

Supporting Information

Inter-Overlapped MoS₂/C composites with Large-Interlayer-Spacing for High-Performance Sodium-Ion Batteries

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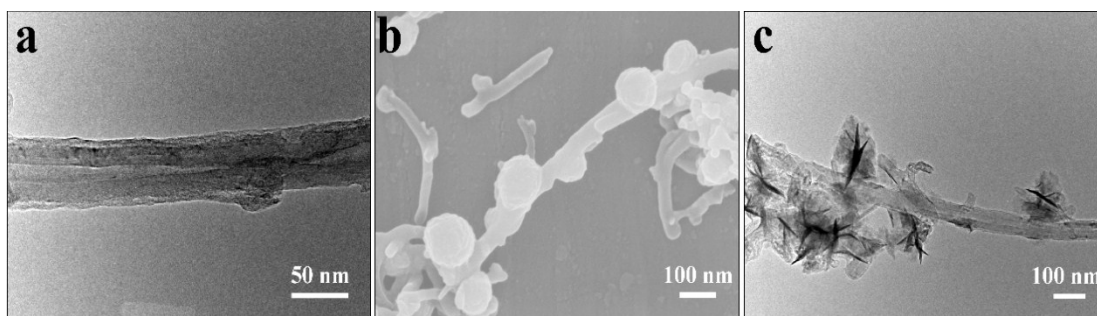


Fig. S1 (a) TEM image of the CNT@NCT. (b, c) SEM and TEM image of the CNT@NCT@MoS₂.

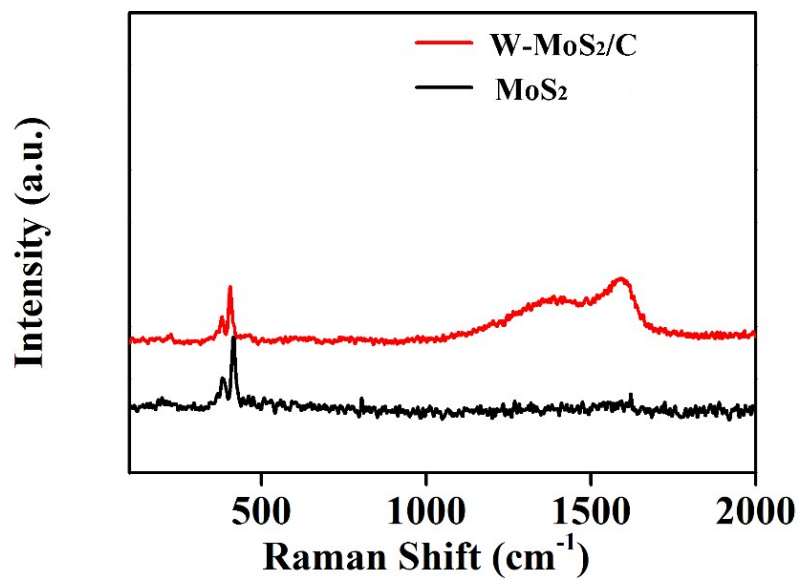


Fig. S2 Raman spectra of the MoS₂ and W-MoS₂/C.

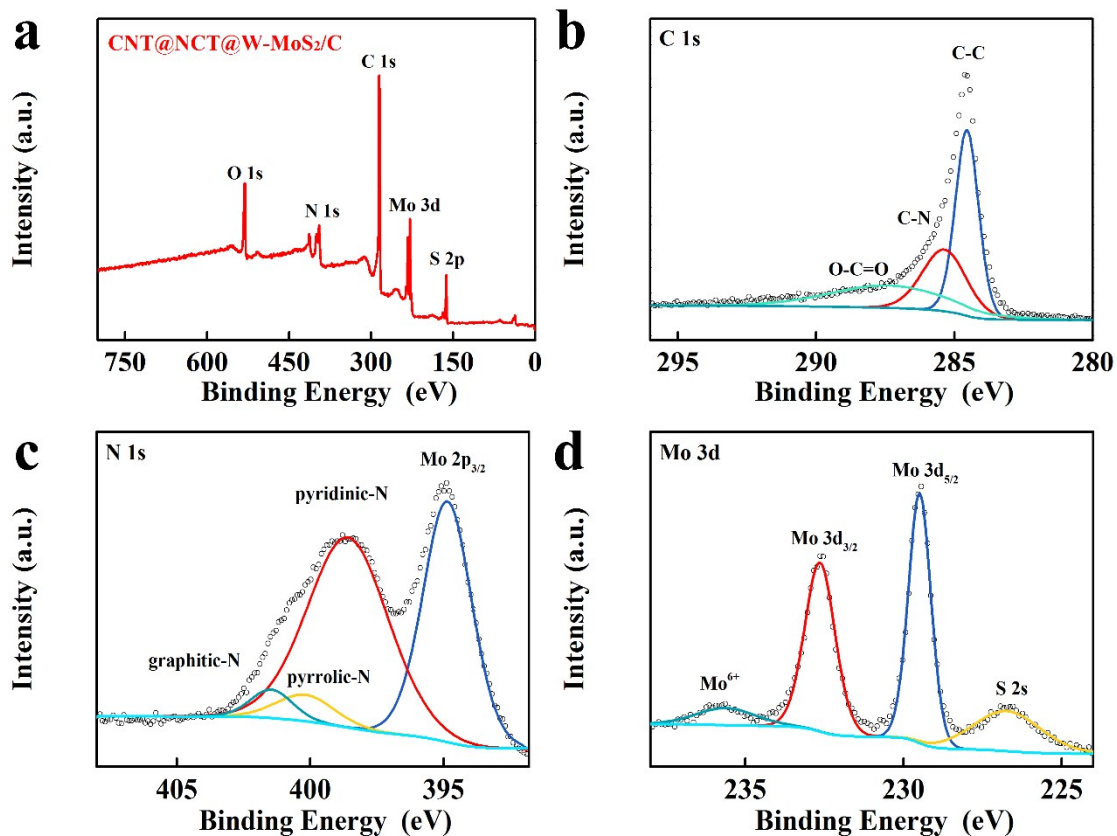


Fig. S3 (a) XPS survey spectrum of the CNT@NCT@W-MoS₂/C. (b-d) High-resolution XPS spectra of the C 1s peak, N 1s peak, and Mo 3d peak in the CNT@NCT@W-MoS₂/C.

Table. S1 Elemental compositions of CNT@NCT@W-MoS₂/C composites.

Element	C	N	S	Mo
CNT@NCT@W-MoS ₂ /C	79%	3.3%	11.6%	6.1%

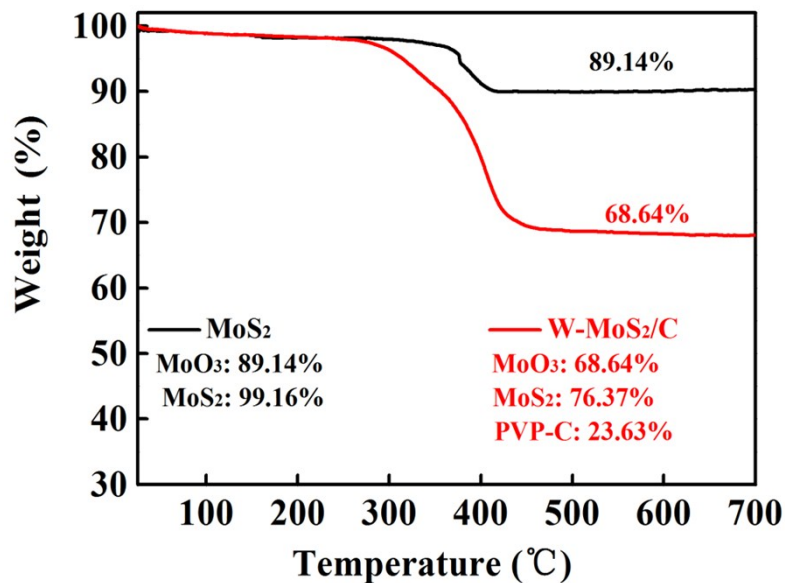


Fig. S4 TG curves of the MoS₂ and W-MoS₂/C.

The MoS₂ content in the CNT@NCT@W-MoS₂/C, W-MoS₂/C and pure MoS₂ was obtained by heating in oxygen atmosphere from room temperature to 700 °C. First, according to Fig. S4, it can be seen that MoS₂ starts to change to MoO₃ at around 370 °C, the mass ratio of MoS₂ in W-MoS₂/C can be calculated using Equation (1). And the ratio of PVP-C to MoS₂ in W-MoS₂/C is 1:3.2.

$$MoS_2 (wt \%) = \frac{\text{Molecular mass of } MoS_2}{\text{Molecular mass of } MoO_3} \times \text{total residual weights} \times 100 \% \quad (1)$$

According to the TG curve of the CNT@NCT@W-MoS₂/C (Fig. 3d), it showed a major weight loss at between 270 °C and 600 °C, during which, the carbon component was completely removed by O₂ oxidation and MoS₂ was oxidized completely to MoO₃. Known by Equation (1), the MoS₂, PVP-C and CNT@NCT content is 42.89 %, 13.27 %, and 43.84 %, respectively.

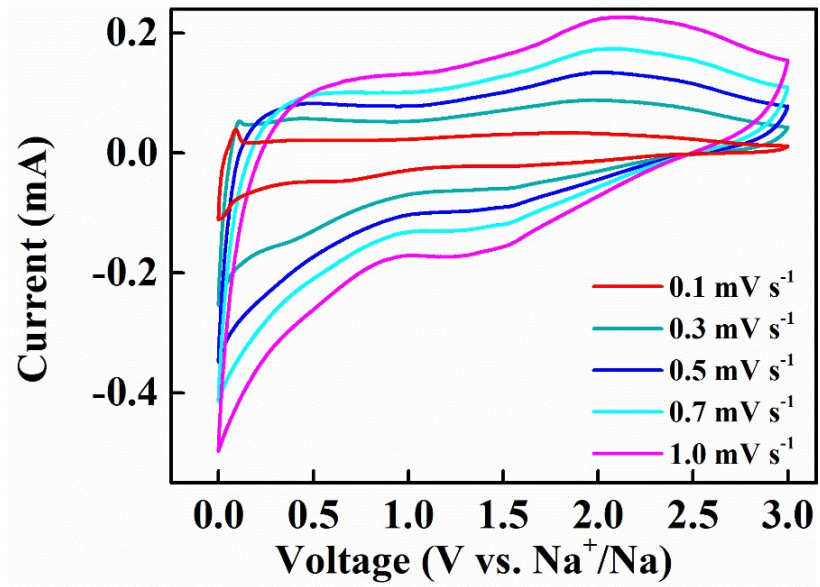


Fig. S5 Typical CV curves of the CNT@NCT@W-MoS₂/C cathode.

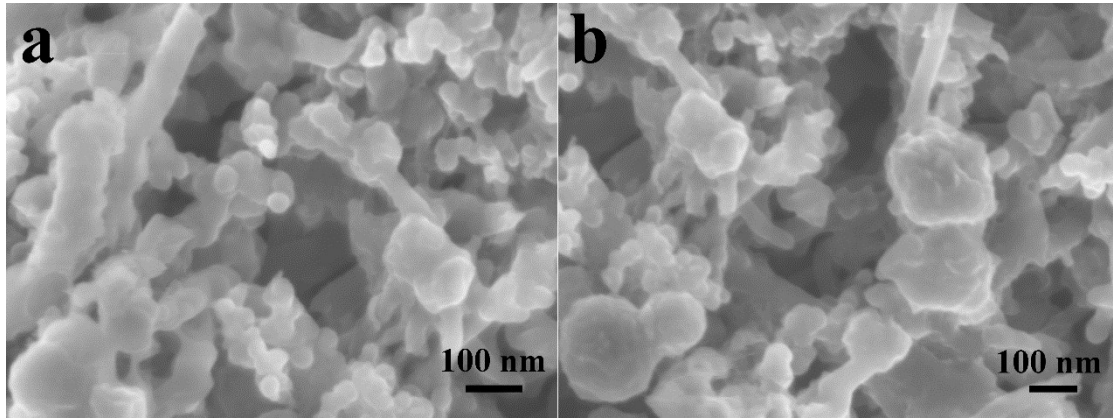


Fig. S6 (a, b) SEM images of CNT@NCT@W-MoS₂/C electrode after 200 cycles at 1 A g⁻¹.

Table S2. A comparison of the rate capability between this work and the work previously reported in literature.

Samples	Current density /mA g ⁻¹	Cycle number /n	Maintained capacity /mA h g ⁻¹	Reference
MoS ₂ -Li ₄ Ti ₅ O ₁₂	1200	200	101	1
MoS ₂ nanosheets	320	100	251	2
MoS ₂ /carbon fibers	1000	100	181	3
PEO-MoS ₂ composites	670	70	150	4
MoS ₂ /rGO composites	50	100	203	5
60MoS ₂	25	20	218	6
MoS ₂ /Graphene composites	320	300	227	7
MoS ₂ nanowires	100	200	200	8
Mo(Se _{0.85} S _{0.15}) ₂ :CNT	2000	100	40	9
G-C@MoS ₂	100	100	155	10
CNT@NCT@MoS ₂ /C	1000	136	90	Control sample
CNT@NCT@W-MoS ₂ /C	1000	200	256	This work

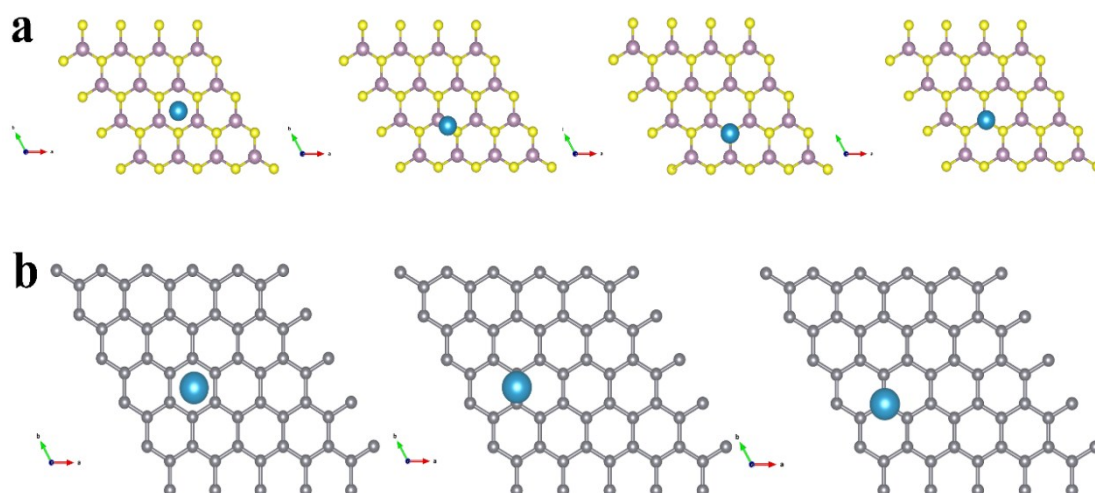


Fig. S7 (a) Optimized adsorption configurations of Na atom on the hollow, bridge, top

of S atom and top of Mo atom site on the MoS₂ layer. (b) Optimized adsorption configurations of Na atom on the hollow, bridge and top of C atom site on the graphene sheet.

Table S3. Calculate adsorption energies of Na atom at various active sites of CNT@NCT@W-MoS₂/C and CNT@NCT@ MoS₂.

	Active site	E _{ad} /eV
CNT@NCT@MoS ₂	Hollow	-0.734
	Bridge	5.476
	Top-S	8.479
	Top-Mo	8.479
CNT@NCT@W-MoS ₂ /C	Hollow	-0.971
	Bridge	-0.999

	Top-C	-0.937
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