## **Supplementary Information**

# Mo-P bond induced MoS<sub>2</sub> fast electron transfer improves the

# lithium storage performance of MoS<sub>2</sub>-MoP heterojunction

Shasha Wang<sup>a,b</sup>, Jiaqi Guo, Jiaqi Huo, Lu Wen, Jingyao Tang, Bo Cao<sup>a</sup>, Yan Cheng<sup>a</sup>\*

a Inner Mongolia Industrial Technology Engineering Center of Special Resources Development, Utilization and Ecological Environment Protection, College of Chemistry and Environment Science, Inner Mongolia Normal University, Hohhot 010022, China b Institute of Environmental and Health, Inner Mongolia Normal University, Hohhot, 010022, China

<sup>\*</sup> Corresponding author: Y. Chen, Email: ycheng@imnu.edu.cn

#### **1** Experimental

#### 1.1. Preparation

#### 1.1.1. Synthesis of graphene oxide

A modified Hummers method was developed to synthesize GO. The typically synthesis process is shown as below: 1 g of graphite, 120 mL of  $H_2SO_4$  (98 %) and 13.3 mL  $H_3PO_4$  was added into a 250 mL round-bottom flask, 5 g of KMnO<sub>4</sub> was slowly introduced subsequently. Then, the flask with mixture was stirred in an ice water bath for 30 min and then kept at 35 °C for 12h. After that, the flask with mixture was stirred at 50 °C for another 24 h. Finally, 150 mL of water and 10 mL of 30 %  $H_2O_2$  were added to closing the reaction. Then, the suspension was centrifuged and washed for several times and then freeze-dried.

#### 1.1.2. Synthesis of silica KIT-6/G template

N-modified KIT-6/G template was synthesized by previous reported method. The typically synthesis process is as follows: 1 g GO was dissolved in 217 mL of distilled water and ultrasonic for several hours, then 6 g of P123, 6 g of 1-butanol (Aldrich, 99.4 %) and 11.8 g of HCl (35 %) were introduced slowly. Then, the solution was stirred for 24 h at 35 °C before 12.9 g of TEOS (Aldrich, 99 %) was added. After being stirred for another 24 h, the mixture was refluxed for 12 h at 80 °C. Finally, the mixture was filtered and dried at 80 °C and further heated up to 400 °C for 2h at a rate of 2 °C/min.

#### 1.1.3. Synthesis of 2D meso-MoS<sub>2</sub>-MoP/G.

2D meso- MoS<sub>2</sub>-MoP/G was prepared via a "nanocasting" method. In this process, KIT-6/G was used as template, thiourea was acted as sulfur source, ammonium molybdate ( $NH_4$ )<sub>6</sub>Mo<sub>7</sub>O<sub>24</sub>·4H<sub>2</sub>O) was adopted as a molybdenum source, and sodium hypophosphite ( $NaH_2PO_2$ ) was used as phosphorus source. Typically, 0.2 g of KIT-6/G template, 0.2 g of ammonium molybdate, and 0.2 g of sulfourea were dissolved in 30 mL of distilled water. The solution was then stirred for 24 h and dried under vacuum at 50 °C to obtain precursor. The precursor was put at the right zone of the tube furnace and sodium hypophosphite was kept at the left zone. After being heated up to 700-800 °C for 3h at a rate of 2 °C·min<sup>-1</sup> under nitrogen atmosphere and removing KIT-6 template using NaOH (2 M) as an etchant, the 2D meso-MoS<sub>2</sub>-MoP/G can be obtained.

### 1.1.4 Synthesis of meso-MoS<sub>2</sub>/G hybrids

Meso-MoS<sub>2</sub>/G hybrids were prepared via a "nanocasting" method. Typically, 0.2 g of KIT-6/G template, 0.2 g of ammonium molybdate and 0.2g of sulfourea were dissolved in 30 mL of distilled water. Then, the mixed solution was stirred for 24 h and dried under vacuum at 50 °C to obtain precursor composites. Next, the precursor composites were heated up to 400 °C, 450 °C and 500 °C for 4 h at a rate of 2 °C·min<sup>-1</sup> in a mixed gas flow of 10 % H<sub>2</sub> and 90 % Ar. After further removing KIT-6 template using NaOH (2 M) as an etchant, the meso-MoS<sub>2</sub>/G hybrids were achieved.

#### 2.2. Characterization

PANalytical Empyrean XRD system was used to record the powder X-ray diffraction (XRD) pattern and scanning rate is  $0.026^{\circ} \cdot s^{-1}$ . The model of field emission scanning electron microscope and field emission transmission electron microscopy are Hitachi S-4800 and Tecnai F20 respectively. Valence states were recorded by XPS measurement (XSAM800 X-ray photoelectron spectrometer) with an Al Ka (1486.67 eV) excitation source. Surface area measurements were tested on Brunauere-Emmette-Teller ASAP 2020 analyser. Raman spectra were recorded by RENISHAW inVia Microscope Raman with a 532-nm laser.

#### 2.3. Electrochemical measurements

Active materials, conductive carbon black, and poly(vinyl difluoride) (PVDF) were used to prepare working electrodes, the weight ratio is 80:10:10. N-methyl

pyrrolidinone (NMP) act as a dispersing agent. The slurry was pasted on pure Cu foil and dried under vacuum at 90 °C for 12 h. During the preparation process of working electrodes, polypropylene film was act as separator and pure lithium foil was employed as a counter electrode. The solution of 1 M LiPF<sub>6</sub> in ethylene carbonate (EC)/dimethyl carbonate (DMC) (1:1 by volume) was used as electrolyte. The assembled process was operated in glove box which is filled with argon. Land BT2013A battery test instrument (Wuhan, China) was used to test the galvanostatic discharge-charge experiments, the voltage range is 0.01-3 V. Electrochemical impedance spectroscopy (EIS) measurement was performed by Zennium electrochemical workstation (Zahner, Germany) and the frequency range of from 10 kHz to 100 mHz.

**Table S1**. The BET and BJH properties of meso-MoS<sub>2</sub>-MoP/G (700°C), meso-meso-MoS<sub>2</sub>-MoP/G (750°C) and meso-MoS<sub>2</sub>-MoP/G (800°C) hybrids.

| Sample                               | $S_{BET}(m^2 \cdot g^{-1})$ | $D_{p}(nm)$ | $V_p (cm^3 \cdot g^{-1})$ |
|--------------------------------------|-----------------------------|-------------|---------------------------|
| meso-MoS <sub>2</sub> -MoP/G (700°C) | 74.5                        | 3.4         | 0.11                      |
| meso-MoS <sub>2</sub> -MoP/G (750°C) | 99.0                        | 3.2         | 0.23                      |
| meso-MoP@MoS <sub>2</sub> /G (800°C) | 80.9                        | 3.4         | 0.09                      |



Figure S1. XRD patterns of meso-MoS<sub>2</sub>/G calcined at different temperatures.



Figure S2. SEM images of (a and b) meso-MoS<sub>2</sub>/G (400 °C), (c and d) meso-MoS<sub>2</sub>/G (450 °C)



and (e and f) meso-MoS<sub>2</sub>/G (500  $^{\circ}$ C).

Figure S3. XPS spectra of meso-MoS<sub>2</sub>/G (500°C).



Figure S4. (a, c and e) The discharge/charge curves and (b, d and f) the cycle performance and coulombic efficiency of meso-MoS<sub>2</sub>/G calcined at 500°C for 4h.



Figure S5. Cyclicvoltammetry curves of (a) meso-MoS<sub>2</sub>-MoP/G (700 °C), (b) meso-MoS<sub>2</sub>-

### MoP/G (750 °C) hybrids.



Figure S6. XRD patterns of meso-MoP/G calcined at different temperature.



Figure S7. (a-c) SEM images of meso-MoP/G calcined at different temperature. TEM images of



meso-MoP/G calcined at 600°C..



**Figure S8.** (a,c and e) The discharge/charge curves, (b,d and f) the cycle performance and coulombic efficiency of meso-MoP/G(500 $^{\circ}$ C), meso-MoP/G(600 $^{\circ}$ C) and meso-MoP/G(700 $^{\circ}$ C).