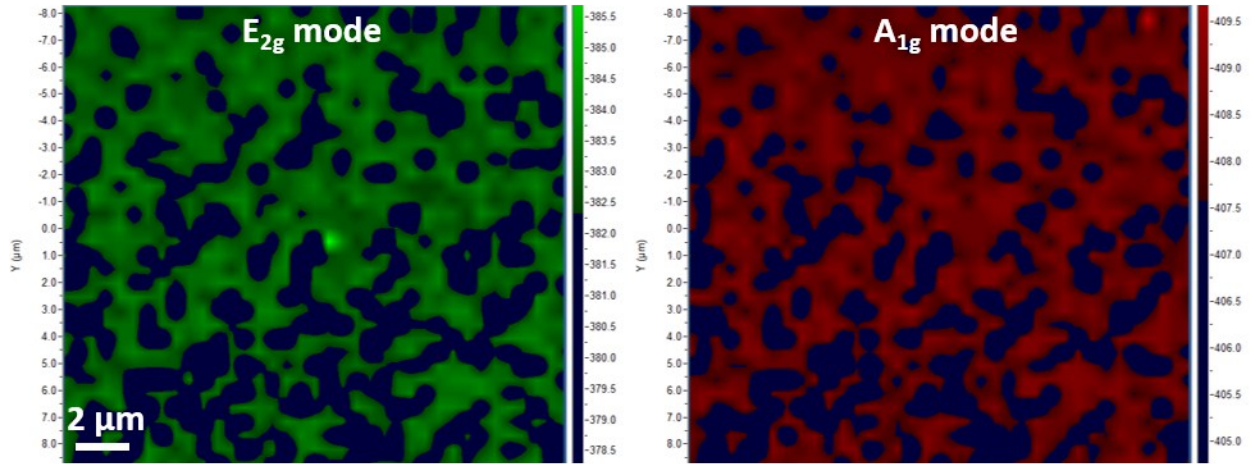




Figure

re S5: (a) Visible light microscope imaging along with Raman spectrum confirms the growth of monolayer MoS<sub>2</sub> on Si substrate. (b) Difference in Raman shift ( $\Delta R \sim 20.2 \text{ cm}^{-1}$ ) observed between E<sub>2g</sub> and A<sub>1g</sub> Raman vibration modes is consistent with earlier reports. Slight contrast variation observed in the Raman mode and intensity mapping indicates the nucleation of seed layers on top of MoS<sub>2</sub> monolayer(c, d).

### a. Raman Modes Mapping



### b. Raman Intensity Mapping

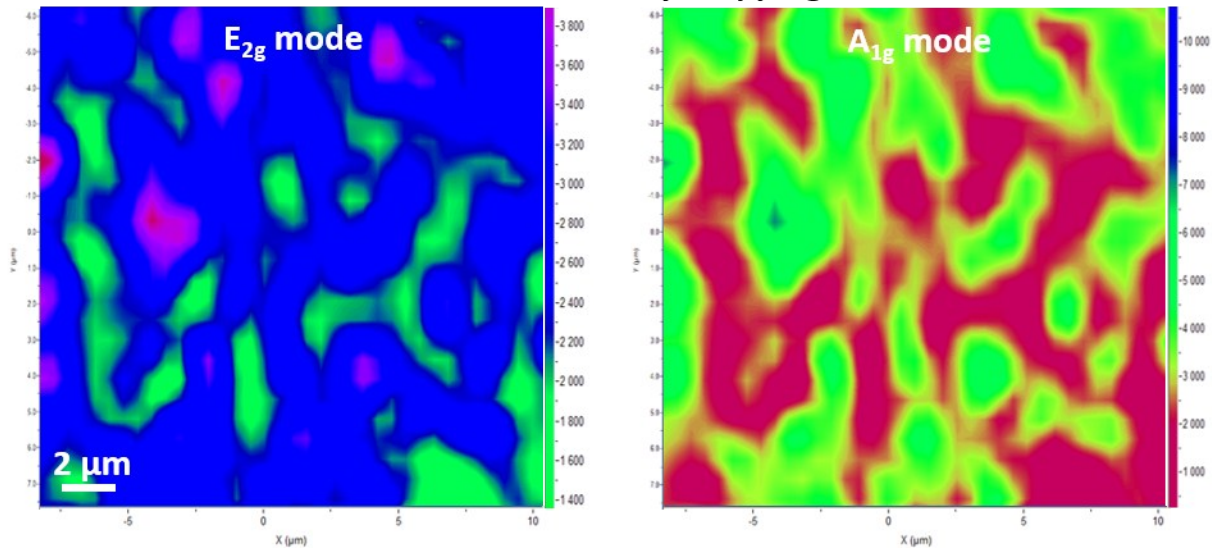


Figure S6: (a) Raman mapping of  $E_{2g}$  and  $A_{1g}$  vibration modes for few layer vertical standing  $MoS_2$  and their corresponding (b) Raman intensity maps. Intensity mapping of  $A_{1g}$  mode shows two fold increase compared to  $E_{2g}$  mode intensity for the same position in vertically aligned  $MoS_2$ .

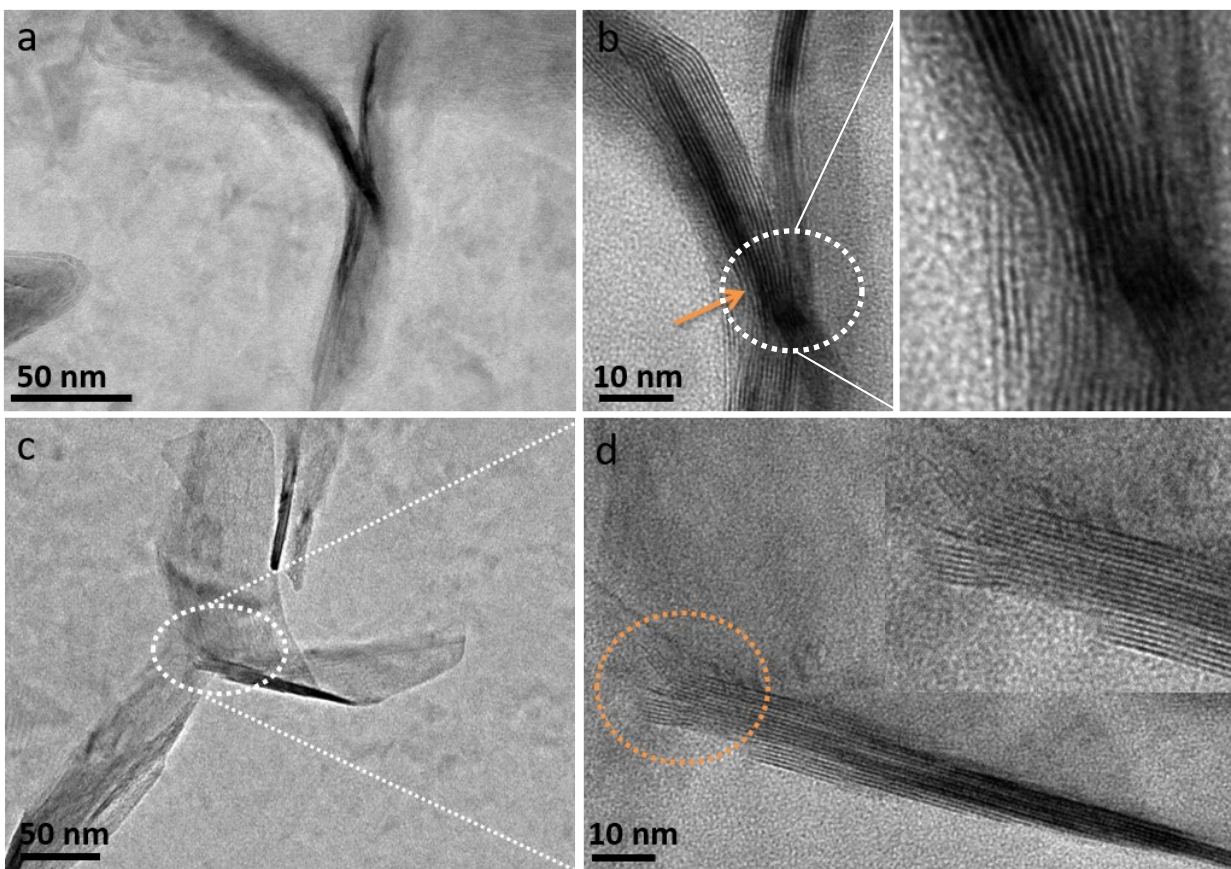
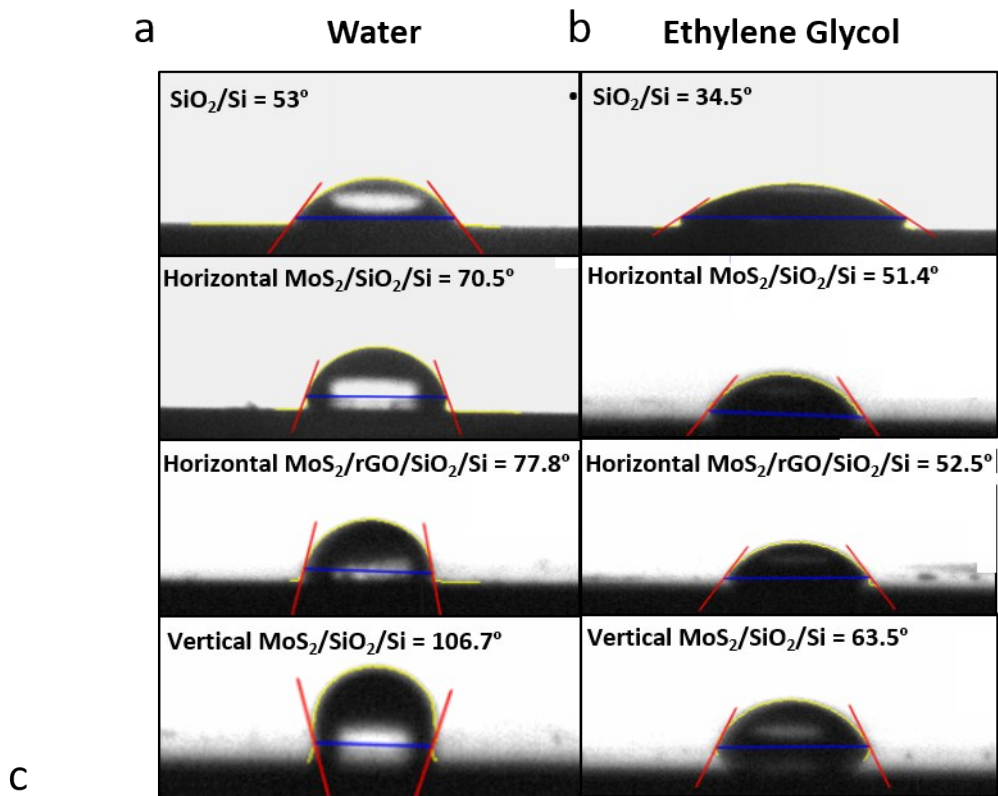


Figure S7: TEM bright field and lattice images of vertically standing  $\text{MoS}_2$  layers undergoing coalescence are shown in (a - c) respectively. Number of atomic thin layers present in each  $\text{MoS}_2$  flake and coalescence induced deformation is evident in (b) along with high resolution image of marked circular portion. Similarly, bending in atomic thin  $\text{MoS}_2$  flakes causes strain between intra layers lead to mechanical deformation (crack) as indicated by circular marked region in figure (d) with inset showing high resolution TEM micrographs.



S. No.	Sample description	Contact Angle		Total Surface Energy (mJ/m <sup>2</sup> )	Surface Energy (mJ/m <sup>2</sup> ) (Polar)	Surface Energy (mJ/m <sup>2</sup> ) (Dispersive)
		Water	Ethylene Glycol			
1.	SiO <sub>2</sub> /Si (Bare Substrate)	53°	34.5°	51.19	47.04	4.15
2.	Flat MoS <sub>2</sub> /SiO <sub>2</sub> /Si	70.5°	51.4°	33.39	27.99	5.40
3.	Vertical MoS <sub>2</sub> /SiO <sub>2</sub> /Si	106.7°	63.5°	22.39	0.26	22.14

Figure S8: Contact angle measurement for horizontally and vertically aligned MoS<sub>2</sub> nanostructure with respect to two different liquid (a) Water and (b) Ethylene glycol having known surface tension. (c) Corresponding calculated surface energies for both oriented MoS<sub>2</sub> nanostructures.



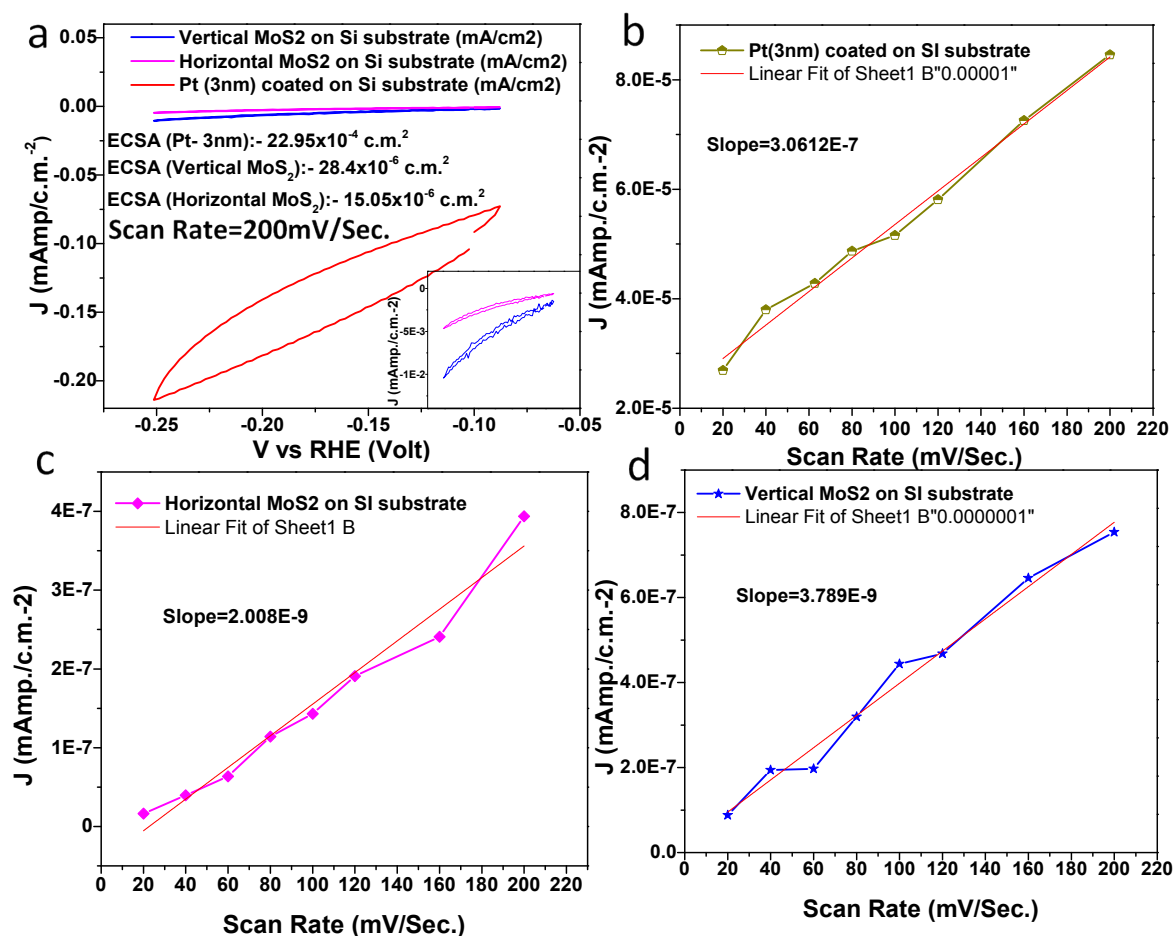


Figure S9: Comparative CV measurement plot at scan rate of 200 mV/sec. and fitted curves for the different scan rate based CV measurement across both nanostructures of MoS<sub>2</sub> as well as Pt. (3nm) coated on Si substrate to calculate  $C_{dl}$  and further analyze the ECSA.

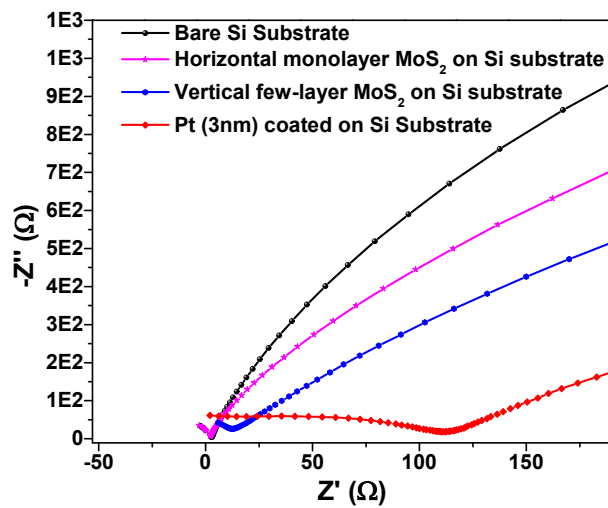


Figure S10: Zoomed region of impedance analysis for different aligned MoS<sub>2</sub> nanostructures with standard Pt. (3 nm).

Table ST1: Controlled growth conditions to achieve horizontal and vertical MoS<sub>2</sub> nanostructures.

Substrate	Growth Parameters	Horizontal MoS <sub>2</sub>	Vertical MoS <sub>2</sub>
Si SiO <sub>2</sub> /Si Si <sub>3</sub> N <sub>4</sub> /Si	Temperature Zone 1 (MoO <sub>3</sub> ) : Zone 2 (S)	650°C : (180°C - 220°C)	700°C : (400°C - 450°C)
	Ar flow	~ 5 sccm	~ 5 sccm
	S - MoO <sub>3</sub> ratio	~18	~22
	S - MoO <sub>3</sub> distance	~15 cm	~12 cm
	Growth Time	~ 3 to 5 min.	~ 10 min.