

Electronic Supplementary Information

Vertical Ultrathin MoS₂ Nanosheets on Flexible Substrate as Efficient Counter Electrode for Dye- Sensitized Solar Cells

Shuai Jiang,^{†ab} Xiong Yin,^{†a} Juntao Zhang,^{ab} Xiaoyang Zhu,^a Jianye Li^{b*} and Meng He^{a*}

¹ CAS Key Laboratory of Nanosystem and Hierarchical Fabrication, National Center for
Nanoscience and Technology, Beijing, 100190, P. R. China

² University of Science & Technology, Beijing, 100083, P. R. China

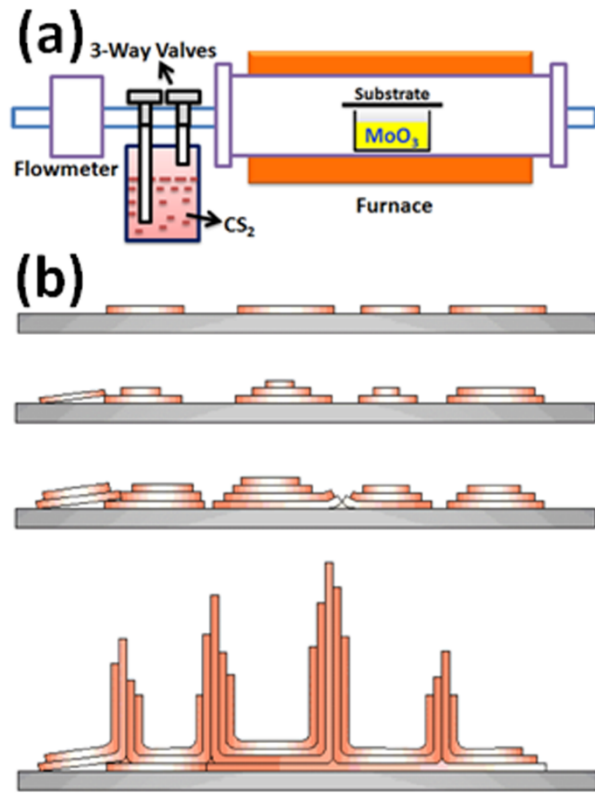
‡These authors contributed equally.

Email: mhe@nanoctr.cn (M. H), jyli@ustb.edu.cn (J. L)

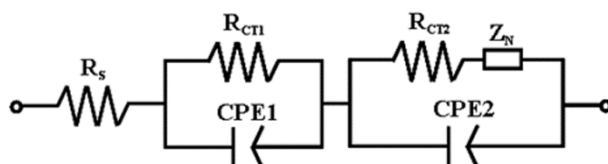
Experimental details of device fabrication and characterization. TiO₂ photoanodes were fabricated on the FTO glass by doctor-blading technique to obtain a 12 μm TiO₂ layer and a 4 μm thick scattering layer. Subsequently, the TiO₂ electrodes were treated in 40mM TiCl₄ at 70 °C for 30 minutes, and then, sintered at 450 °C for 30 min. After the temperature dropped to 85 °C, the electrodes were immersed into 0.3 mM N719 dye solution (mixture of acetonitrile and tertiary butanol with volume ratio 1:1) for 18 hours. The dye-sensitized TiO₂ film and the CE were separated by a hot-melt Surlyn film (25 μm thick) and liquid electrolyte. The liquid electrolyte was composed of 0.1 mol L⁻¹ iodine, 0.6 mol L⁻¹ methylhexylimidazolium iodide, 0.5 mol L⁻¹ tert-butylpyridine and 0.1 mol L⁻¹ lithium iodide in 3-methoxypropionitrile. The plastic TiO₂ electrode was prepared using electrophoretic deposition technique. A pair of plastic PEN-ITO substrates (Kintec, 20 Ω sq⁻¹) was vertically immersed in the P25 TiO₂ suspension and then a 1.6 V cm⁻¹ DC field was applied. After that, the as-prepared TiO₂ electrode was heated at 85 °C on a hotplate for 1.5 h to remove the organic solvents. After cooled to room temperature, the as-prepared TiO₂ electrode was further pressed at 10 MPa for 5 min to yield pressed P25 TiO₂ electrode using a manual hydraulic press at room temperature. The plastic P25 TiO₂ electrodes were then heated at 85 °C for 0.5 h. After that, plastic P25 TiO₂ electrodes were sensitized with 0.5 mM D149 dye (mixture of acetonitrile and tertiary butanol with volume ratio 1:1) for 12 hours. The D149-sensitized P25 TiO₂ electrodes were assembled with corresponding flexible counter electrodes to fabricate flexible devices.

Cyclic voltammetry measurements were carried out on a potentiostat (CHI660E, CHI instruments) by using the blank graphite foil, MoS₂/graphite and Pt as working electrode with working area of 1 cm², a Pt wire as counter electrode, a Ag/AgCl electrode as reference electrode, respectively. The scanning was performed at rate of 50 mV S⁻¹ in an acetonitrile

solution containing LiClO_4 (0.1 mol L^{-1}), LiI (10 mmol L^{-1}) and I_2 (1 mmol L^{-1}). The photocurrent density–voltage characteristics of the DSCs were measured under AM 1.5G illumination (100 mW cm^{-2}) using a solar simulator (Oriel Newport) equipped with a 150 W xenon lamp and a digital source meter (2420, Keithley Instruments, USA). The effective irradiated area was 0.2 cm^2 . Electrochemical impedance spectroscopy (EIS) measurement was carried out using a frequency response analyzer (Solartron SI 1270) and a potentiostat (Solartron 1287) at amplitude of 10 mV and the open-circuit voltage under light irradiation of 100 mW cm^{-2} in the frequency range from 0.1 to 10^5 Hz . The EIS data was fitted using ZView software.



Scheme S1. (a) Schematic of the set up for the growth of vertical MoS₂ nanosheets. (b) The proposed mechanism for the growth of vertical MoS₂ nanosheets.



Scheme S2. Equivalent circuit for fitting the electrochemical impedance spectra.

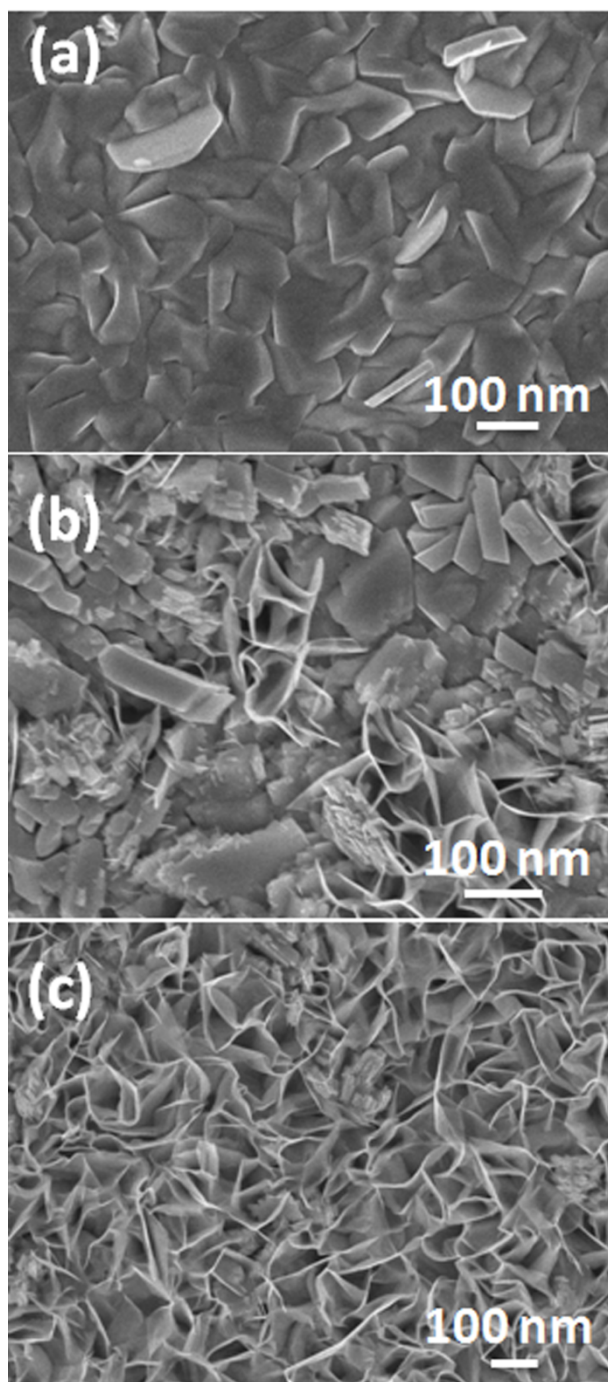


Figure S1. SEM images for products deposited on the (a) central, (b) intermediate and (c) marginal zone of the Si substrate with high concentration of MoO₃ vapor.

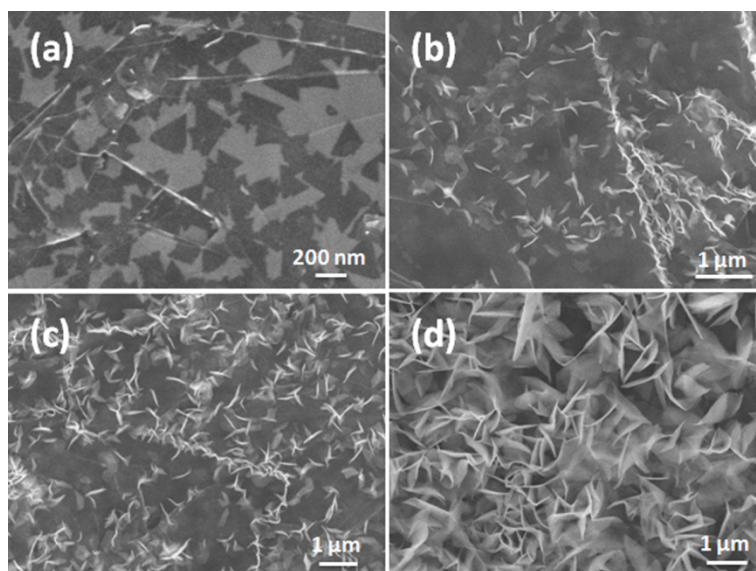


Figure S2. SEM images for MoS₂ deposited on the graphite substrate from the marginal (a) and intermediate (b, c) to the central zone (d).



Figure S3. The photograph of the flexible as-prepared MoS₂/graphite foil electrode.

Table S1. EIS Fitting parameters of the DSCs with different counter electrodes measured under illumination of 100 mW cm⁻² (AM 1.5 G).

Device	R _S / Ω	R _{CT2} / Ω
Blank Graphite	19.43	64.20
MoS ₂ /Graphite	25.60	26.84
Pt	27.41	25.58