

# Low-temperature synthesis of MoS<sub>2</sub> slabs on TiO<sub>2</sub>(110)

Mahesh K. Prabhu and Irene M. N. Groot \*

Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden University, Einsteinweg 55, 2333 CC Leiden, The Netherlands; m.k.prabhu@lic.leidenuniv.nl

\* Correspondence: i.m.n.groot@lic.leidenuniv.nl

Received: 21 October 2020; Accepted: 03 November 2020; Published: date

S1. Comparison of Mo/TiO<sub>2</sub>(110) precursors at Mo coverages of 0.25 ML and 0.49 ML

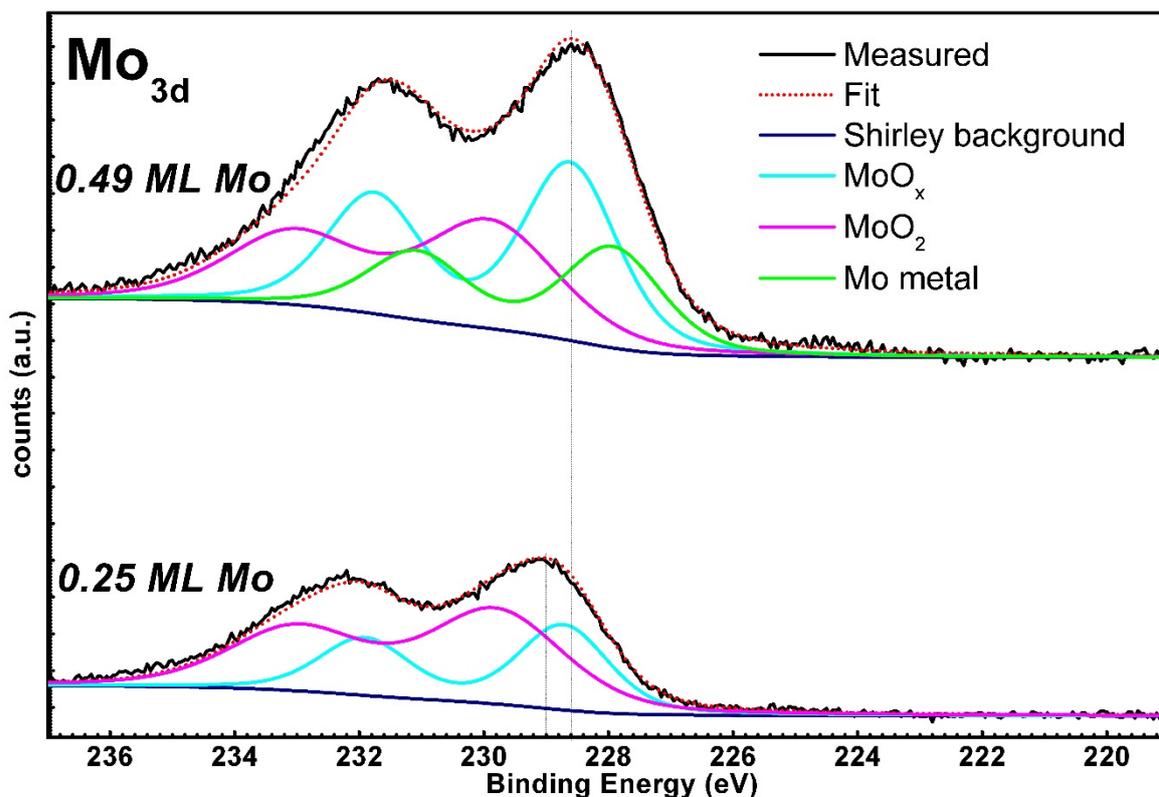
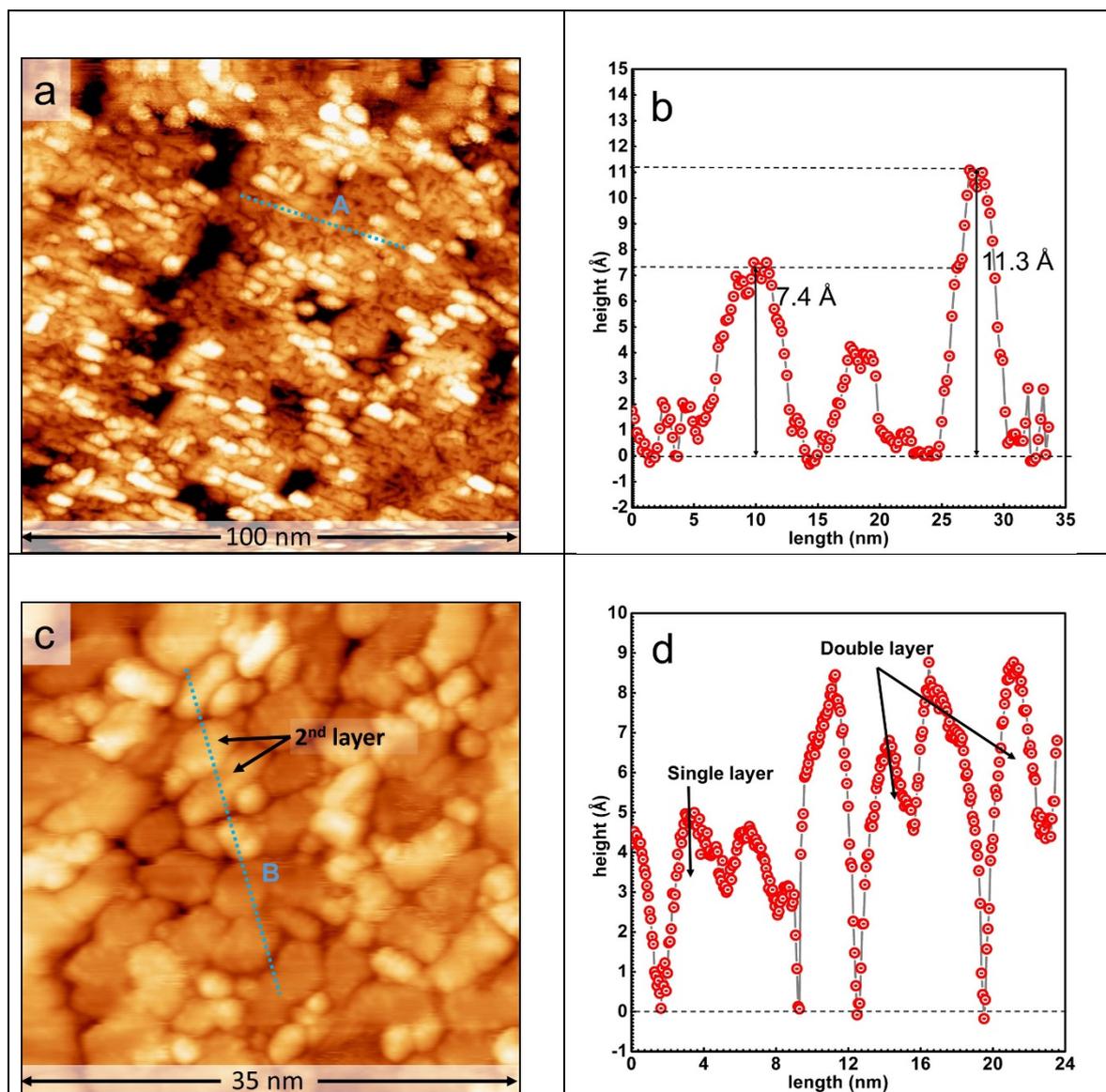


Figure S1. Mo 3d spectra of Mo nanoparticles supported on TiO<sub>2</sub>(110) at initial Mo overages of 0.25 ML and 0.49 ML.

## S2. MoS<sub>2</sub> slabs grown on TiO<sub>2</sub>(110) at Mo coverages of 0.49 and 0.61 ML



**Figure S2.** a) Large-scale STM image of MoS<sub>2</sub> supported on TiO<sub>2</sub>(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 MoS<sub>2</sub> supported on TiO<sub>2</sub>(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.

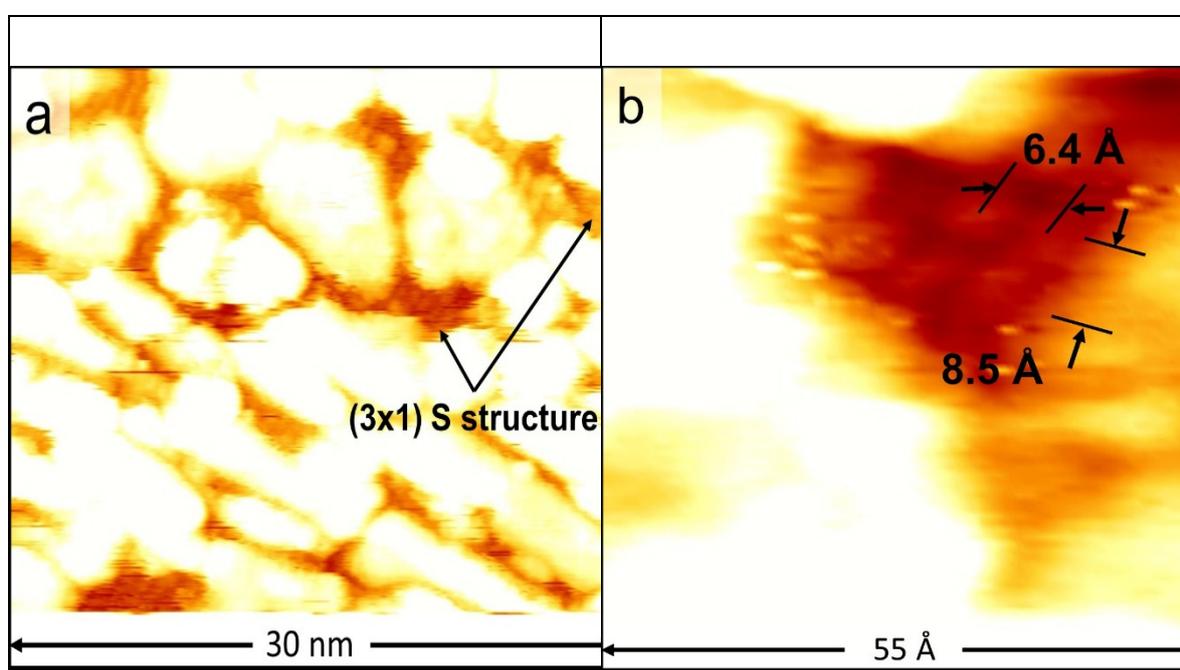
## S3. Estimation of the number density of the elongated structures from STM images

**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

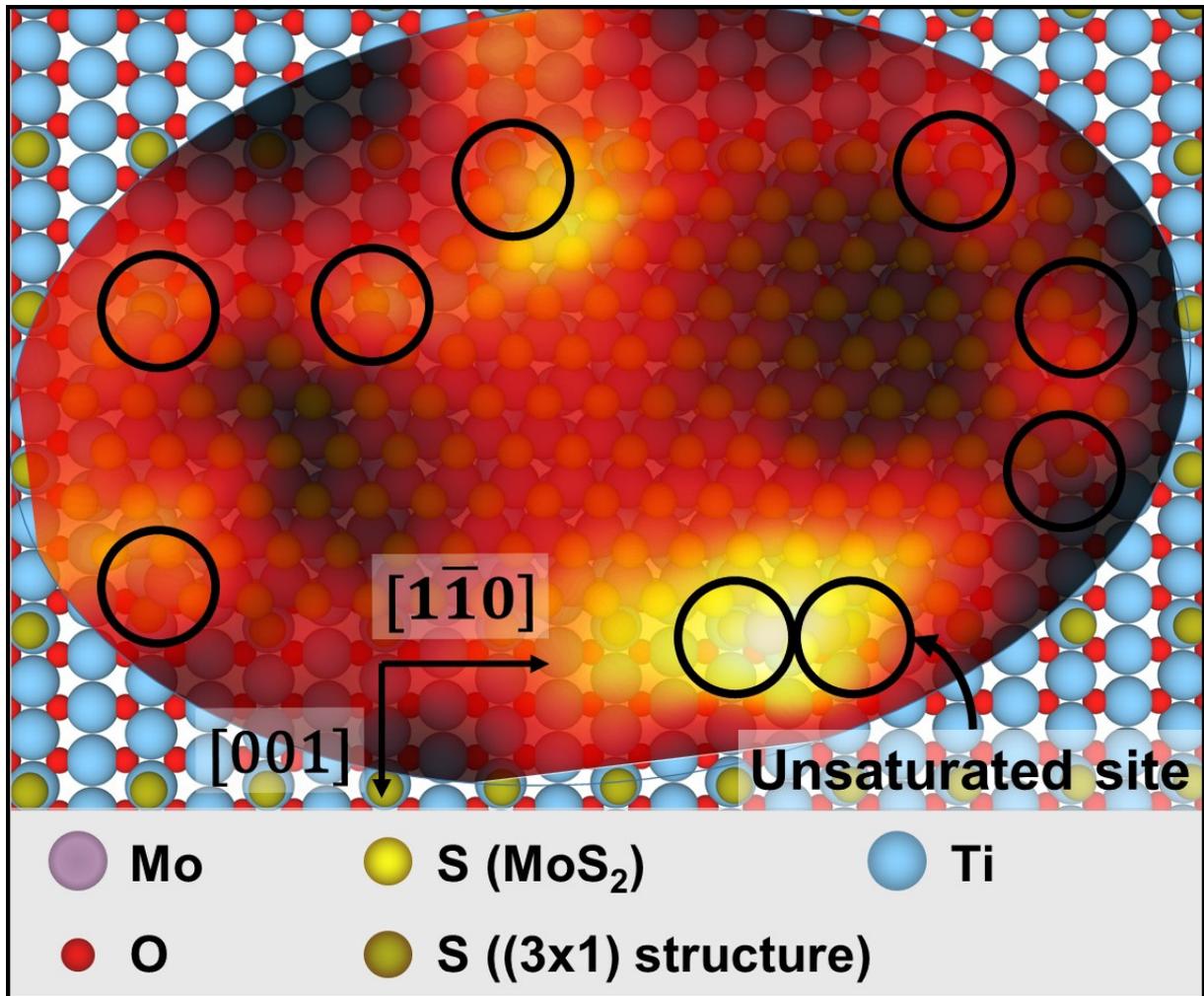
The number of elongated structures per unit area of the substrate is proportional to the projected area fractions as measured from the STM images taking into account the elongated structures with both the intermediate and bright STM contrasts. Estimation of the projected area fraction of the elongated 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  $(3 \times 1)$  sulfur structure; obtained with a sample voltage = +2.3 V and tunneling current = 500 pA. b) Zoom-in of a  $(3 \times 1)$  structure near the edge of a "basal-bonded"  $\text{MoS}_2$  slab.

### S5. Atomic model of “basal-bonded” MoS<sub>2</sub> slabs



**Figure S4.** Atomic model of a “basal-bonded” MoS<sub>2</sub> 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” MoS<sub>2</sub> 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 MoS<sub>2</sub> slabs instead. Analyzing an area of 1.25 μm<sup>2</sup>, we obtain:

Projected area fraction of the “basal-bonded” MoS<sub>2</sub> slabs = 0.117 (*measured from the masks drawn*)

Area occupied by MoS<sub>2</sub> slabs for every (100 × 100) nm<sup>2</sup> of TiO<sub>2</sub>(110) = 1170 nm<sup>2</sup>

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

Therefore, number of Mo atoms in MoS<sub>2</sub> for every (100 × 100) nm<sup>2</sup> of TiO<sub>2</sub> =  $\frac{3\sqrt{3}}{2} \times 67^2$  (area of a regular hexagon) = 11805 atoms

Number of Ti atoms for every (100 × 100) nm<sup>2</sup> of TiO<sub>2</sub> =  $\left(\frac{100}{0.298}\right) \times \left(\frac{100}{0.32}\right)$  where 0.298 and 0.32 nm are the experimentally measured Ti-Ti distances of the TiO<sub>2</sub>(110) unit cell [22][40-42] = 104865 atoms

Since for low coverage, nearly all MoS<sub>2</sub> slabs are single layer, coverage of Mo in “basal-bonded” MoS<sub>2</sub>; = 11805/104865 = 0.113 ML < 0.25 ML estimated from XPS data.