Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Hierarchical MoS_2/Carbon Microspheres as Long-Life and High-Rate Anodes for Sodium-Ion Batteries

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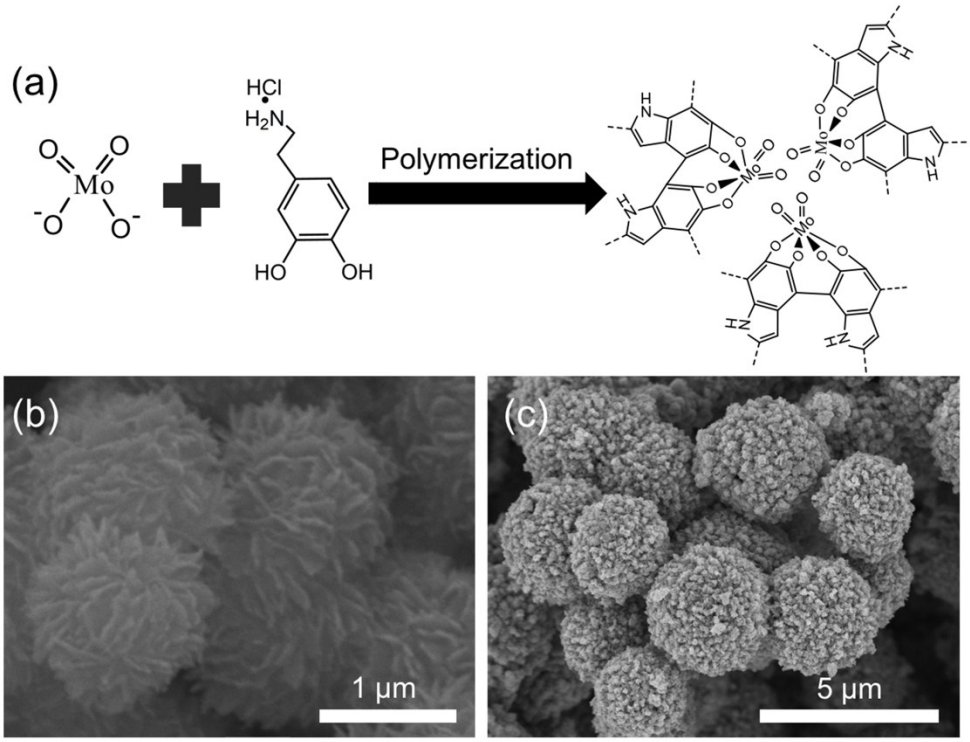

Fig. S1 (a) Illustration of the reaction mechanism between dopamine and the molybdate anion. SEM images of (b) the Mo-dopamine precursor and (c) hy-MoS_2/C

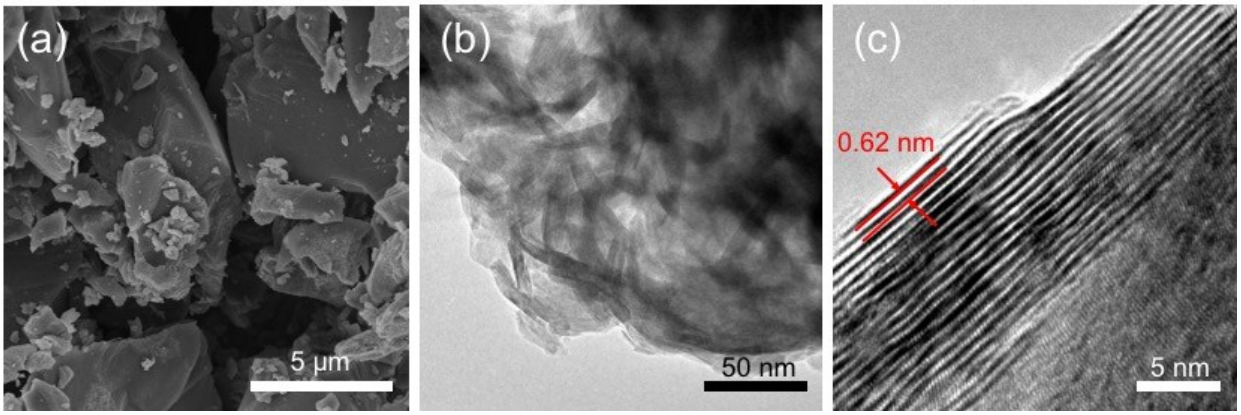

Fig. S2 (a) SEM, (b) TEM and (c) HRTEM images of MoS_2.

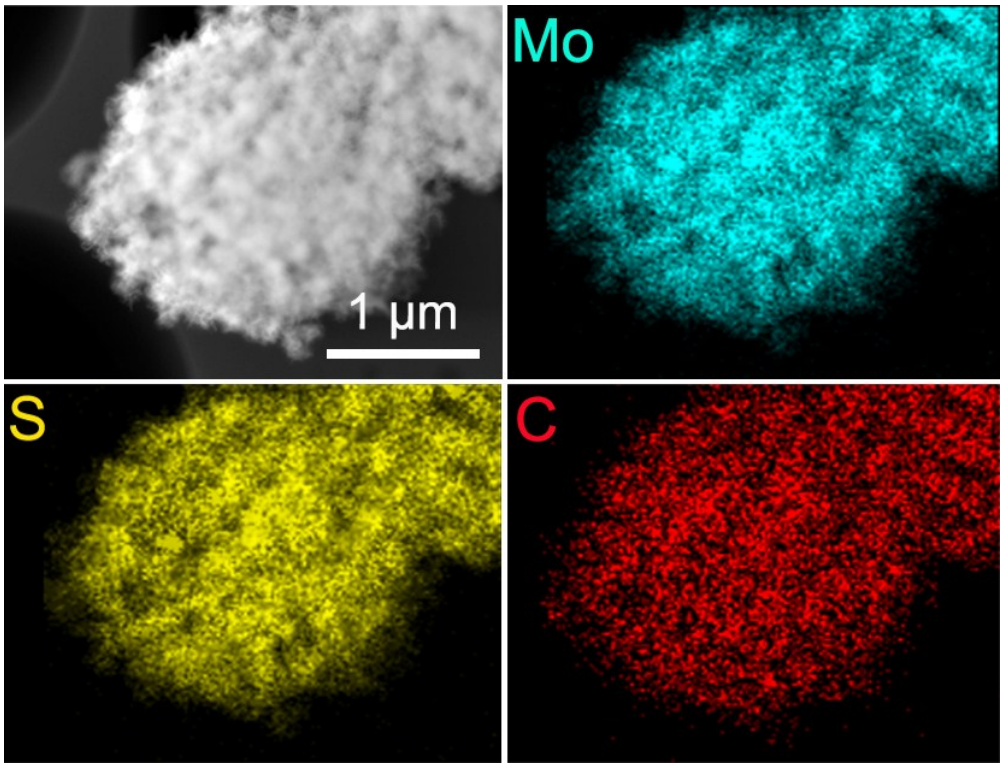

Fig. S3 Elemental maps of MoS_2/C.

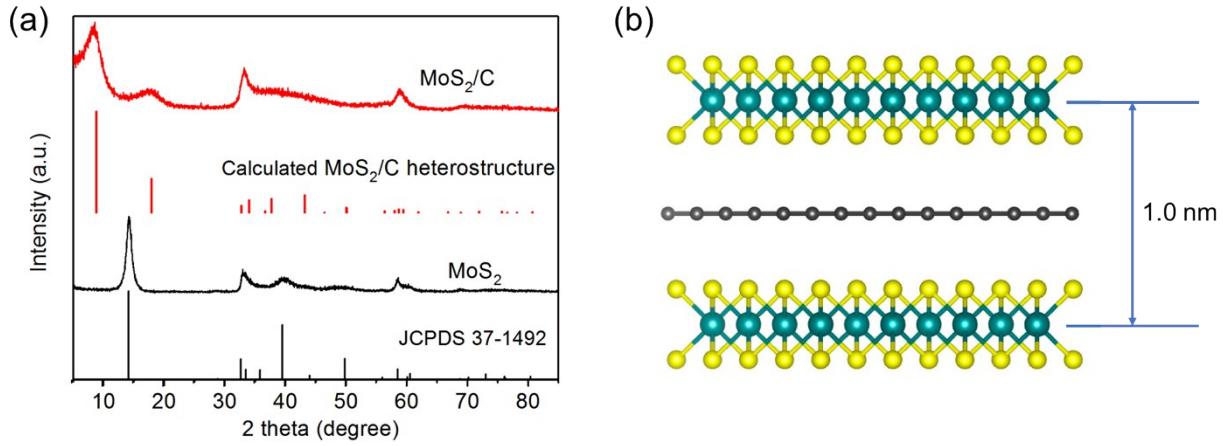

Fig. S4 (a) XRD patterns of MoS_2/C and MoS_2; (b) MoS_2/C heterostructure configuration. The simulated pattern shown in (a) is generated by the structural model shown in (b).

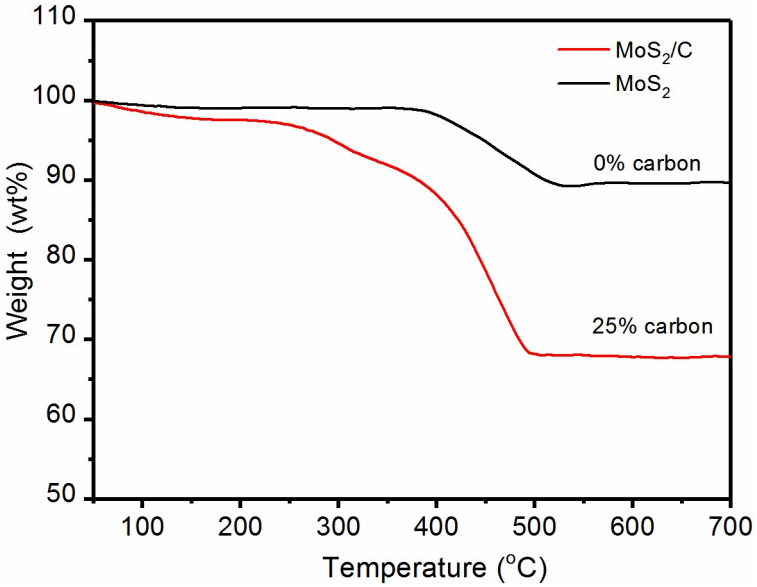

Fig. S5 TGA curves of MoS_2/C and MoS_2.

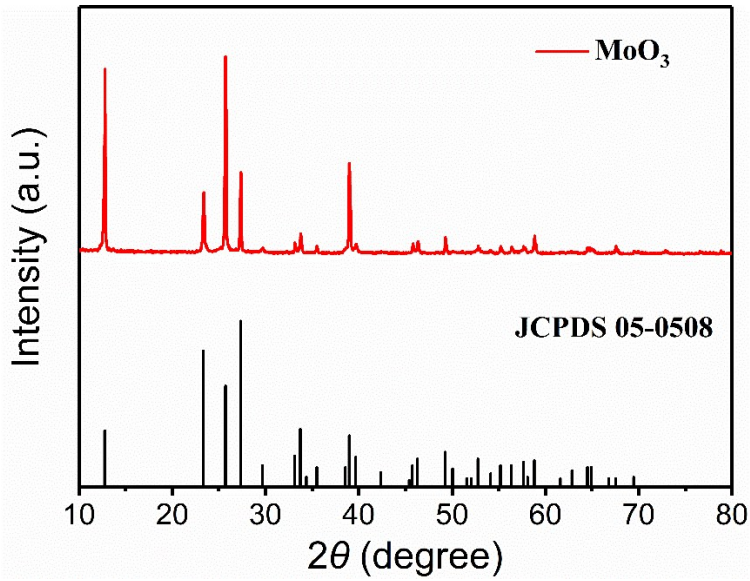

Fig. S6 XRD pattern of MoS_2/C after the TGA measurement. The MoS_2/C was fully oxidized to give MoO_3.

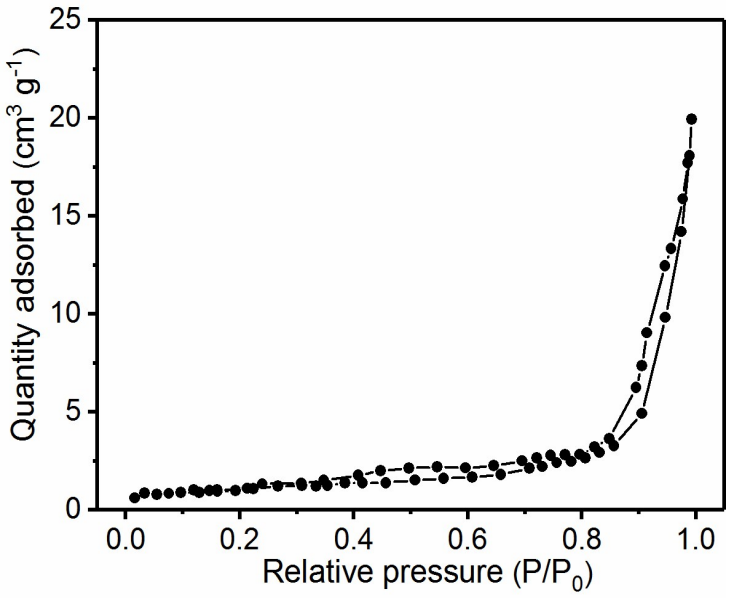

Fig. S7 N_2 adsorption-desorption isotherms of MoS_2.

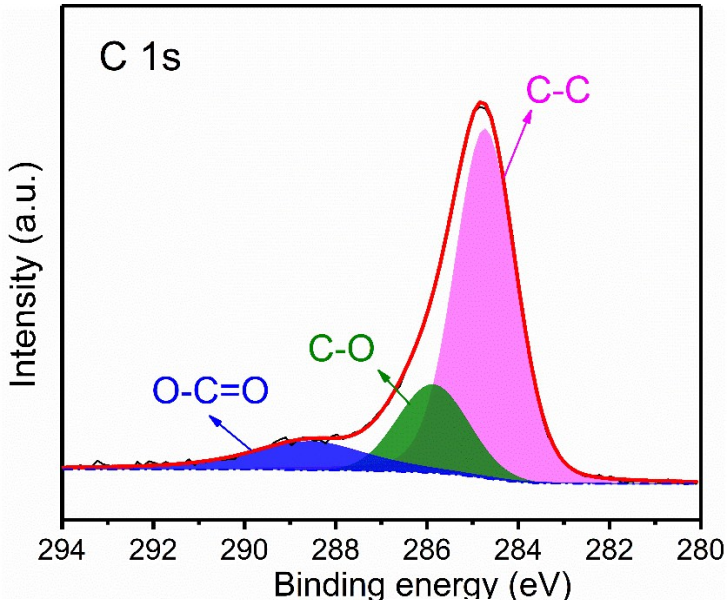

Fig. S8 Deconvolution of the C1s XPS spectrum of MoS_2/C.

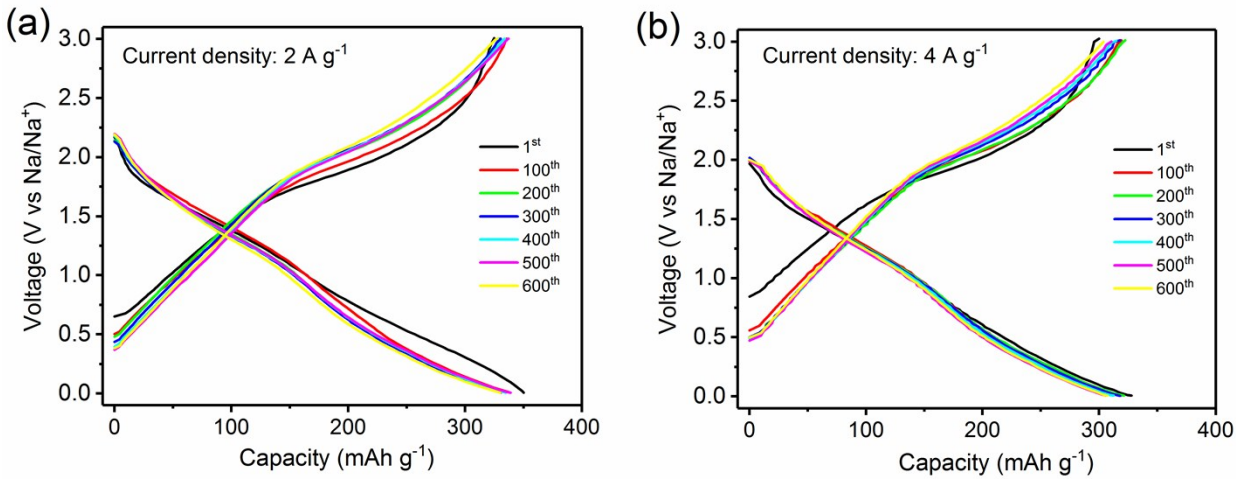

Fig. S9 Charge and discharge profiles of the MoS_2/C electrode at (a) 2 A g^{-1} and (b) 4 A g^{-1}.

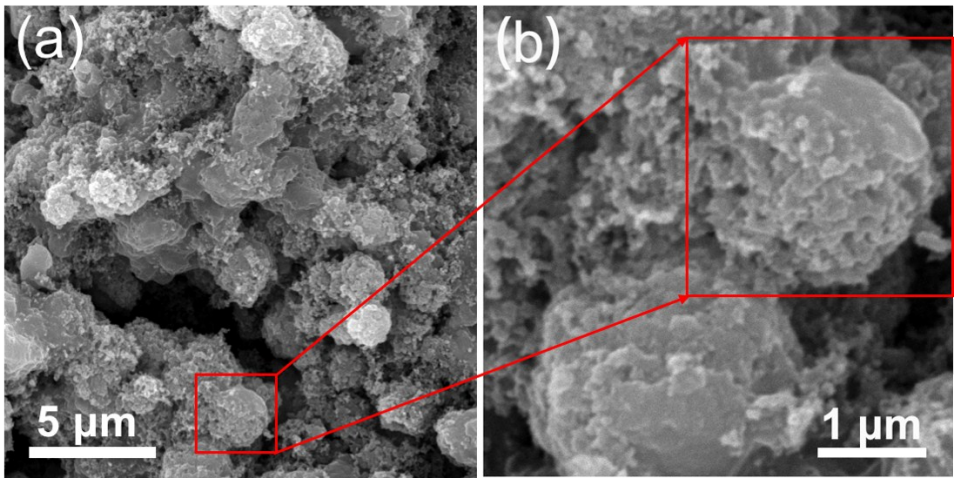

Fig. S10 (a, b) SEM images of MoS_2/C electrode after 500 cycles.

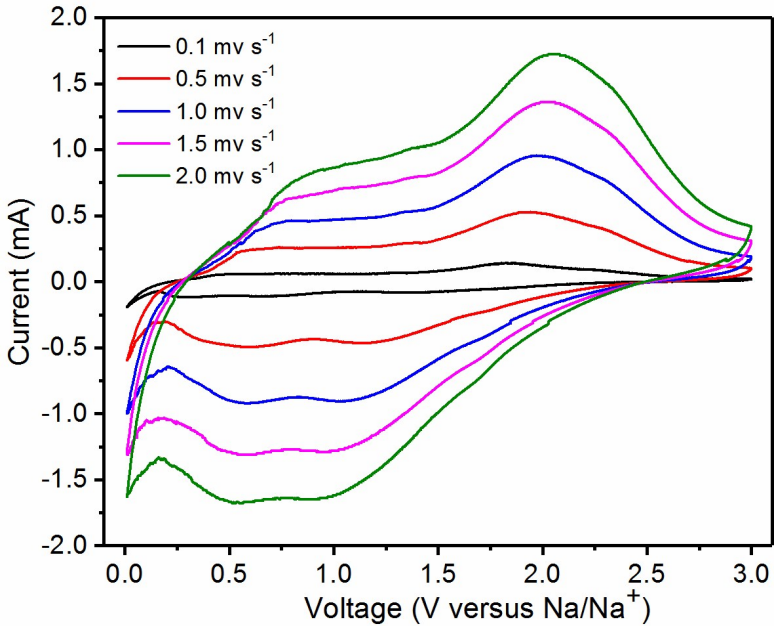

Fig. S11 CV curves of MoS_2 at scan rates ranging from 0.1 to 2 mV s^{-1}.

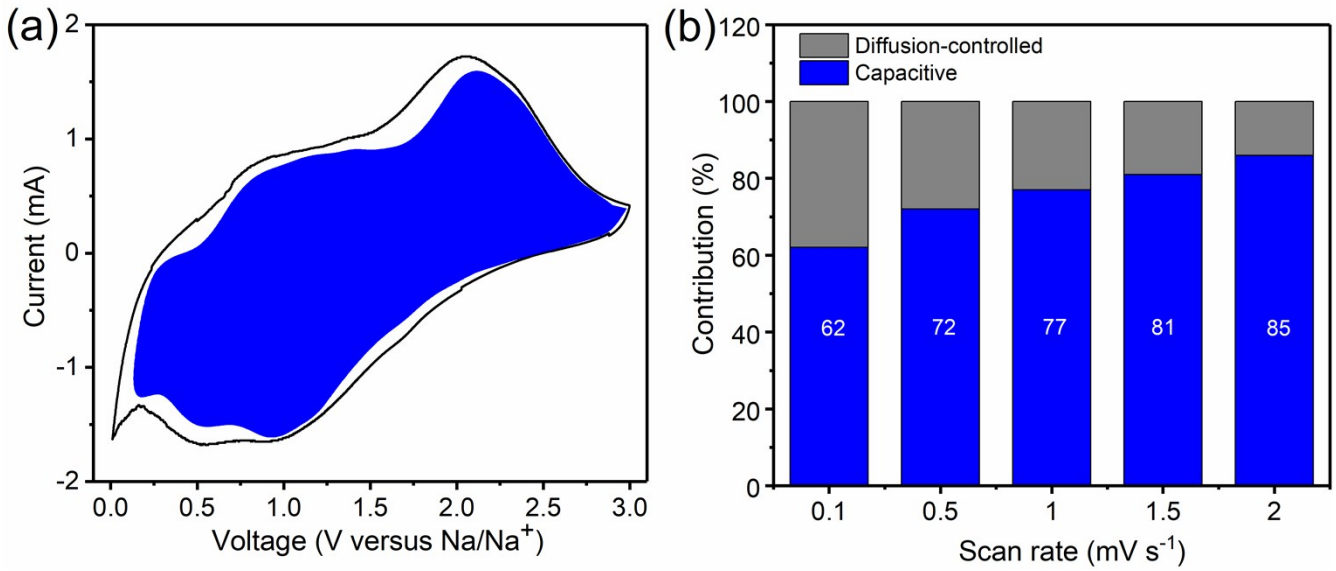

Fig. S12 (a) Capacitive contribution (black region) of MoS_2 electrode at 2 mV s^{-1}; (b) Contributions from capacitive (black) and diffusion-controlled (green) components at different scan rates.

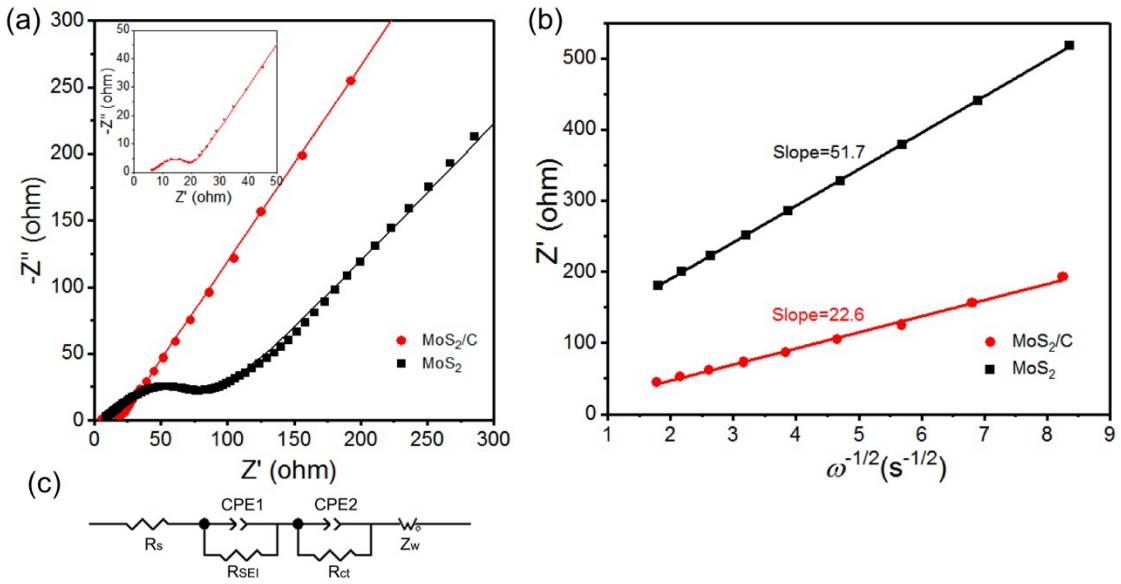

Fig. S13 (a) Nyquist plots of the MoS_2/C and MoS_2 electrodes after 10 cycles. The inset shows the magnified view of MoS_2/C at a low ohmic region. (b) Fitted lines and real part of impedance versus $\omega^{1/2}$ for MoS_2/C and MoS_2 electrodes. (c) Equivalent circuit used for fitting the EIS data.

The EIS data were fitted by the equivalent circuit shown in Fig. S13c, and the obtained impedance parameters are shown in Table S1. In the equivalent circuit, R_s is the ohmic resistance of the electrode system, R_{SEI} and R_{ct} represent the resistances related to the SEI and the charge transfer, respectively. CPE1, CPE2, and Z_w are the capacitances associated with the SEI, the double layer, and the Warburg resistance, respectively.

Table S1 Impedance parameters obtained from EIS spectra in Fig. S13

Sample	R_s (Ω)	R_{SEI} (Ω)	R_{ct} (Ω)
MoS_2	6.5	18.5	64.3
MoS_2/C	5.2	5.9	8.4

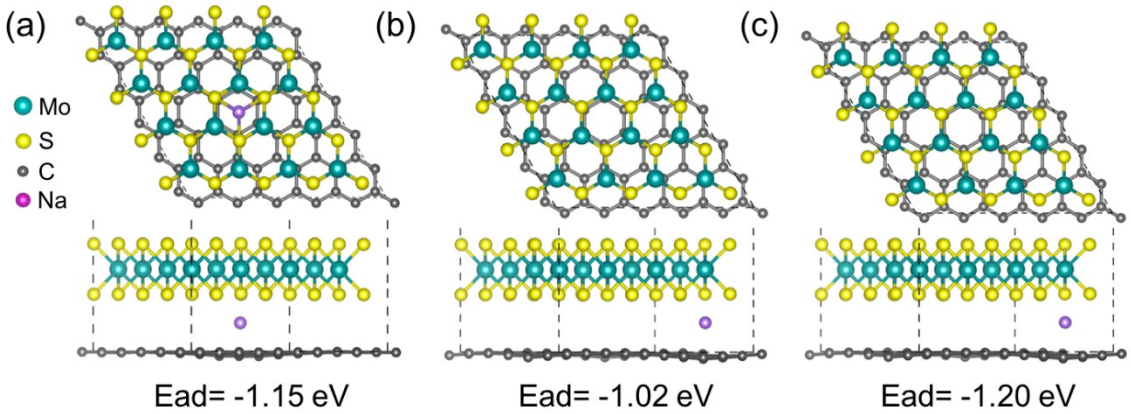

Fig. S14 (a) Optimized structure of the MoS_2/C interface, (b-d) Three representative configurations of a single Na atom adsorbed between the MoS_2/C bilayer structure. (b) Na adsorbed at the MoS_2/C interface of (b) MoS_2(H)/G(H) site, (c) MoS2(T_{Mo})/G(T) site and (d) MoS_2(T_{Mo})/G(H) site. The adsorption energy (E_{ad}) of each case is given.

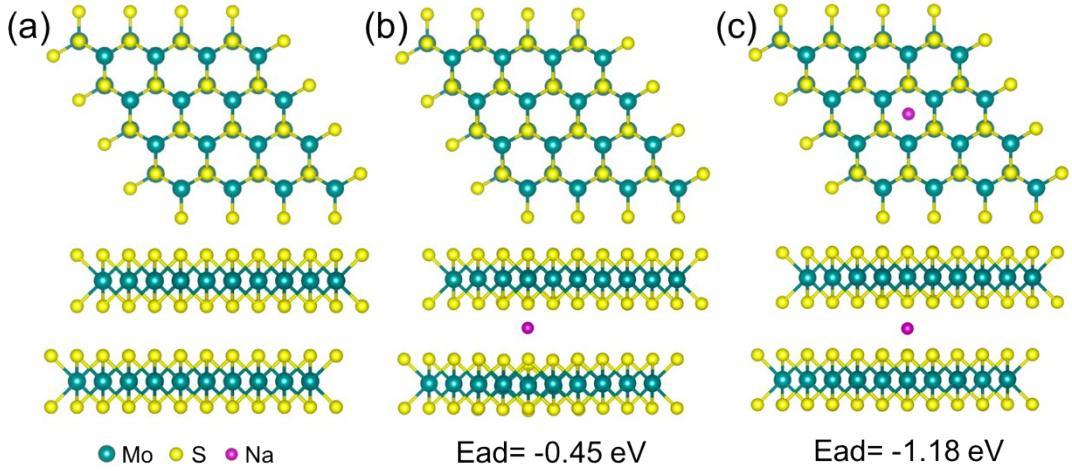

Fig.S15 (a) Optimized configuration of the MoS_2 bilayer. Single Na atom adsorption at tetrahedral (Th) sites (b) and octahedral (Oh) site (c) in the MoS_2 bilayer.

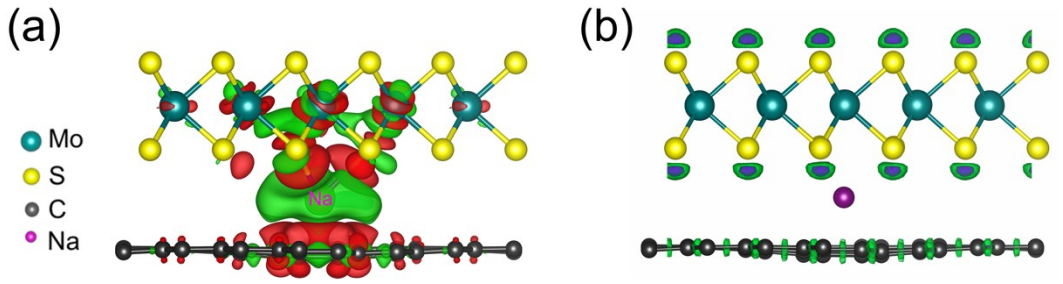

Fig. S16 (a) Charge density difference plot. The charge difference plot is calculated by $\Delta\rho$ = ρ(total)-ρ(MoS_2)-ρ(C)-ρ(Na), where ρ(total), ρ(MoS_2), ρ(C) and ρ(Na) are the total charge of the system, MoS_2, C and Na atom, respectively. The green and dark red areas indicate the electron depletion and accumulation in the space with an isovalue of ±0.0005 e $Å^{-3}$. (green for -0.0005 and red for +0.0005) (b) ELF plot. The isovalues in ELF plot are 0.8 (outside, green) and 0.85 (inner, purple), respectively.

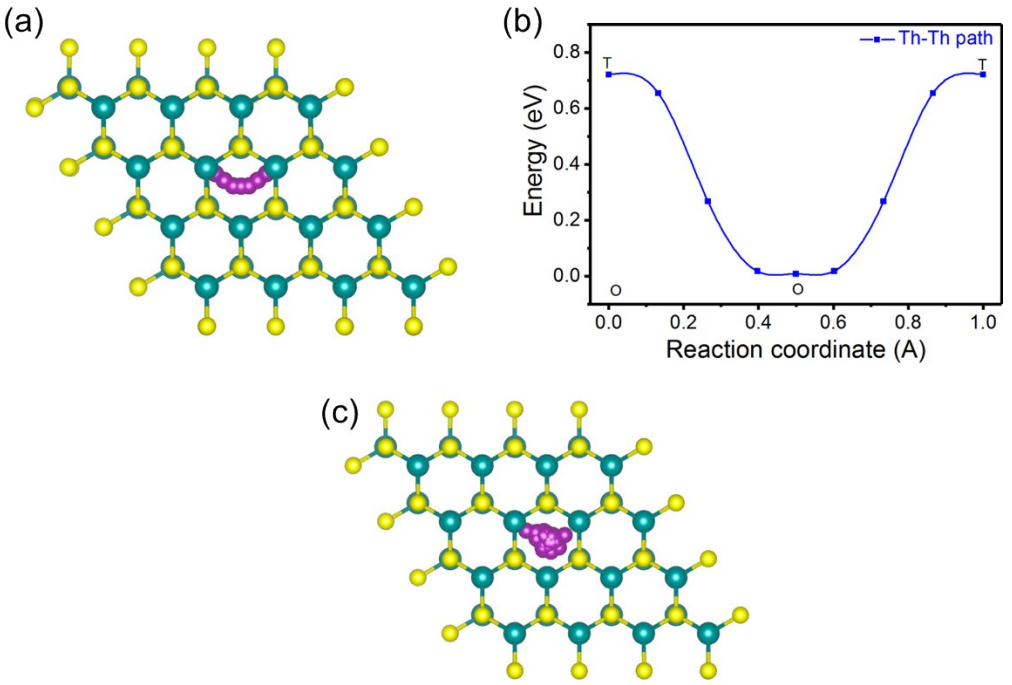

Fig. S17 (a) Na migration path between two adjacent Th sites at the MoS_2/MoS_2 interface, and (b) the associated energy profiles along the diffusion path. (c) Na trajectories at the MoS_2/MoS_2 interface (Na initially located at Th site) during 10 ps by AIMD simulations at 600 K.