Electronic Supplementary Information

Facile synthesis of MoS₂/graphene composites: effects of different cationic surfactants on microstructures and electrochemical properties of reversible lithium storage

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As shown Table 1, the carbon contents in the three composite samples (MoS₂/GNS-D, MoS₂/GNS-O and MoS₂/GNS-T) are different, respectively. In general, the different carbon contents of the composites will have different effects on the electrochemical performance of the anode materials for reversible lithium storage. In order to exclude the influence of the carbon content in the MoS₂/GNS composites, other two composites (MoS₂/GNS-S1 and MoS₂/GNS-S2) were synthesized by same liquid phase chemical reduction route and heat treatment. The carbon content of the MoS₂/GNS-S1 (or MoS₂/GNS-S2) composite was controlled to be very close (or almost equal) to that of MoS₂/GNS-D (or MoS₂/GNS-O) by changing the amounts (or ratios) of starting materials. The amounts of starting materials are shown in Table S1. The microstructure and element composition of MoS₂/GNS-S1 and MoS₂/GNS-S2 composites were characterized by X-ray diffraction (XRD, D8 ADVANCE X-ray diffractometer with Cu K α radiation λ =0.15405 nm), transmission electron microscopy (TEM, JEOL JEM-200CX microscope operating at an acceleration voltage of 200 kV), high resolution transmission electron microscopy (HRTEM) and energy dispersive X-ray spectroscopy (EDX, GENENIS-4000). Electrochemical performances of MoS₂/GNS-S1 and MoS₂/GNS-S2 composites were tested using two-electrode coin cells (CR2025) by galvanostatic charge/discharge cycling between the voltage limits of 0.005 and 3.0 V on a LANHE 2001A Battery Tester.

Composites	GOS /mmol	Surfactant	$(NH_4)_2MoS_4$ /mmol
MoS ₂ /GNS-S1	8.07	100 mL of 0.01 M	2.69
		DIAB solution	
$MoS_2/GNS-S2$	9.42	No using	2.69

 Table S1 The amounts of starting materials for preparing MoS₂/GNS-S1 and MoS₂/GNS-S2 composites



Fig. S1 XRD patterns of (a) MoS₂/GNS-S1 and (b) MoS₂/GNS-S2 composites

XRD patterns of MoS₂/GNS-S1 and MoS₂/GNS-S2 composites are shown in Fig. S1. Both MoS₂/GNS-S1 and MoS₂/GNS-S2 composites clearly displays diffraction peaks of MoS₂, which can be indexed to the (002), (100), (103), (105), (110) and (201) planes of the 2H-MoS₂ (JCPDS card No. 37-1492), respectively. For both composites, the interlayer space $d_{(002)}$ of MoS₂ is calculated to be 0.62 nm according to the (002) peak at 2θ =14.17°. As shown in Fig. S1, MoS₂/GNS-S1 displays broadening and lower (002) reflection compared to MoS₂/GNS-S2, indicating the layer number of MoS₂ in MoS₂/GNS-S1 is less than that in MoS₂/GNS-S2.

Fig. S2 shows the TEM/HRTEM images of MoS₂/GNS-S1 and MoS₂/GNS-S2 composites. As shown in Fig. S2(a, b), MoS₂/GNS-S1 displays that few-layer MoS₂ sheets (3~5 layer) dispersed on the wrinkled graphene surface can be clearly found. Fig. S2(c, d) shows that for MoS₂/GNS-S2 composite, the layered MoS₂ sheets (about 7~11 layer) supported on the wrinkled graphene surface can also be found. HRTEM images of MoS₂/GNS-S1 and MoS₂/GNS-S2 composites clearly show the few-layered or layered MoS₂ structure with $d_{(002)}$ of 0.62 nm, which agree with their XRD analysis.



Fig. S2 TEM/HRTEM images of (a, b) MoS₂/GNS-S1 and (c, d) MoS₂/GNS-S2 composites.

Table S2 Elemental compositions of MoS2/GNS-S1 and MoS2/GNS-S2 composites

Composites	C /wt%	O/wt%	Mo /wt%	S /wt%	MoS_2 /wt%	S:Mo
MoS ₂ /GNS-S1	26.95	8.51	38.91	25.63	64.54	1.97
MoS ₂ /GNS-S2	21.63	5.32	43.45	29.60	73.05	2.04

(S: Mo represents the atomic ratio)

The elemental compositions of $MoS_2/GNS-S1$ and $MoS_2/GNS-S2$ were examined by EDX as summarized in Table S2. The atomic ratios of S to Mo calculated for both samples are very approaching to the stoichiometry of MoS_2 . The strong presences of C in the composites are clearly derived from the reduced GO and amorphous carbon from the carbonization of the surfactant (DTAB). A small amount of O should be provided by residual oxygenic functional groups of reduced GO and amorphous carbon. As shown in Table S2, the content of $MoS_2/GNS-S1$ is 26.95 *wt*%, which is very close to that (26.29 *wt*%) of $MoS_2/GNS-D$ composite. The content of $MoS_2/GNS-S2$ is 21.63 *wt*%%, which is almost equal to that (21.32 *wt*%%) of $MoS_2/GNS-O$ composite.



Fig. S3 Cycling performances of (a) $MoS_2/GNS-1$ and (b) $MoS_2/GNS-2$ composites at a current density of 100 mA g⁻¹.

Fig. S3 shows the cycling performances of $MoS_2/GNS-S1$ and $MoS_2/GNS-S2$ composites at a constant current density of 100 mA g⁻¹. At the first cycle, the lithiation capacity is 1453 and 1253 mAh g⁻¹ for $MoS_2/GNS-S1$ and $MoS_2/GNS-S2$ composite, respectively. The corresponding reversible capacity is 892 and 793 mAh g⁻¹ with the Columbic efficiencies of 61.4% and 63.3%. The irreversibility in the first cycle is due to the irreversible electrode process such as the formation of the SEI film, the electrochemically driven electrolyte degradation, reduction of oxygen-containing groups and being trapped of a small amount of lithium in the defect sites or disordered structures. As shown in Fig. S3, both $MoS_2/GNS-S1$ and $MoS_2/GNS-S2$ composite electrodes exhibit stable cycling performance. After 50 cycles, $MoS_2/GNS-S1$ and $MoS_2/GNS-S2$ composite electrodes remain the reversible capacity of 869 and 762 mAh g⁻¹, respectively.



Fig. S4 Rate capability of (a) MoS₂/GNS-S1 and (b) MoS₂/GNS-S2 composites at different charging/discharging current densities.

Fig. S4 shows the rate capability of $MoS_2/GNS-S1$ and $MoS_2/GNS-S2$ composites at the different charging/discharging current densities. At a high current density of 1000 mA g⁻¹, the reversible capacity of $MoS_2/GNS-S1$ and $MoS_2/GNS-S2$ electrodes is 549-524 mAh g⁻¹ and 472-458 mAh g⁻¹, respectively.

The electrochemical performances comparison of $MoS_2/GNS-S1$ and $MoS_2/GNS-D$, $MoS_2/GNS-S2$ and $MoS_2/GNS-O$ for reversible lithium storage are summarized in Table S3. As listed in Table S3, even if the carbon content of $MoS_2/GNS-S1$ is very close to that of $MoS_2/GNS-D$ composite, $MoS_2/GNS-S1$ exhibits lower reversible capacity and poor rate capability than $MoS_2/GNS-D$ composite. In particular, the carbon content of $MoS_2/GNS-S2$ is almost equal to that of $MoS_2/GNS-O$ composite, but $MoS_2/GNS-S2$ exhibits much lower reversible capacity and poor rate capability in comparison with $MoS_2/GNS-D$ composite. Therefore, the factor of the carbon content in the composites can be excluded.

MOS ₂ /GNS-S2 and MOS ₂ /GNS-O for reversible fitnium storage						
Composites	Carbon content /wt%	Cycling performance	Reversible capacity at 100 mA g^{-1} (mAh g^{-1})	Rate-capability at 1000 mA g ⁻¹ (mAh g ⁻¹)		
MoS ₂ /GNS-S1	26.95	Excellent	~893	549-524		
$MoS_2/GNS-D$	26.29	Excellent	~932	676-657		
$MoS_2/GNS-S2$	21.63	Good	~793	472-458		
MoS ₂ /GNS-O	21.32	Excellent	~1050	731-716		

Table S3 Electrochemical performance comparison of MoS₂/GNS-S1, MoS₂/GNS-D, MoS₂/GNS-S2 and MoS₂/GNS-O for reversible lithium storage