## Supporting information

## Guest-host interactions and their impacts on structure and performance of nano-MoS $_2$

Xuefeng Wang, Zhaoruxin Guan, Yejing Li, Zhaoxiang Wang\* and Liquan Chen

## **Experimental section**

All the chemicals were of analytical grade and used as received without further purification. Commercial MoS<sub>2</sub> powder (purity > 99%) was ordered from Alfa. Typically, nano-MoS<sub>2</sub> was prepared by hydrothermal treatment of Na<sub>2</sub>MoO<sub>4</sub> and NH<sub>2</sub>CSNH<sub>2</sub> mixture at 200 °C for 12h and denoted as GMS. GMS-C was fabricated with glucose as the additive and subsequent annealing to the hydrothermal reaction product at 800°C for 2h with Ar flowing. Sample MoS<sub>2</sub>-PVP was obtained by adding polyvinyl pyrrolidone (PVP) in the Na<sub>2</sub>MoO<sub>4</sub>/NH<sub>2</sub>CSNH<sub>2</sub> mixture and hydrothermal treatment. By replacing Na<sub>2</sub>MoO<sub>4</sub> with an inorganic-organic hybrid MoO<sub>3</sub>-EDA (EDA for ethylenediaminetrimolybdate) in the hydrothermal reaction for GMS, MoS<sub>2</sub>-EDA was synthesized according to the reference<sup>1, 2</sup>.

The structure of the samples were characterized on powder X-ray diffractometer (D8 Advance with a LynxEye\_XE detector, Bruker) with Cu K $\alpha$ 1 radiation ( $\lambda$ =1.5405 Å). The morphology of the composite was observed on an FEI XL30 Sirion FEG digital scanning electron microscope (SEM). Thermogravimetric (TG) analysis was performed on a Netzsch STA 449 C apparatus to analyze the thermal stability of MoS<sub>2</sub> and determine the MoS<sub>2</sub> content in the composite between room temperature and 800 °C in flowing Ar and O<sub>2</sub> (90:10 v/v, 18 mL min<sup>-1</sup>) at 10 K min<sup>-1</sup> heating rate. Fourier-transformed infrared (FTIR) spectra of the powder dispersed in dry KBr were recorded on a Bruker VERTEX 70v spectrometer. Ultraviolet-visible (UV-vis) absorption spectra were collected on a Varian Cary 5000 spectrometer (532 nm radiation) with a resolution of 2 cm<sup>-1</sup>. X-ray photoelectron spectroscopy (XPS) was carried out on an Escalab 250 XPS spectrometer (Perkin Elmer). The spectra were calibrated to C1s of adventitious carbon at 284.8 eV.

The working electrode for Li- and Na-ion batteries was prepared by casting a slurry of the active material (75 wt%), carbon nano-tubes (10 wt%) and sodium alginate (15 wt%) on a clean Cu current collector. Test cells were assembled with Li or Na foil as the counter electrode and Celgard 2400 or glass fiber as the separator, respectively, in an Ar-filled glove box. A mixture of EC/DMC (1:1 v/v) containing 1.0 mol L<sup>-1</sup> LiPF<sub>6</sub> was used as the electrolyte for Li-ion batteries while 1.0 M NaClO<sub>4</sub> in EC/DEC (4:6 v/v) for the Na-ion batteries. The electrochemical performances of the materials were evaluated at a current density of 50 mA g<sup>-1</sup> between 0.01 and 3.0 V versus Li<sup>0</sup> or Na<sup>0</sup> on Land BT2000 battery testers (Wuhan, China) at room temperature. The cyclic voltammetry (CV) tests were carried out on a CHI600D electrochemical workshop (Shanghai, China) at a scan rate of 0.05 mV s<sup>-1</sup>.

<sup>1.</sup> S. Zhuo, Y. Xu, W. Zhao, J. Zhang and B. Zhang, Angew Chem Int Ed Engl, 2013, 52, 8602-8606.

<sup>2.</sup> Q. Gao, S. Wang, H. Fang, J. Weng, Y. Zhang, J. Mao and Y. Tang, J. Mater. Chem., 2012, 22, 4709-4715.