Supporting Information for Nanoscale

Sodium Storage in Promising MoS$_2$-Carbon Anode: Elucidating Structural and Interfacial Transition in Intercalation Process and Conversion Reactions

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Fig. S1 (a) XRD patterns of MoS$_3$ and MoS$_3$-PVP, (b) SEM image of MoS$_3$, (c) SEM image of MoS$_3$-PVP, (d) FTIR spectrum of PVP, MoS$_3$, MoS$_3$-PVP. MoS$_3$-PVP represents the precursor for MoS$_3$-AC-100 sample. The XRD patterns of MoS$_3$ and MoS$_3$-PVP show the typical profile of amorphous MoS$_3$. MoS$_3$ and MoS$_3$-PVP precursors display the granular morphology in nanosize.$^{51,52}$ The grain size of MoS$_3$-PVP is slightly larger than that of MoS$_3$, most likely due to PVP coating. The absorption peaks of FTIR from the chemical groups of PVP including C-N, C-O and CH$_2$ can be observed in MoS$_3$-PVP samples prepared with additional PVP.$^{53}$
Fig. S2 SEM images for morphology characterization. (a) and (b) for MoS$_2$, (c) and (d) for MoS$_2$-AC-20, (e) and (f) for MoS$_2$-AC-50, (g) and (h) for MoS$_2$-AC-100, (i) and (j) for MoS$_2$-AC-200.

Fig. S3 (a) SEM image of selected area for EDS test for MoS$_2$-PVP-100 and the corresponding element mappings: (b) C element, (c) Mo element and (d) S element.
Fig. S4 Rate capability for MoS$_2$-AC compared to other intercalated anodes in reported literatures: hard carbon$^{54}$ MXenes$^{55}$ expanded graphite$^{56}$ Na$_2$Ti$_3$O$_7$,$^{57}$ P$_2$Na$_{0.66}$Li$_{0.22}$Ti$_{0.78}$O$_2$,$^{58}$ and soft carbon.$^{59}$

Fig. S5 Long-term cycling performance of MoS$_2$-AC-100 at a current density of 5 A g$^{-1}$ within two potential ranges of 0.4-3.0 V and 0.01-3.0 V.
Fig. S6 (a) Rate performance for MoS$_2$-AC electrodes at various current densities from 0.1 to 10 A g$^{-1}$ within a working potential range of 0.4-3.0 V. (b) Rate performance for MoS$_2$-AC electrodes at various current densities from 0.1 to 10 A g$^{-1}$ within a working potential range of 0.01-3.0 V. (c) and (d) Long-term cycling performance for MoS$_2$-AC electrodes at 1 A g$^{-1}$ within two working potential ranges: 0.4-3.0 V and 0.01-3.0 V, respectively.
**Fig. S7** Initial charge/discharge process for MoS$_2$-AC-100 at a current density of 0.1 A g$^{-1}$ and the corresponding ex-situ XRD patterns for MoS$_2$-AC-100 during the cycles within two trade-off potentials: (a) 0.4 V and (e) 0.01 V. The notes: 1-pristine material, 2-initial sodiation, 3-initial desodiation. The note for 4 is the desodiated state after long cycles of 1200 cycles for (a) and 200 cycles for (b) at a current density of 1 A g$^{-1}$. HRTEM images of MoS$_2$-AC-100 sample cycled within 0.4-3.0 V: (b) the initial sodiation to 0.4 V (vs. Na/Na$^+$), (c) initial desodiation to 3.0 V (vs. Na/Na$^+$), (d) 1200$^{th}$ cycle to 3.0 V (vs. Na/Na$^+$). HRTEM images of MoS$_2$-AC-100 sample cycled within 0.01-3.0 V: (f) the initial sodiation to 0.01 V (vs. Na/Na$^+$), (g) initial desodiation to 3.0 V (vs. Na/Na$^+$), (h) 200$^{th}$ cycle to 3.0 V (vs. Na/Na$^+$). The current density is 0.1 A g$^{-1}$, except for 1 A g$^{-1}$ for long cycles for (d) and (h).
Fig. S8 Electrochemical kinetics analysis of MoS$_2$-AC-100 electrode. (a) CV curves at various scan rates from 1 to 10 mV s$^{-1}$. (b) Determination of the $b$-value using the relationship between anodic peak current and scan rate. (c) Separation of the capacitive and diffusion currents at a scan rate of 5 mV s$^{-1}$, respectively. (d) Contribution ratio of the capacitive charge versus scan rate.
Fig. S9 Charge/discharge curves of MoS$_2$-AC-100 within two different potential windows (0.4-3.0 V (red line) and 0.01-3.0 V (black line)) and PDPC versus Na/Na$^+$, respectively. The specific current density is 1 A g$^{-1}$.

Fig. S10 (a) CVs of as-fabricated MoS$_2$-AC//PDPC-4.2 V at various scan rates from 2 to 50 mV s$^{-1}$. (b) Charge/discharge curves of as-fabricated MoS$_2$-AC//PDPC-4.2 V SIC at the different current densities from 0.1 to 2 A g$^{-1}$. 
References


