Electronic Supplementary Information

for

In Situ TEM Observing Structural Transitions of MoS_2 upon Sodium Insertion and Extraction

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Supplemental Methods

The Preparation of MoS_2 nanosheets

Pristine MoS_2 powder was purchased from commercial products MoS_2 powder Beijing Dekedaojin Co. Ltd. China. The experiment is performed with a self-developed apparatus. The device mainly contains four parts: gas cylinder, chiller, pump, and reactor. The schematic drawing of experimental setup is shown in Fig. S1. The exfoliation of MoS_2 by supercritical CO_2 fluid shear has been carried out in reactor vessel with volume of 1.5 L and maximum operation pressure of 40 MPa. A magnetic stirring motor whose rotating speed can be adjusted is designed on the top of reactor. An electric heating jacket on the outside of machine is used to control reaction temperature. The reactor was filled with CO_2 through the pump and heated until it reached to the supercritical state. After reaction, the vent valve was opened to emit CO_2 and then the exfoliated MoS_2 nanosheets were collected from the sampling valve at reactor bottom.

Supplemental Figures

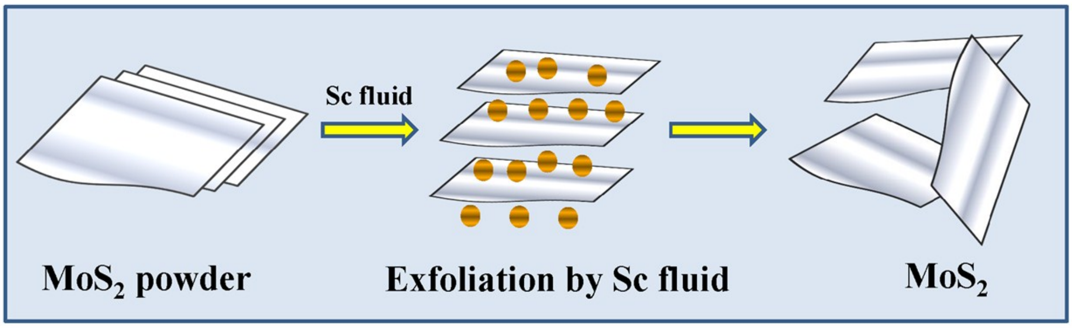

Fig. S1 The schematic drawing of exfoliating MoS_2 by using supercritical (Sc) CO_2 fluid shear.

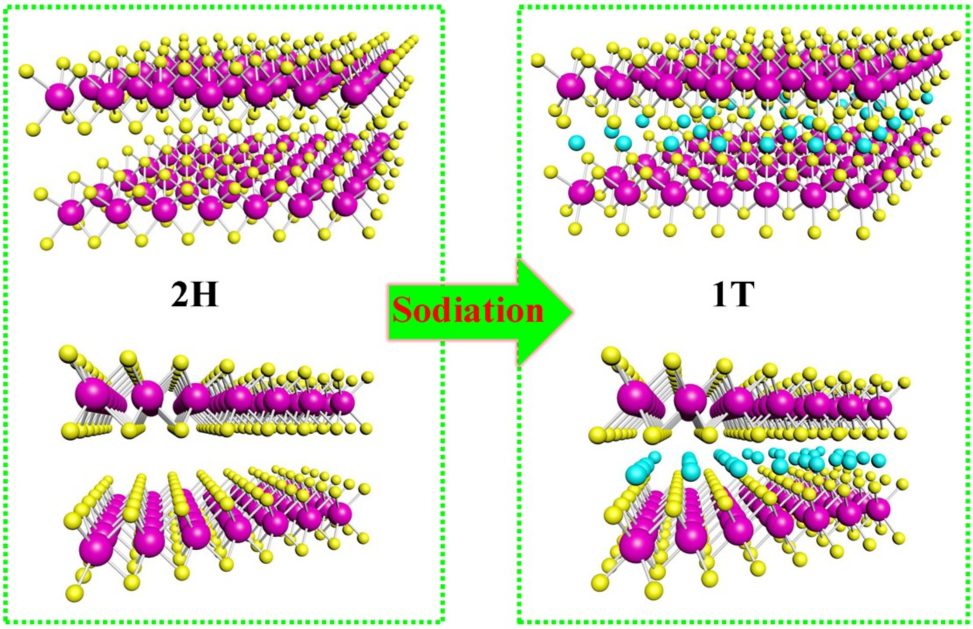

Fig. S2 (Color Online) A schematic diagram of MoS_2 nanosheet during the sodiation process. The pristine MoS_2 is a semiconductor in its trigonal (2H) structure, where the S atoms locate in the lattice position of a hexagonal close-packed structure. Planes of Mo atoms are sandwiched between two atomic layers of S, so that each Mo is coordinated to six S atoms in a trigonal prismatic geometry (2H) and the atomic stacking sequence (S-Mo-S) is of ABA. The parallel and neighboring slabs are interconnected with weak van der Waals force. After Na ions occupying these interlayers, the large strain and unfavorable energy induce glide of the sulfur plane along an interlayer atomic plane and phase transition from 2H- to 1T-MoS_2, where the Mo atom-coordination transfers from trigonal to octahedral resulting in a straight chain of S-Mo-S. The 1T-MoS_2 shows atomic stacking sequence (S-Mo-S') of ABC where the bottom S' plane occupies the hollow center of 2H hexagonal lattice, that is why the EDP in Fig. 2(e) generates some new dim spots between every two pristine spots.

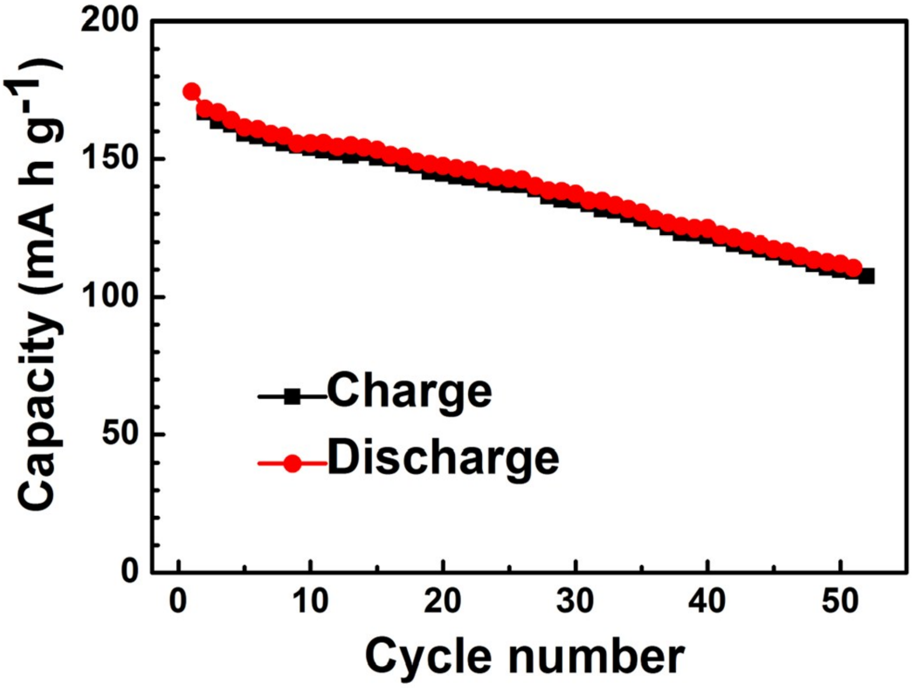

Fig. S3 Cycle performance of the Na/MoS_2 cell.

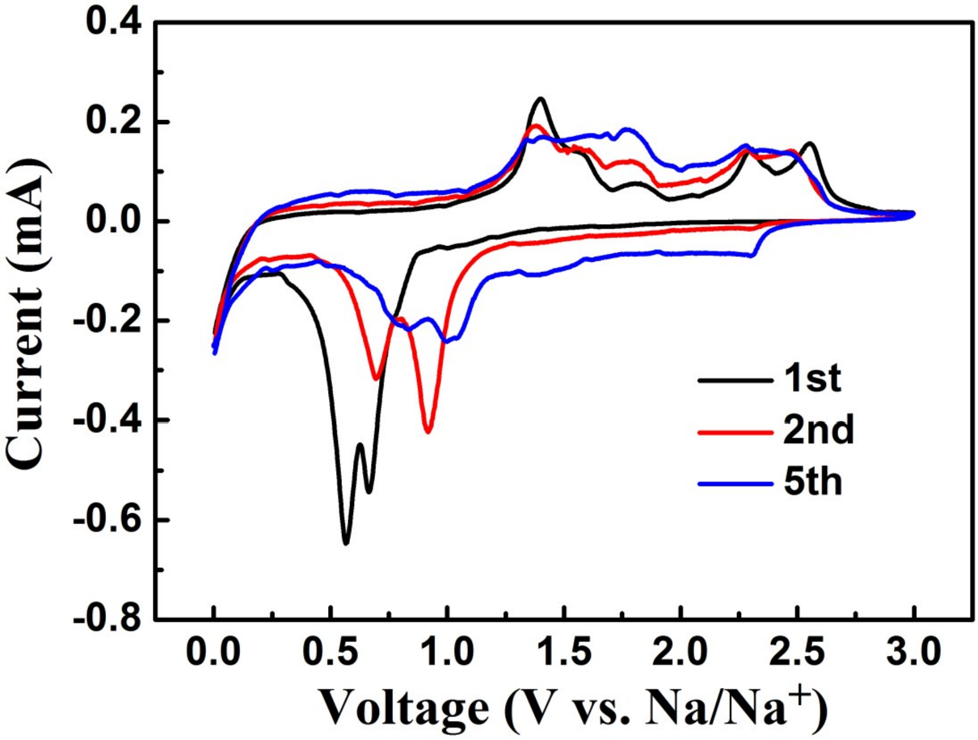

Fig. S4 Cyclic Voltrammogram (CV) curves of the Na/MoS_2 cell at a scan rate of 0.2 mV/s.

Supplemental Movies

Movie S1 An *in situ* TEM movie showing the propagation of the reaction front during the first sodiation of a MoS_2 nanosheet. The video was recorded at 4 frames/second, and played at 24× speed.

Movie S2 An *in situ* TEM movie showing the morphology changes of Na/MoS_2 nanosheets during the first desodiation. The video was recorded at 4 frames/second, and played at 24× speed.