**Electronic Supplementary Information** 

## Prevention of sulfur diffusion using MoS<sub>2</sub>-intercalated 3Dnanostructured graphite for high-performance lithium-ion batteries

Anand P. Tiwari<sup>†1</sup>, HeeJoun Yoo<sup>†3</sup>, JeongTaik Lee<sup>2</sup>, Doyoung Kim<sup>3</sup>, JongHyeok Park<sup>2</sup> and Hyoyoung Lee<sup>\*1</sup>

- Centre for Integrated Nanostructure Physics (CINAP), Institute of Basic Science (IBS), Department of Chemistry, Sungkyunkwan University, 300 Cheoncheon-Dong, Jangan-Gu, Suwon, Gyeonggi-Do 440-746, South Korea E-mail: <u>hyoyoung@skku.edu</u>
- Department of Chemical and Biomolecular Engineering, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 120-749, Republic of Korea
- Department of Energy Science, Sungkyunkwan University, 2066 Seoburo, Jangan-gu, Suwon, Gyeonggi-do 440-746, Republic of Korea
  - \* Equally contributed
  - \* Corresponding Author: hyoyoung@skku.edu (Prof. Hyoyoung Lee)



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 ~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<sub>2</sub>. 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<sub>5</sub> and sulfur to form MoS<sub>2</sub> sheets.



**Figure S2. HRTEM image of EGS-M1 sample.** It can be seen that the MoS<sub>2</sub> sheets are intercalated between the graphite layers and form the repeated 3D-nanostructure as graphite/MoS<sub>2</sub>/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<sub>2</sub> in the composites. The mass fraction of MoS<sub>2</sub> 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<sub>2</sub> to MoO<sub>3</sub>.



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 pcocess**. It is illustrated from Figure S5(b) that during the cycling, there are aglomoration of the particles in EGS-M2 composite due to curling up of vertically grown MoS<sub>2</sub>. 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 respons.