Supporting Information

for

Tuning the optical absorption performance of MoS_2 monolayers by compressive strain

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This file includes:

S1 Topography characterizations of monolayer MoS_2

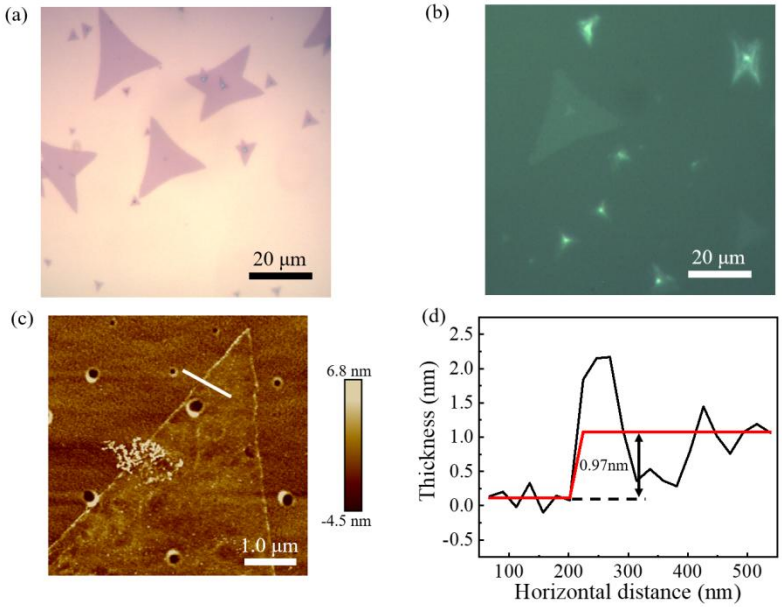

Figure S1. Characterization of monolayer MoS_2. (a) Optical microscopy image of monolayer MoS_2 grown on SiO_2/Si substrate by CVD method. (b) Optical microscopy image of monolayer MoS_2 transferred onto PET substrate. (c) AFM image of monolayer MoS_2. (d) Height profile along the white line as shown in (c). The thickness of the sample terrace is measured to be around 0.97 nm, indicating its monolayer nature.

Monolayer MoS_2 samples were synthesized by a chemical vapor deposition (CVD) method. Optical microscopy images of the monolayer MoS_2 samples directly deposited on SiO_2/Si substrate and transferred onto flexible polyethylene terephthalate (PET) substrate, are displayed in **Figure S1**a and S1b, respectively. Morphology characterization of monolayer MoS_2 was performed by atomic force microscope

(AFM) technique (Figure S1c). Figure S1d presents the measured height profile of the MoS_2 sample along the white line as shown in Figure S1c. The sample thickness is measured to be about 0.97 nm, as an indication of the monolayer nature.

S2 Schematic diagram of sample transfer process

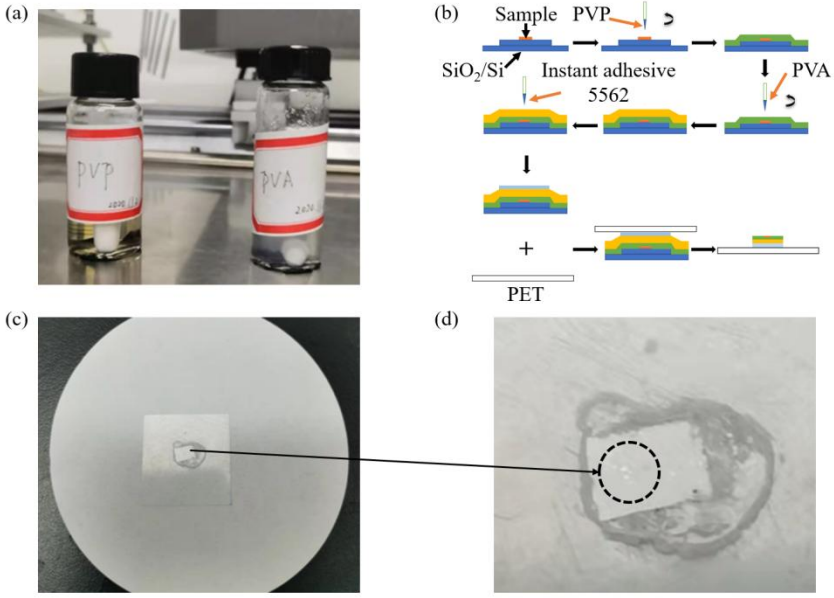

Figure S2. Schematic diagram of transfer process for 2D materials. (a) PVP and PVA aqueous solutions. (b) Schematic diagram of sample transfer process. (c, d) Photographs of a sample transferred onto PET.

Figure S2a presents the fully dissolved polyvinyl pyrrolidone (PVP) and polyvinyl alcohol (PVA) organic solvent aqueous solutions, which are used to transfer the large-area MoS_2 monolayers. The transfer experimental procedure is schematically presented in Figure S2b. SiO_2/Si wafer is cut into a step-like shape for convenient transfer. And then, 9 wt% PVP ($[C_6H_9NO]_n$) and 10 wt% PVA ($[C_2H_4O]_n$) aqueous solutions are spin-coated in sequence onto the entire SiO_2/Si wafer. Afterwards, a 0.5 mm PET flexible film is glued atop the PVA/PVP composite membrane, with the assistance of an instant adhesive 5562. After left for 24 h, the composite membrane with 2D samples can be easily peeled from SiO_2/Si wafer. Figure S2c and S2d display the photographs of the membrane transferred onto PET flexible substrate, denoted by the dashed circle.

S3 Photograph of the home-made strain loading equipment

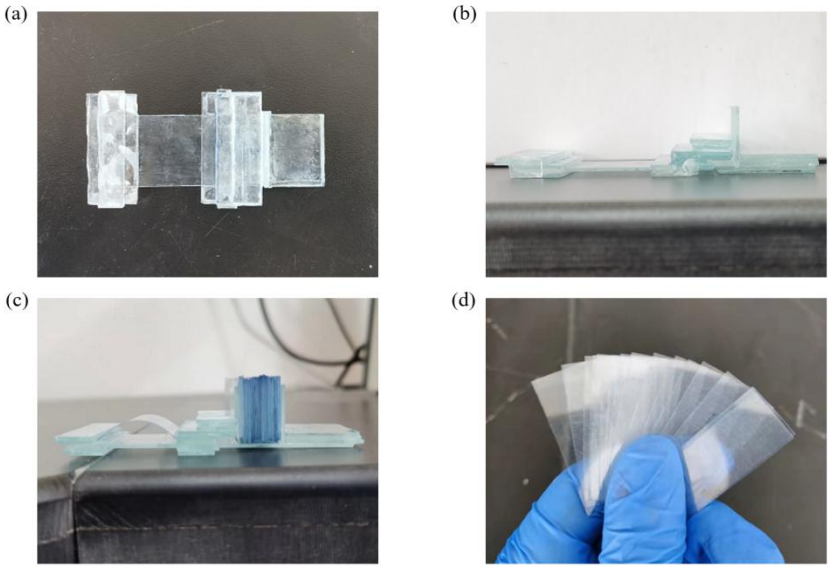

Figure S3. The home-made strain loading equipment. (a-c) Photographs of the strain loading equipment from different views. (d) Photograph of calibration cards, used for strain loading.

Figure S3a-c display the structure of the strain loading equipment from different views, which is made of glass slides and flexible PET. Figure S3d shows the calibration cards used for strain loading. The calibration card is made of PET and the thickness of each calibration card is 0.18 mm.

S4 Monolayer MoS_2 in a bent state

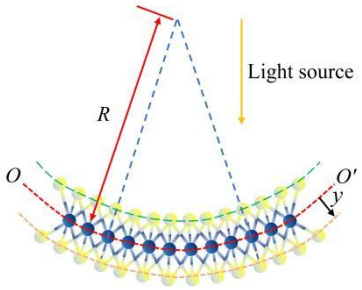

Figure S4. Schematic diagram of monolayer MoS_2 in a bent state.

As shown in **Figure S4**, in the curved substrates with developable surfaces, 2D semiconductors bear uniaxial strain with tension and compression simultaneously when bending the substrate[S1]. The strain applied to monolayer MoS_2 is determined by the bending stress formula: $\varepsilon=y/R$, where ε is the strain value, y is the distance away from the neutral layer OO', and R is the radius of curvature of the neutral layer OO'. Since the y value along the concave side of MoS_2 (green dashed curve shown in Figure S4) is negative, the corresponding ε value is negative, as an indication of applying compressive strain.

S5 Schematic diagram of optical absorption measurement equipment

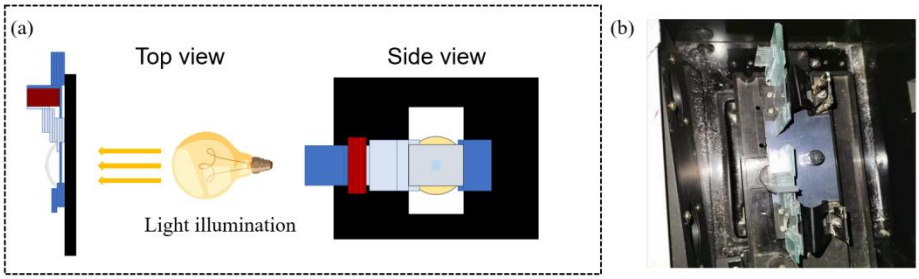

Figure S5. Schematic diagram and photograph of optical absorption measurement equipment. (a) Schematic diagrams of optical absorption measurement equipment for 2D materials under compression. (b) Photograph of optical absorption measurement equipment for 2D materials under compression.

Figure S5a schematically display the experimental setup for optical absorption spectrum measurement, which is used for collecting optical signals from 2D materials under compression. Figure S5b present the photograph of the absorption measurement system for 2D materials under compression.

S6 Optical absorption spectra obtained from different samples

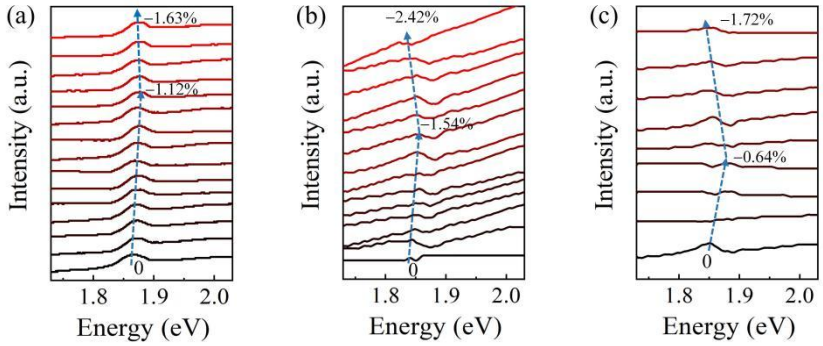

Figure S6. Optical absorption spectra obtained from different MoS_2 samples under compression.

The optical absorption spectra measurements were performed on three different samples, as presented in **Figure S6**. The highest value of the compressive strain loaded in this work was −2.42%. The trend of first blueshift and then redshift under the increasing compression has been observed for all measured MoS_2 samples, proving the good repeatability of our experiment. Due to the sample variation, the critical values of the applied compressive strain are different, with −1.12% for sample (a), −1.54% for sample (b), and −0.64% for sample (c).

Reference:

[S1] J. Du, H. Yu, B. Liu, M. Hong, Q. Liao, Z. Zhang and Y. Zhang, *Small Methods*, 2021, **5**, 2000919.