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Supplementary Material

New insight into growth of monolayer MoS₂ flakes by indigenously developed CVD setup: A study on shape evolution and spectroscopy

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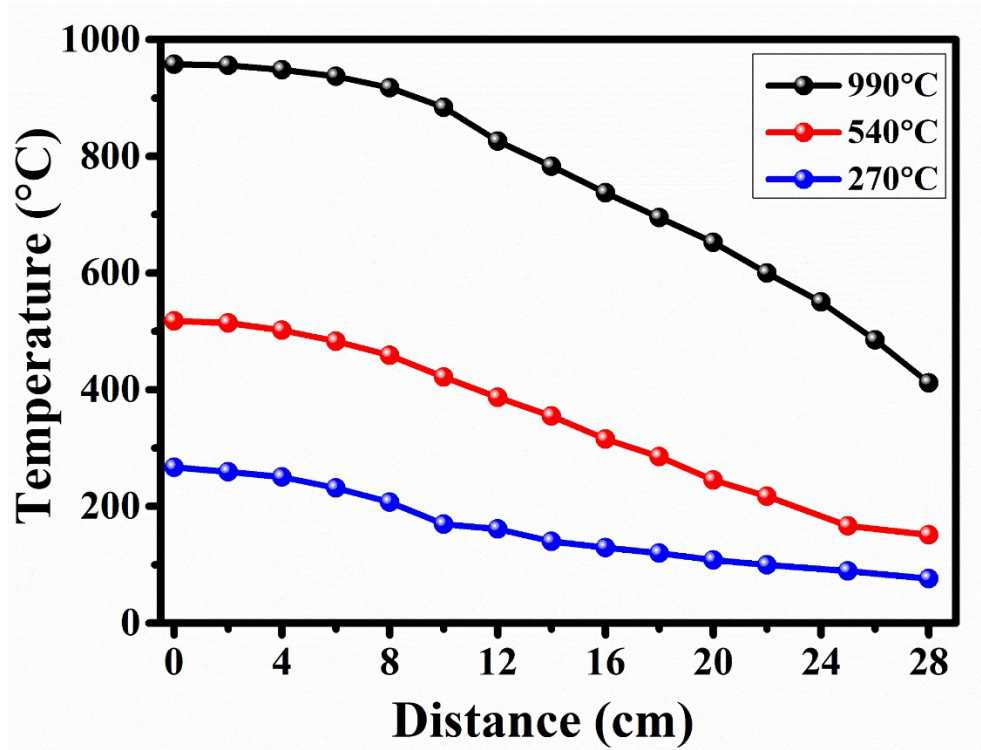


Figure S1. The temperature profile of quartz tuSSbe towards the upstream direction from center location of the zone at three different temperatures (990 °C, 540 °C, and 270 °C). The profiles show the actual temperature at different locations across the tube and the legend displays the set temperature of the single zone furnace.

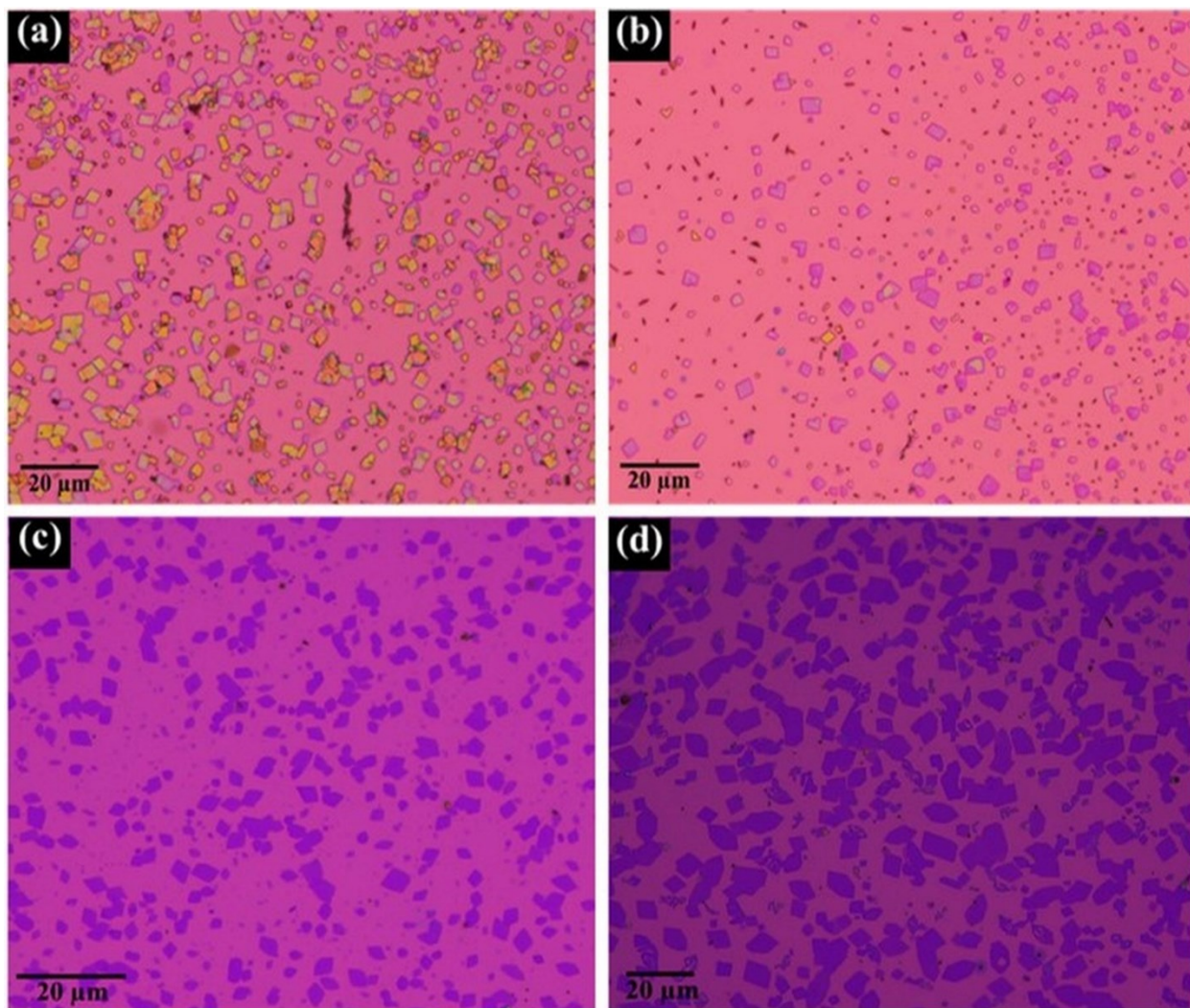


Figure S2. The optical images of CVD grown MoO₂ flakes over Si substrate having SiO₂ thickness of 300 nm (Substrate-I), close to MoO₃ powder. (a) The optical image at the growth temperature of 700°C and ~1:8.6 weight ratio of MoO₃ and S precursors. (b) The optical image at the growth temperature of 725°C and weight ratio of ~ 1:7.1. (c,d) The optical images at the growth temperature of 750°C and weight ratio of ~ 1:3.

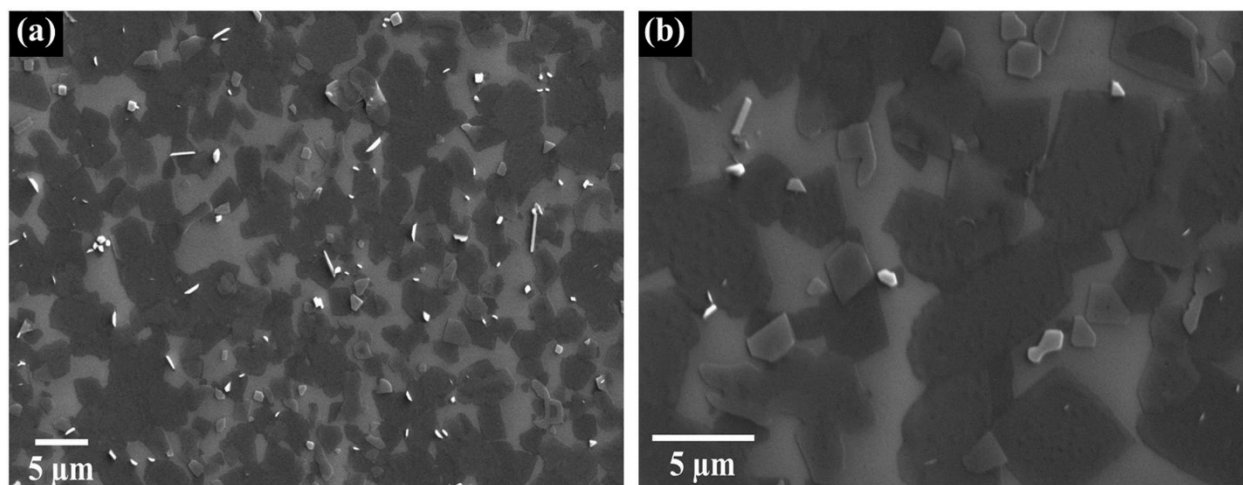


Figure S3. (a,b) The SEM images of different MoO₂ flakes on Substrate-I at the growth temperature of 750°C and weight ratio of ~ 1:3.

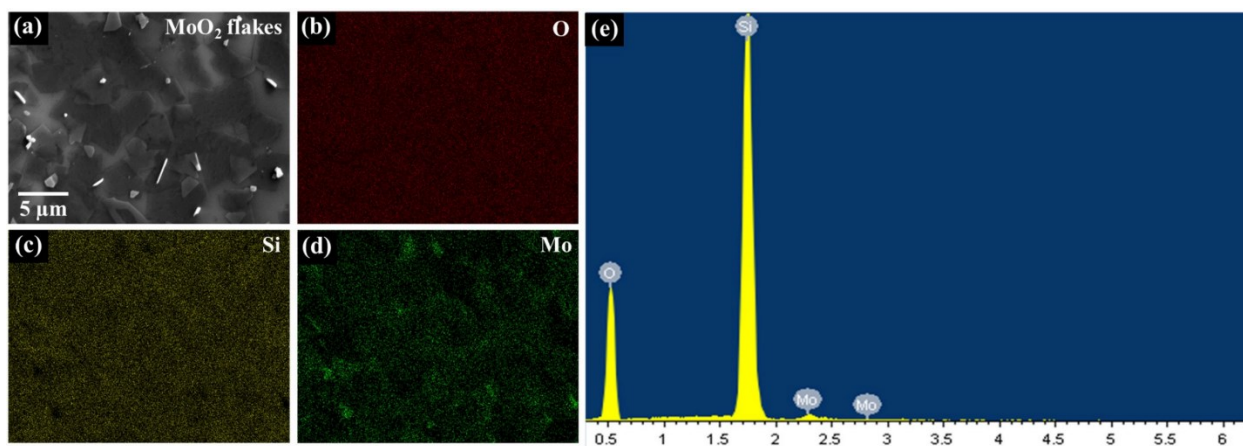


Figure S4. (a-d) shows the EDX elemental mapping images of O, Si, and Mo in MoO₂ flakes. (e) Elemental analyses of the MoO₂ flakes over Si/SiO₂ substrate (Substrate-I).

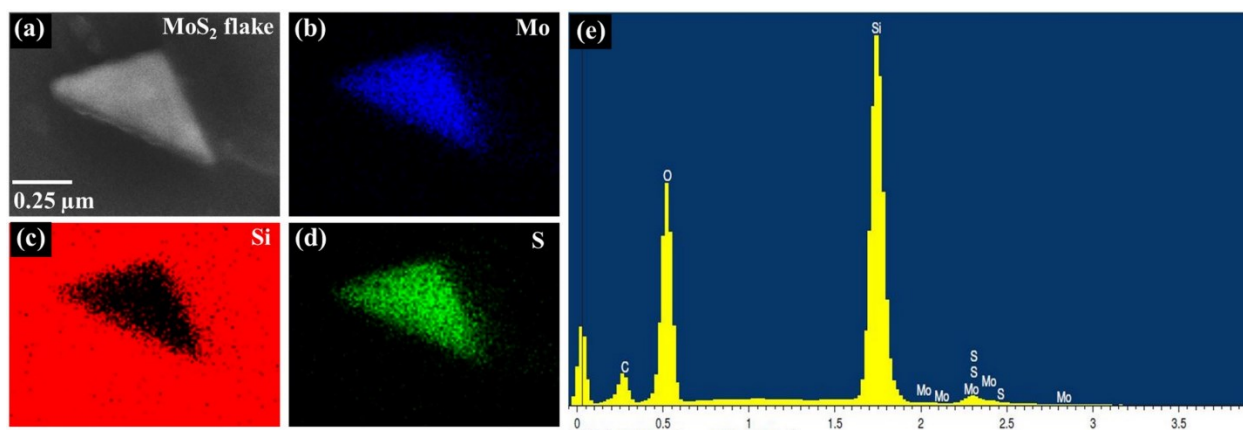


Figure S5. (a-d) shows the EDX elemental mapping images of Mo, Si, and S in MoS₂ flakes. (e) Elemental analyses of the MoS₂ flakes over Si/SiO₂ substrate (Substrate-II).

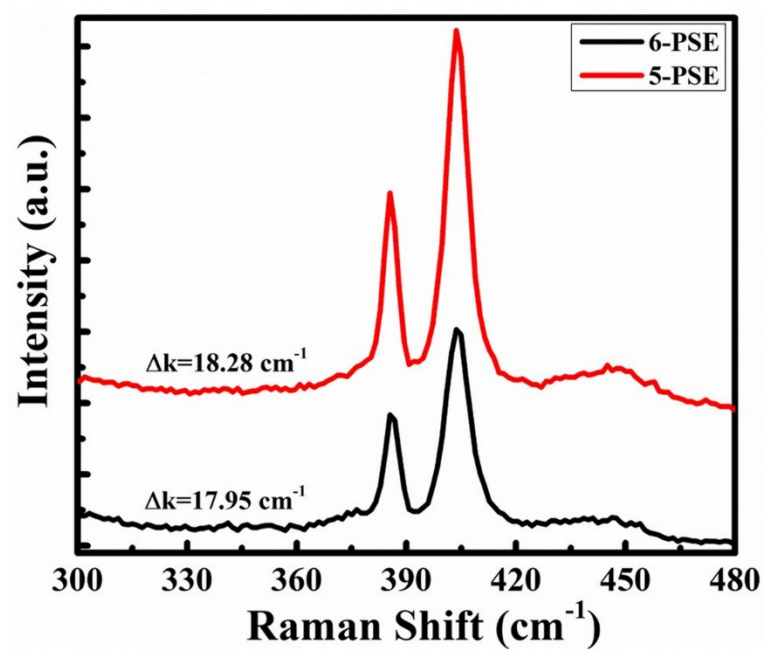


Figure S6. Raman spectra are captured on the edge of five-point star and six-point star MoS₂ flakes deposited over Si/SiO₂ substrate.

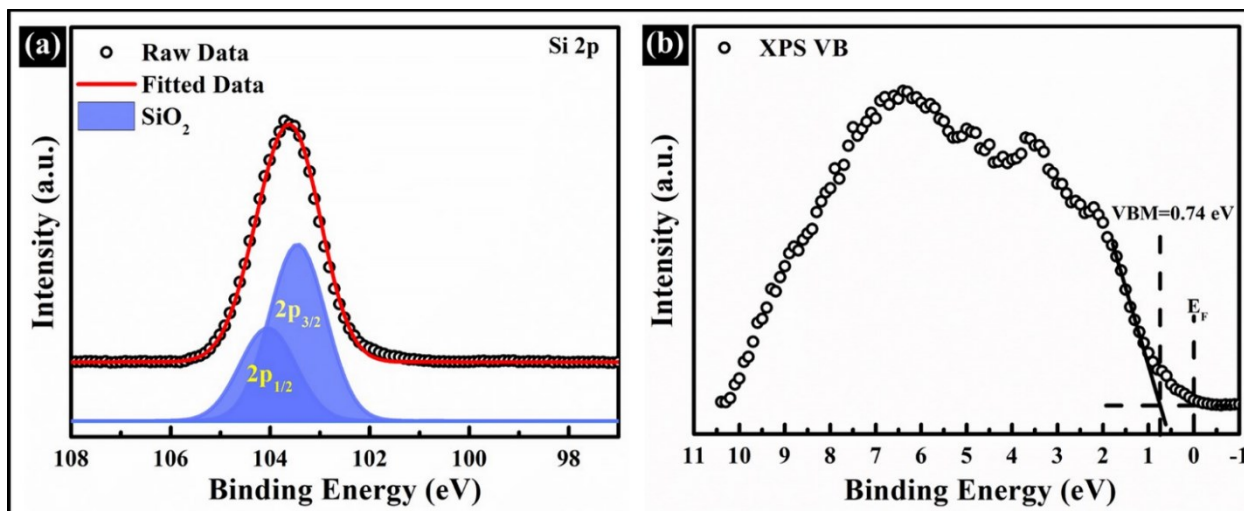


Figure S7. (a) High-resolution XPS spectra of Si 2p. (b) XPS-VB spectra are recorded at room temperature, and the valence band maxima position is located at 0.74 ± 0.05 eV below the Fermi level.

Table S1. Fitting parameters of the PL spectra in various shapes of MoS₂ flakes deposited on Si/SiO₂ substrate.

Shapes (MoS ₂ flakes)	A ⁻ trion (eV)	A ⁰ exciton (eV)	B exciton (eV)	VBS (meV)
Triangle (normal)	–	1.82663	1.97937	152.74
Triangle (sharp)	1.76775	1.82098	1.96045	139.47
Truncated Triangle	1.77075	1.81766	1.94566	128.00
Three point star	–	1.81385	1.96559	151.74
Four point star	1.76973	1.81293	1.94385	130.92
Five point star	1.77303	1.83342	1.95728	123.86
Six point star	1.77941	1.82049	1.94592	125.43
Tilt boundary	1.76906	1.81521	1.94673	131.52
Mirror boundary	1.76975	1.82162	1.94456	122.94