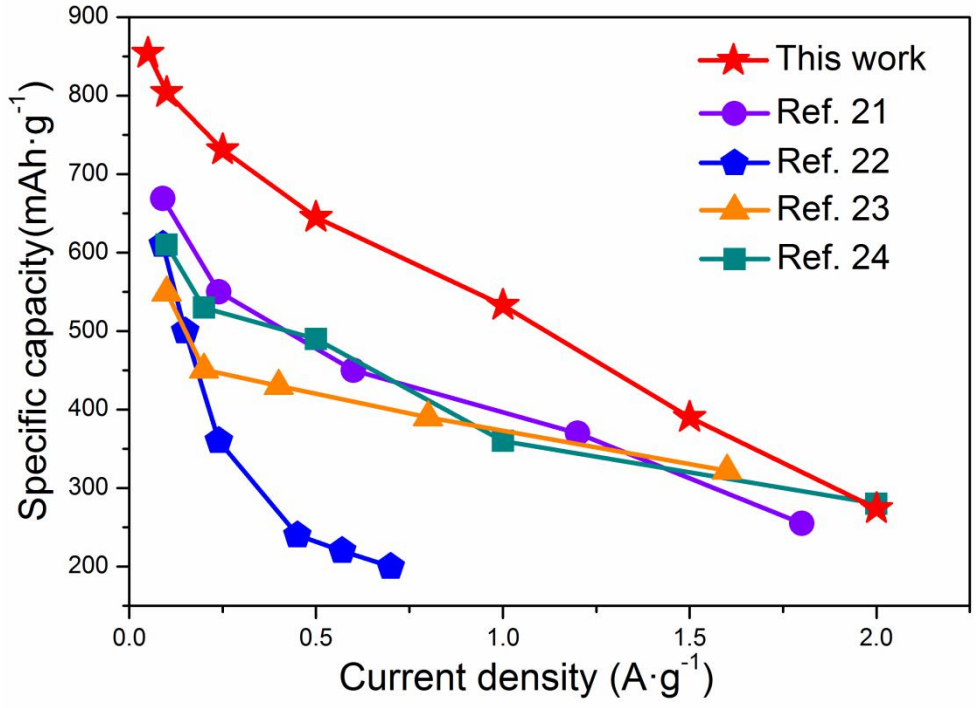
Supplementary Material

Lithium molybdate composited with carbon nanofibers as a high-capacity and stable anode material for lithium-ion batteries



Supplementary Figure 1. Comparative rate performance of Li_2MoO_4@C anode materials between this work and those reported in the literature.

Supplementary Table 1. Comparative long-cycle performance of Li_2MoO_4@C anode materials between this work and those reported in the literature.

	Current density ($A \cdot g^{-1}$)	The initial coulomb efficiency	Capacity ($mAh \cdot g^{-1}$)	Cycle number
Ref. 21	0.09	63.4%	400	58
Ref. 22	0.09	63.7%	550	50
Ref. 23	0.1	—	473	200
Ref. 24	0.1	66.1%	504	150
This work	0.1	68.2%	761	100

(LMO@CNF)	0.5	64.2%	531	360
	1	60.5%	290	800

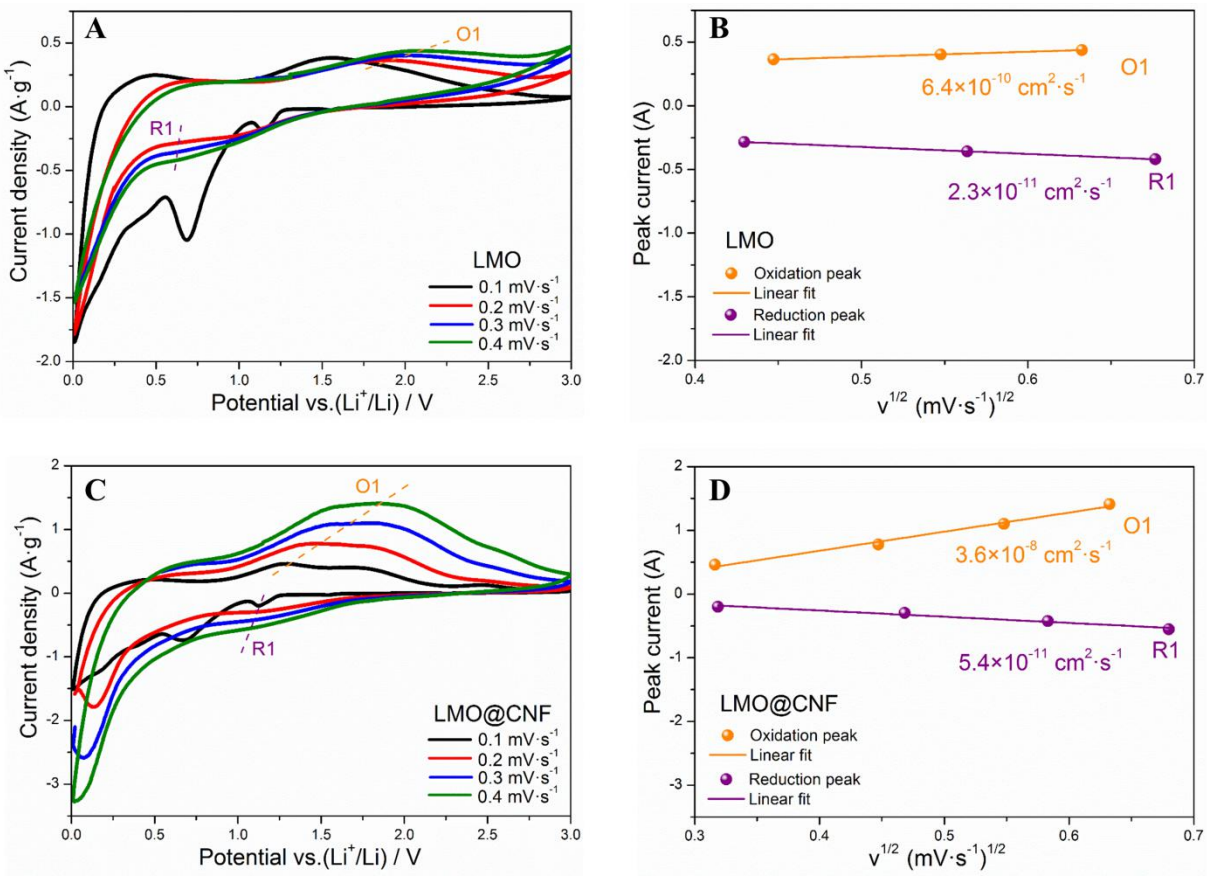
The Li-ion diffusion coefficient of LMO@CNF was further tested and analyzed by CV at different scanning rates (0.1/0.2/0.3/0.4 $mV \cdot s^{-1}$). The diffusion coefficient D_{Li+} of Li-ion can be calculated by Randles-Sevchik formula:

$$i_p = (2.69 \times 10^5) n^{3/2} A {D_{Li+}}^{1/2} v^{1/2} C_{Li+}$$

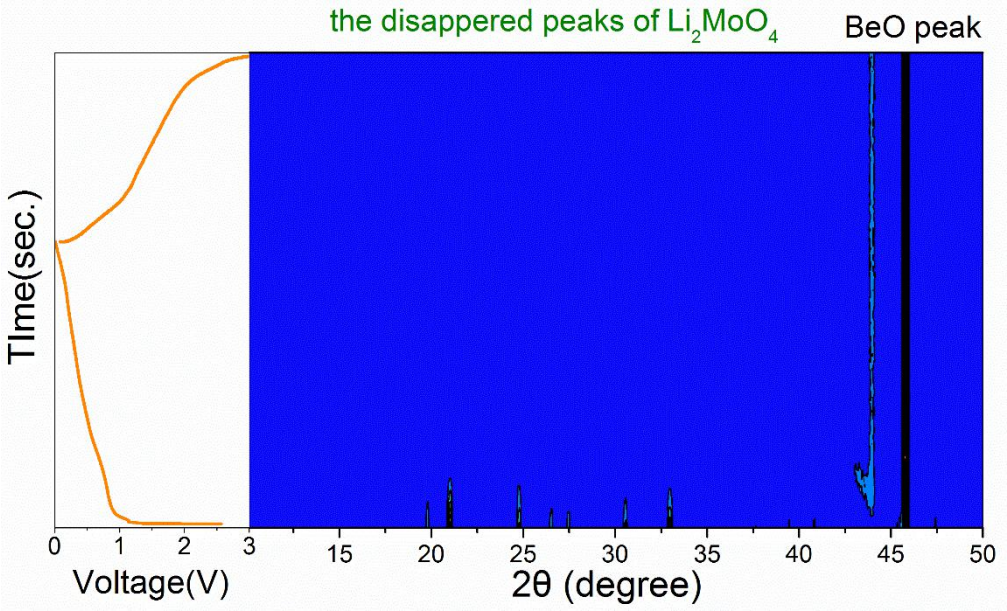
In this formula, i_p denotes the peak current value of the redox peak, n is the number of electron transfer, A is the contact area between electrode and electrolyte, D_{Li+} is the diffusion coefficient of Li^+, v means the scanning rate, C_{Li+} is the concentration of Li-ion in the active substance. By linear fitting of i_p and $v^{1/2}$, the diffusion coefficient D_{Li+} of Li-ion can be calculated as shown in Supplementary Table 2. The O1/R1 redox peaks correspond to the delithiation/lithiation of Li-Mo-O compounds. The higher diffusion coefficient of LMO@CNF indicates that the CNF conductive network combined with nanoparticles enables faster Li-ion transfer.

Supplementary Table 2. Diffusion coefficients, D_{Li+}, measured from cyclic voltammetry.

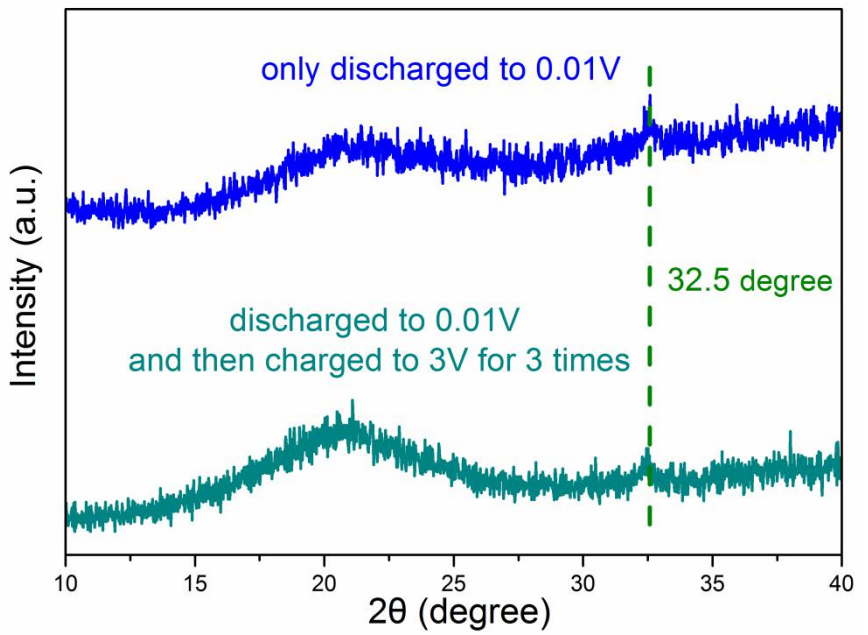
Diffusion coefficient, D_{Li+} ($cm^2 \cdot s^{-1}$)	O1	R1
LMO	6.4×10^{-10}	2.3×10^{-11}
LMO@CNF	3.6×10^{-8}	5.4×10^{-11}



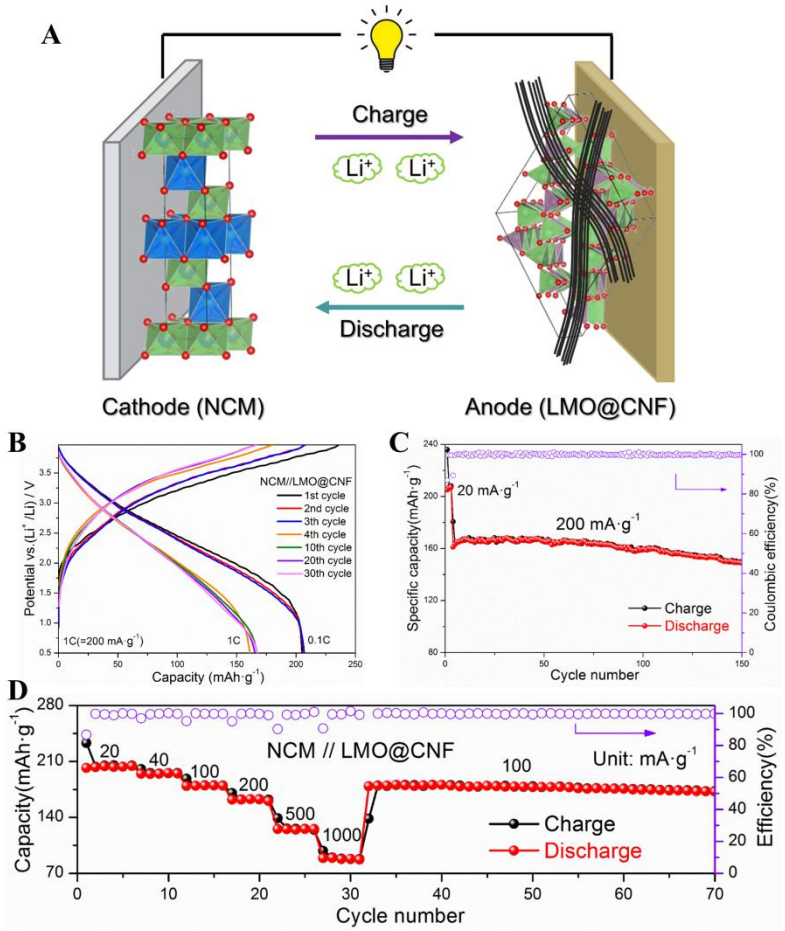
Supplementary Figure 2. The cyclic voltammetry curves of (A) LMO and (C) LMO@CNF at different scanning rates and (B) and (D) the corresponding fitting results of the relationship between the peak current and the square root of the scanning rate.



Supplementary Figure 3. *In situ* XRD examination of LMO@CNF electrode during the first charge/discharge cycle.



Supplementary Figure 4. *Ex situ* XRD examination of LMO@CNF with a weak peak around 32.5 degrees.



Supplementary Figure 5. (A) Schematic diagram of NCM//LMO@CNF full battery structure, (B) charge-discharge curves, (C) long-cycle performance at 1 C (1 C=200 mA g^{-1}), (D) rate performance.