Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Hierarchical MoO_3/SnS_2 Core-Shell Nanowires with Enhanced Electrochemical Performance for Lithium-Ion Batteries

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S1. TG analysis of MoO_3/SnS_2

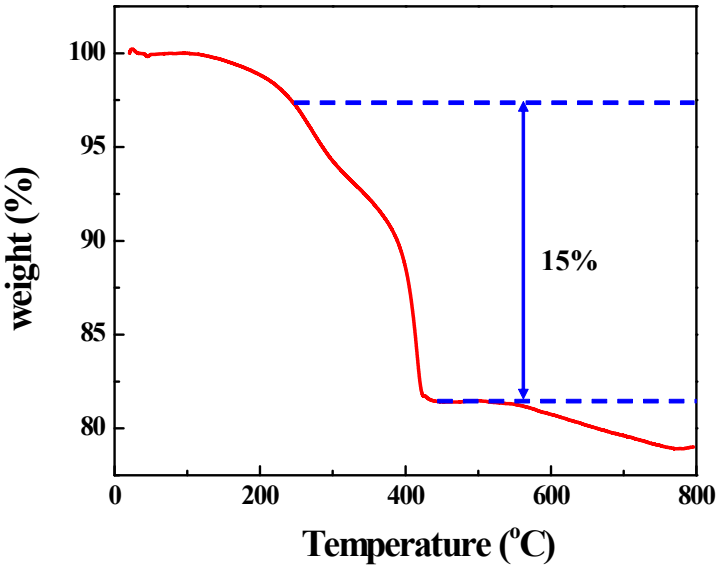

Fig. S1 TG analysis of MoO_3/SnS_2 composite material performed in air at a heating rate of 10 ºC/min. The initial weight loss (up to ~250 ºC) is due to removal of physisorbed and chemisorbed water and sulfur. Subsequent weight loss between 250 and 450 ºC is mainly due to oxidation of SnS_2 to SnO_2 (a weight loss of ~15%).

S2. CV Curves of MoO_3 and SnS_2 electrodes

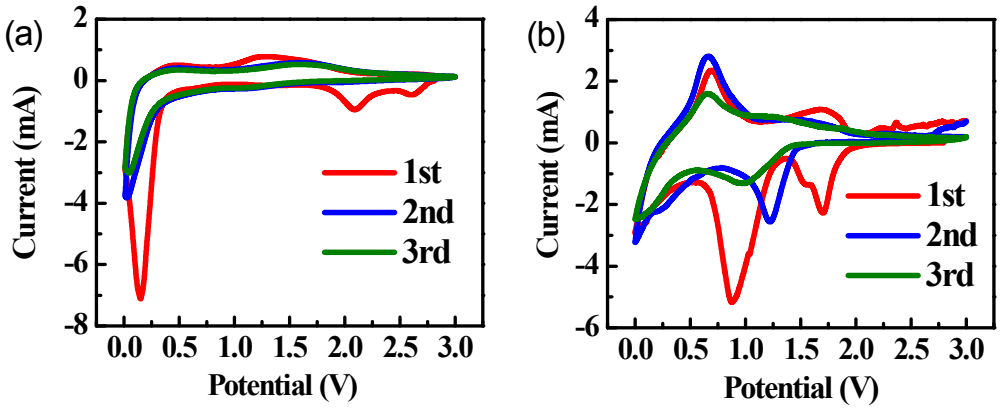

Fig. S2 Cyclic voltammetry curves of (a) MoO_3 and (b) SnS_2 electrodes at a scan rate of 0.2 mV/s in the potential range of 0.01 and 3.0 V (vs Li/Li^+)..

S3. Atomic Structure of MoO_2

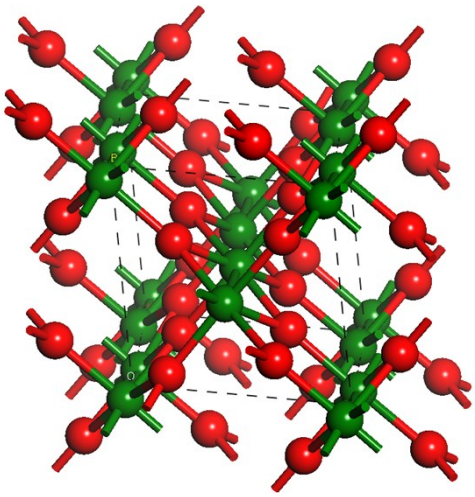

Fig. S3 Atomic structure of MoO_2 (a = 0.5611 nm, b = 0.4856 nm, c= 0.5629 nm, space group P121/c1). The green and red balls represent Mo and O atoms, respectively.

S4. Movies for recording the AIMD simulation results

Movie S1: The movie records the trajectories for lithiated SnS_2 nanosheet at 300 K within 6 ps.

Movie S2: The movie records the trajectories for lithiated MoO_3 nanosheet at 300 K within 6 ps.

Movie S3: The movie records the trajectories for lithiated MoO_3/SnS_2 heterostructure at 300 K within 6 ps.

In above three movies, green, red, cyan, yellow, and purple balls represent Mo, O, Sn, S, and Li atoms, respectively.