Supporting Information

CTAB-assisted synthesis of single-layer MoS₂/graphene composites as anode materials of Li-ion battery

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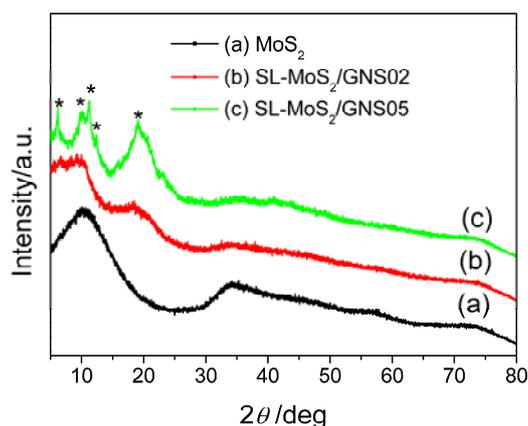
Fig. S1 XRD patterns of (a) as-prepared MoS₂, (b) as-prepared SL-MoS₂/GNS02 and (c) as-prepared SL-MoS₂/GNS05 composite precursors.

Fig. S1 shows the XRD patterns of the as-prepared MoS₂ and as-prepared SL-MoS₂/GNS composite precursors before annealing. All the samples hardly reveal the characteristic peaks corresponding to layered MoS₂ crystal. This fact indicates that crystalline of MoS₂ is too poor to reflect its XRD peaks before annealing. As shown in Fig. S1c, the as-prepared SL-MoS₂/GNS05 composite precursor displays several small and sharp peaks (marked by *), which are related to being included of surfactant

ion CTA$^+$ into the composite precursor. The fact agrees with that reported by Bezverkhyy.[1] In order to confirm the reduction of MoS_4^{2-} to MoS_2, the element composition of the as-prepared samples were characterized by EDX. Repeat EDX analysis revealed that the atomic ratio of Mo to S is close to the stoichiometry of MoS_2, confirming that MoS_4^{2-} has been reduced to MoS_2. It was reported that the strong reduction character of hydrazine can make MoS_4^{2-} reduced to MoS_2 during refluxing according the overall reaction:[2]

$$2MoS_4^{2-}+N_2H_4 =2MoS_2 +N_2+S^{2-}+H_2S$$

While GOS was in-situ reduced to GNS by hydrazine solution under refluxing at 95 ^{o}C.

MoS$_2$ and SL-MoS$_2$/GNS composites were characterized by TGA as shown in Fig. S2. Fig. S2 shows that MoS_2 starts to lose weight at approximately 430 ^{o}C due to the oxidation of MoS_2 to MoO_3. The SL-MoS$_2$/GNS composites exhibit two weight losses. The first one appears at approximately 270 ^{o}C, which can probably be attributed to the removal of oxygen-containing groups. The second is only one large continuous weight loss in the range of approximately 365-550 ^{o}C. This thermal behavior might be caused by the decomposition of the amorphous carbon and graphene, and oxidation of MoS_2 in the composites. It is very difficult to distinguish the content of graphene from the TGA curves of SL-MoS$_2$/GNS composites due to the presence of amorphous carbon. In order to calculate the content of graphene in the SL-MoS$_2$/GNS composites, the MoS$_2$/GNS (1:2) composite was prepared by the same process without CTAB and characterized by TGA as shown in Fig. S2b. Fig. S2a shows that the pure MoS$_2$ has an overall weight loss of 91.1%, which well agrees with

the theoretic value (89.9%) of the oxidization reaction of MoS_2 to MoO_3. It was reported that the amorphous carbon and graphene were completely oxidized under 700 °C in air, thus the remaining product of the MoS_2/GNS composites under 700 °C was only MoO_3.[3-5] According to Fig. S2b, the content of MoS_2 in the MoS_2/GNS (1:2) composites was calculated to be about 83.66% and the content of graphene was 16.33%. Because the three composites have the same molar ratio of MoS_2 to graphene, we can estimate the contents of MoS_2, graphene and amorphous carbon in the SL-MoS_2/GNS composites and the results are summarized in Table S1. In addition, according the elemental compositions of the samples examined by EDX, we can directly calculate the content of MoS_2 in the composites (see Table 1), which matches well with the results of the TGA analysis.
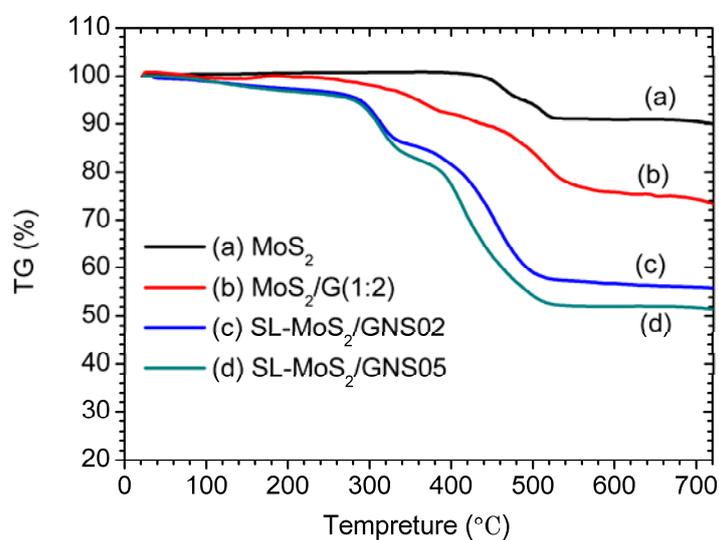
Fig. S2 TGA curves of (a) MoS_2, (b) MoS_2/GNS (1:2), (c) SL-MoS_2/GNS02 and (d) SL-MoS_2/GNS05 composites measured at a heating rate of 10 °C min^{-1} in a flowing air.

Table 1. The compositions of the samples calculated from the TGA

Samples	MoS_2 /wt%	Graphene /wt%	Amorphous carbon /wt%
MoS_2	100	—	—
MoS_2/GNS(1:2)	83.66	16.33	—
SL-MoS_2/GNS02	63.12	12.32	24.56
SL-MoS_2/GNS05	56.94	11.12	31.94
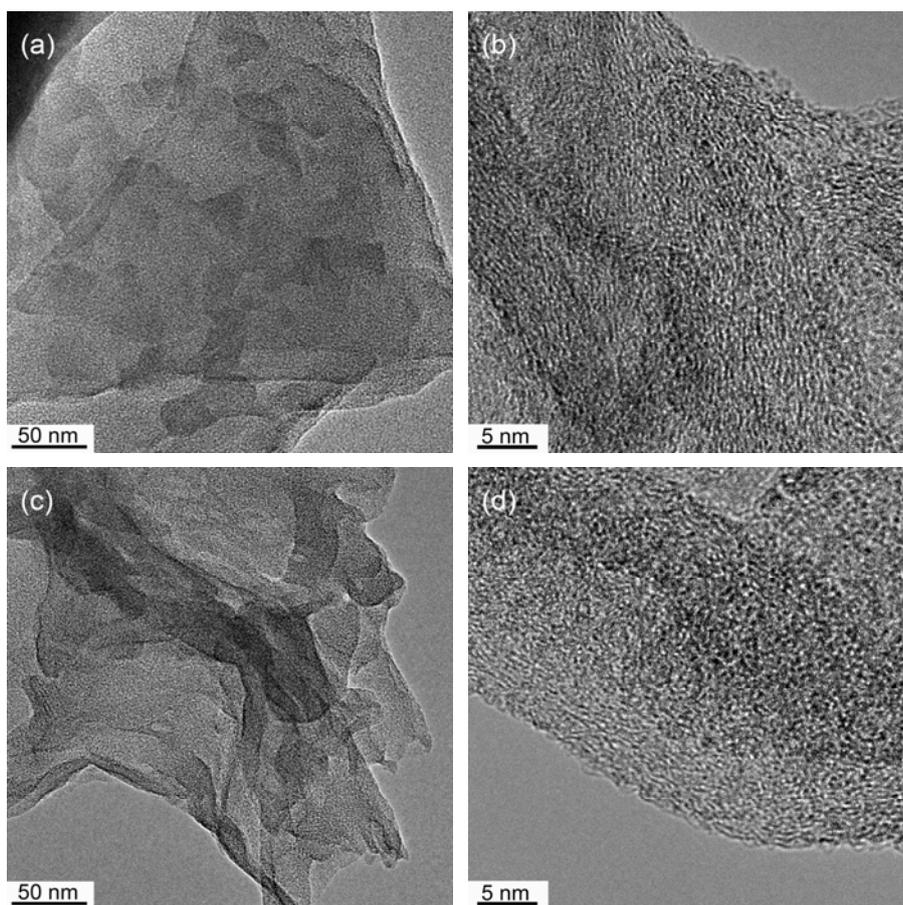
Fig. S3 TEM and RTEM images of (a, b) as-prepared SL-MoS_2/GNS02 and (c, d) as-prepared SL-MoS_2/GNS05 composites.

The TEM and HRTEM images of the SL-MoS_2/GNS products before heat-treatment were carried out as shown in Fig. S3. From the HRTEM images, it can be seen that the very short MoS_2 fringes with poor-crystalline are highly dispersed in the composites. Due to the very short fringes and extremely poor-crystalline of MoS_2,

the XRD patterns of the as-prepared SL-MoS$_2$/GNS composite precursors before heat treatment hardly display the characteristic peaks of MoS$_2$ crystal as shown in Fig. S1.

Refernces

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