

Low-temperature synthesis of MoS₂ slabs on TiO₂(110)

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S1. Comparison of Mo/TiO₂(110) precursors at Mo coverages of 0.25 ML and 0.49 ML

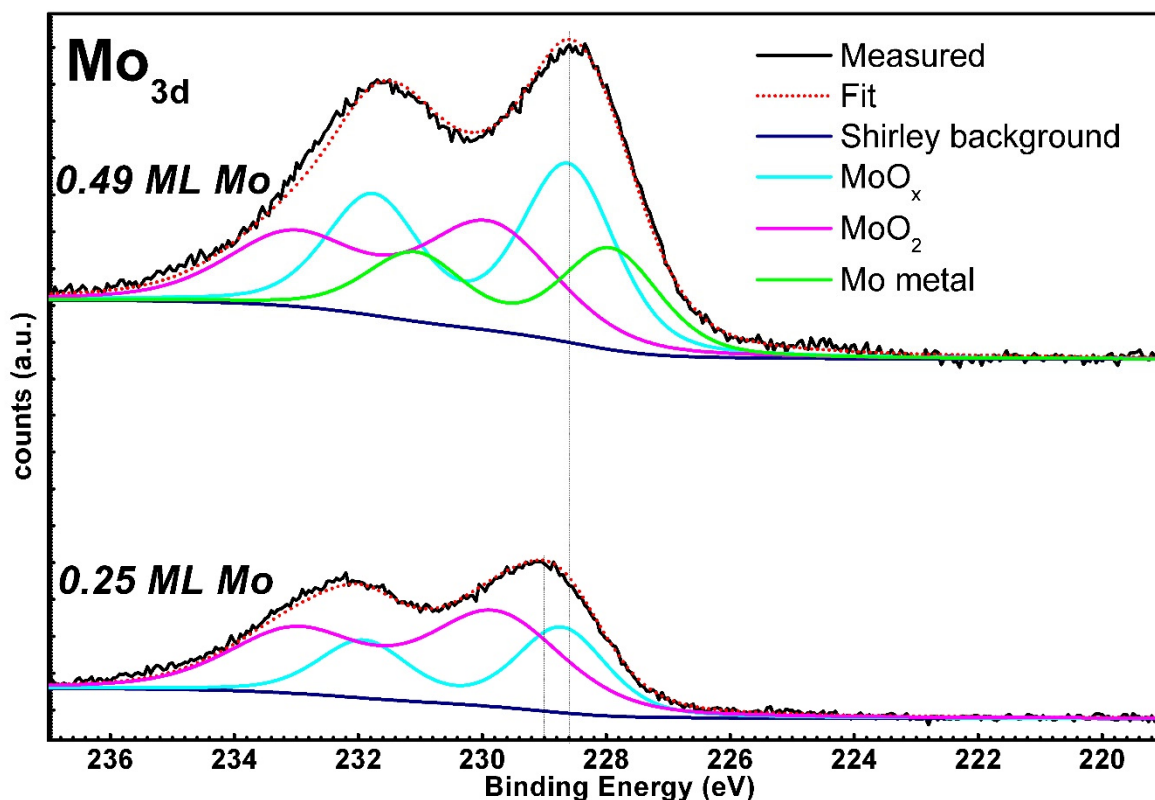


Figure S1. Mo 3d spectra of Mo nanoparticles supported on TiO₂(110) at initial Mo overages of 0.25 ML and 0.49 ML.

S2. MoS₂ slabs grown on TiO₂(110) at Mo coverages of 0.49 and 0.61 ML

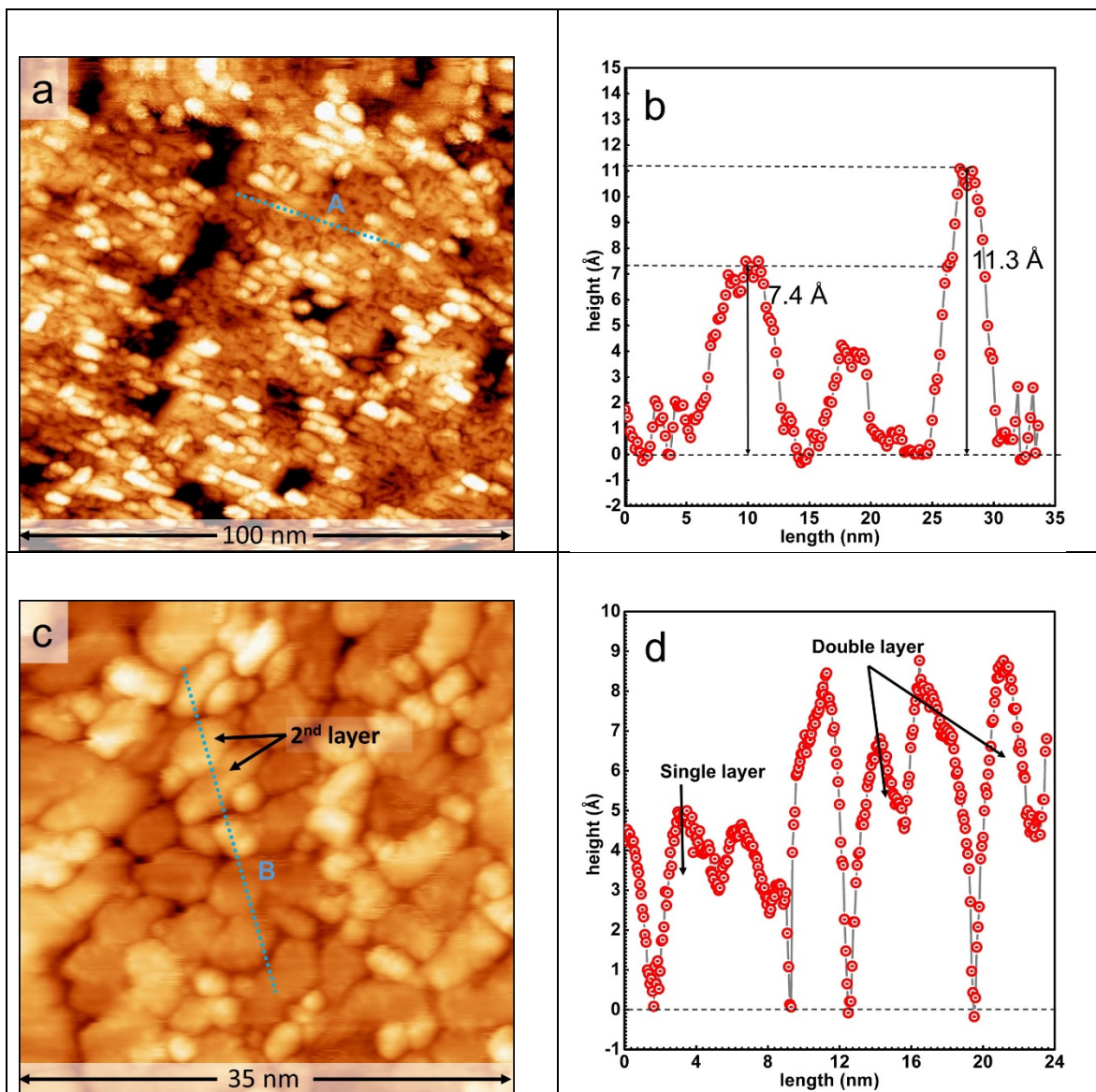


Figure S2. a) Large-scale STM image of MoS₂ supported on TiO₂(110) obtained with a sample voltage = +2.2 V and tunneling current = 250 pA. The coverage of Mo is 0.61 ML. b) Measured height along the line marked A in Figure S2a. c) Large-scale STM image of MoS₂ supported on TiO₂(110) obtained with a sample voltage = +2.1 V and tunneling current = 300 pA. The coverage of Mo is 0.49 ML. d) Measured height along the line marked B in Figure S2c.

S3. Estimation of the number density of the elongated structures from STM images

Table S1. Table for estimation of the projected coverages of the elongated structures from STM images of various locations of the samples.

absolute Mo coverage from XPS	Area fraction–elongated structure
0.25	0.44 ± 0.02
0.49	0.32 ± 0.04
0.61	0.29 ± 0.03

The number of elongated structures per unit area of the substrate is proportional to the projected area fractions as measured from the STM images taking into account the elongated structures with both the intermediate and bright STM contrasts. Estimation of the projected area fraction of the elongated structures requires statistical averaging of the number of pixels over large substrate areas. For this, STM images of various areas of substrate totaling to $\sim 2 \mu\text{m}^2$ for each of the three Mo coverages were analyzed. Using the Gwyddion 2.47 software, masks were drawn over areas occupied by the elongated structures. The statistically averaged area coverages of the elongated structures are mentioned in Table S1.

S4. STM images of the exposed areas of the $\text{TiO}_2(110)$ substrate

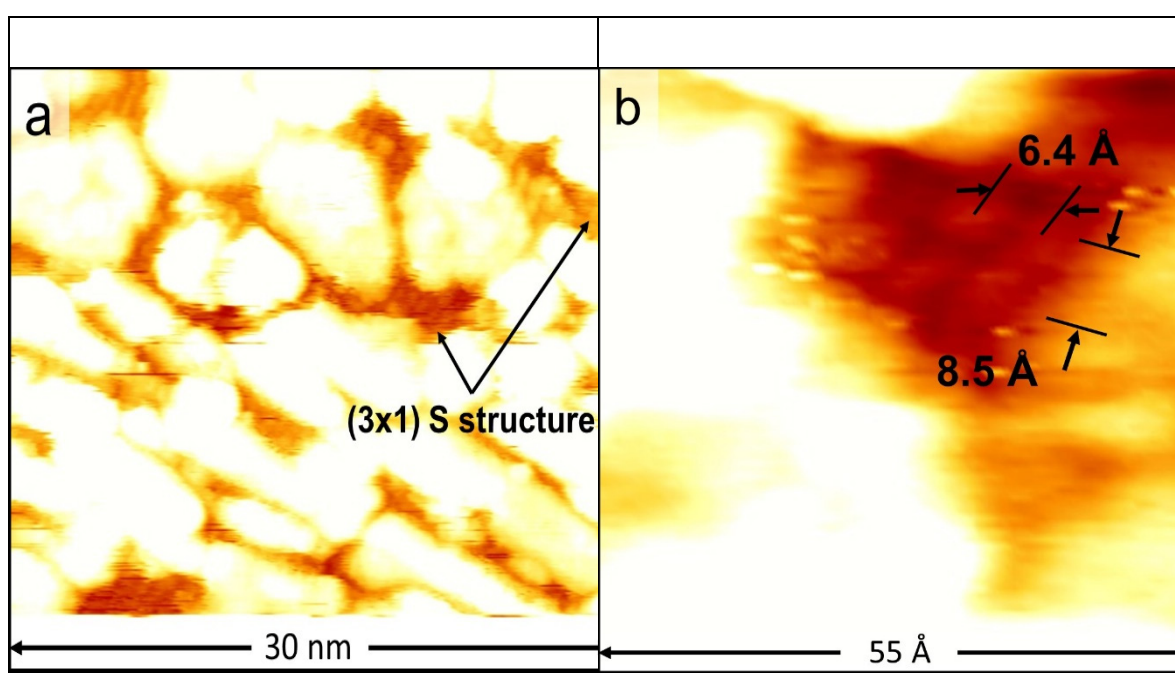


Figure S3. a) High-contrast STM image highlighting the exposed $\text{TiO}_2(110)$ substrate with the (3×1) sulfur structure; obtained with a sample voltage = +2.3 V and tunneling current = 500 pA. b) Zoom-in of a (3×1) structure near the edge of a "basal-bonded" MoS_2 slab.

S5. Atomic model of “basal-bonded” MoS₂ slabs

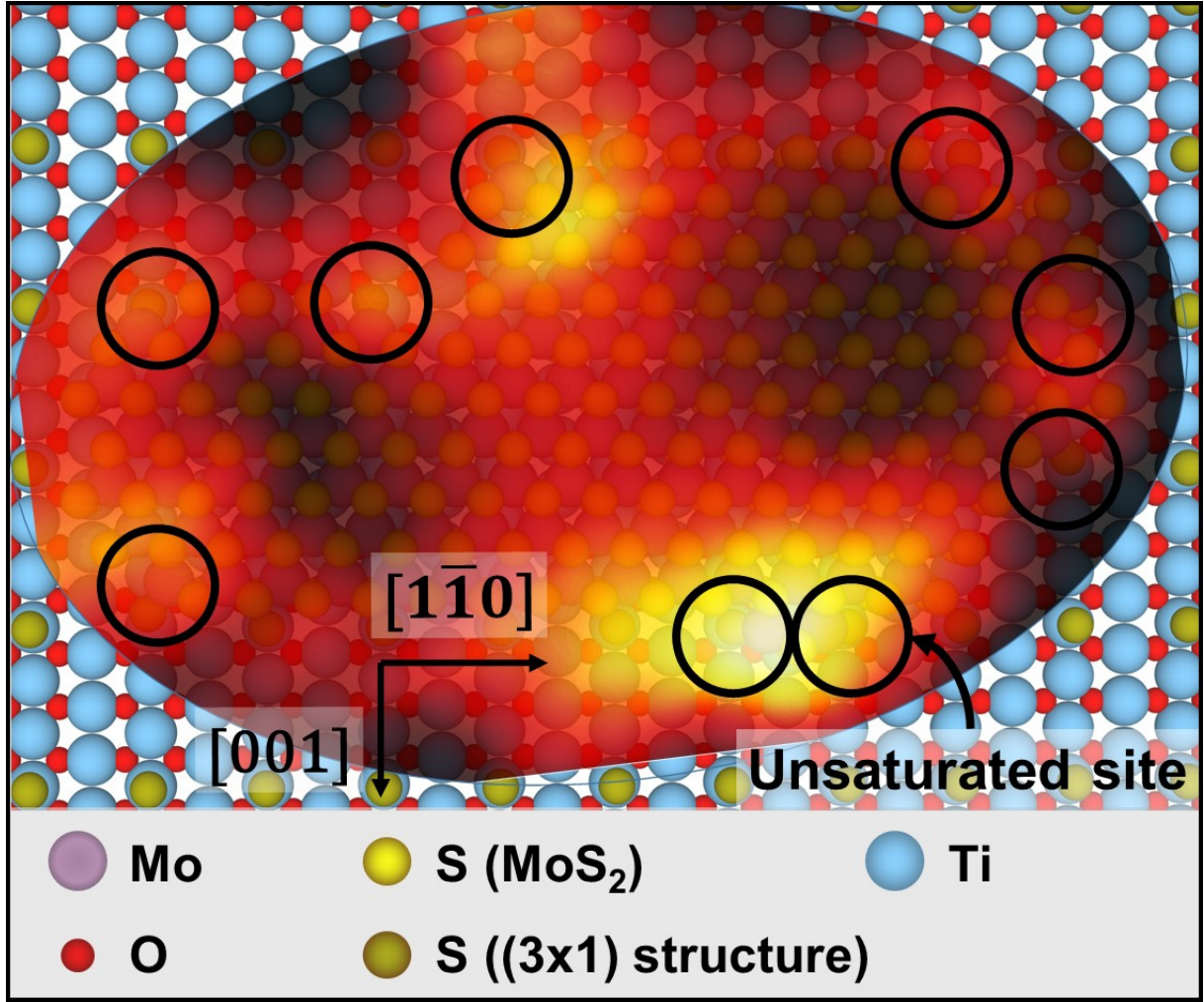


Figure S4. Atomic model of a “basal-bonded” MoS₂ slab from Figure 7a with the STM image of the slab marked 1 in Figure 3c superimposed. Note the close match between the bright spots and the coordinatively unsaturated corner Mo sites marked with black circles.

S6. Estimation of Mo coverage from the STM images

In order to estimate the amount of Mo present in the “basal-bonded” MoS₂ slabs, the statistically averaged projected area needs to be determined. For this purpose, we make use of the same method as in S3, but mask the areas occupied by the MoS₂ slabs instead. Analyzing an area of 1.25 μm², we obtain:

Projected area fraction of the “basal-bonded” MoS₂ slabs = 0.117 (*measured from the masks drawn*)

Area occupied by MoS₂ slabs for every (100 × 100) nm² of TiO₂(110) = 1170 nm²

Side length of a hexagon of the same area = $\{(1170) \times \frac{2}{3\sqrt{3}}\}^{1/2}$ (*assuming that the MoS₂ slabs are perfectly hexagonal*) = 21.23 nm = 21.23/0.315 Mo atoms, (*S-Mo-S distance in MoS₂ is 0.315 nm.*) ~ 67 atoms

Therefore, number of Mo atoms in MoS₂ for every (100 × 100) nm² of TiO₂ = $\frac{3\sqrt{3}}{2} \times 67^2$ (area of a regular hexagon) = 11805 atoms

Number of Ti atoms for every (100 × 100) nm² of TiO₂ = $\left(\frac{100}{0.298}\right) \times \left(\frac{100}{0.32}\right)$ where 0.298 and 0.32 nm are the experimentally measured Ti-Ti distances of the TiO₂(110) unit cell [22][40-42] = 104865 atoms

Since for low coverage, nearly all MoS₂ slabs are single layer, coverage of Mo in “basal-bonded” MoS₂; = 11805/104865 = 0.113 ML < 0.25 ML estimated from XPS data.