Prevention of sulfur diffusion using MoS$_2$-intercalated 3D-nanostructured graphite for high-performance lithium-ion batteries

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Figure S1. XPS analysis of (a) EGS-M1 and (b) EGS-M2.

To determine the chemical composition of MoS\(_2\) intercalated graphite 3D-nanostructured composites EGS-M1 and EGS-M2, X-ray photospectroscopy (XPS) measurements were carried out in the region of 0 \(\sim\)1100 eV. Figures S1 (a) and (b) show that the sample contains the C, Mo and S elements and the atomic ratio of the elements is summarized in the insert of Figures S1 (a) and (b). The calculated atomic ratio of Mo to S element is 1 to 2.11 and 1 to 2.23 for EGS-M1 and EGS-M2 samples, approaching the theoretical value of MoS\(_2\). The high-resolution of C1s can be seen apart from the “C = C” bond. In addition, we did not observe chlorine peaks in XPS measurement, which implies that 10 min microwave treatment is sufficient for the reaction between MoCl\(_5\) and sulfur to form MoS\(_2\) sheets.
Figure S2. HRTEM image of EGS-M1 sample. It can be seen that the MoS\textsubscript{2} sheets are intercalated between the graphite layers and form the repeated 3D-nanostructure as graphite/MoS\textsubscript{2}/graphite.
Figure S3. TGA curve of EGS-M1 and EGS-M2 samples: The EGS-M1 and EGS-M2 samples exhibit two weight losses. The first weight loss appears between 230-250 \(^{\circ}\)C, which can probably be illustrated to the removal of oxygen-containing groups. The second weight loss is continuous in the range of 300-450 \(^{\circ}\)C. This thermal behavior might be caused by the decomposition of the amorphous carbon and graphite, and oxidation of MoS\(_2\) in the composites. The mass fraction of MoS\(_2\) in the EGS-M1 and EGS-M2 samples can be determined to be around 5.43 wt\% and 13.87 wt\%, respectively, assuming the complete conversion from MoS\(_2\) to MoO\(_3\).
Figure S4. FESEM images of (a) sulfur intercalated edged open graphite and (b) edged open graphite.

Figure S5. FESEM images of (a) EGS-M1 and (b) EGS-M2 composites after the 100 cycles of charging and discharging process. It is illustrated from Figure S5(b) that during the cycling, there are agglomeration of the particles in EGS-M2 composite due to curling up of vertically grown MoS$_2$. However, the structure of EGS-M1 is not changed.
Figure S6 (a) Nyquist plots of EGS-M1 and EGS-M2 electrodes obtained by applying a sine wave with amplitude of 5.0mV over the frequency range from 100 kHz to 0.01 Hz, and (b) The equivalent circuit model for the impedance response.