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Tuning ZnSe/CoSe in MOF-derived N-doped porous carbon/CNTs for high-performance lithium storage

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Table S1. A comparison of the electrochemical properties of Se-based TMC anode materials.

Electrode materials	Capacity (mAh g^{-1}) (cycle number)	Current density	Ref.
CoSe@C	711 (100)	0.5 A g^{-1}	1
$Co_{0.85}Se$	295 (50)	0.5 A g^{-1}	2
$MoSe_2$/C	788 (100)	0.1 A g^{-1}	3
CoSe@C	708 (500)	1 A g^{-1}	4
ZnSe/C	705 (300)	0.1 A g^{-1}	5
$MoSe_2$/rGO	637 (1000)	1 A g^{-1}	6
ZnSe@C	960 (400)	0.2 A g^{-1}	7
ZnSe/rGO	778 (400)	1 A g^{-1}	8
Fe_2SeS	397 (100)	0.1 C	9
ZCS@NC/CNTs	1272 (120)	0.2 A g^{-1}	This work
	873 (500)	0.5 A g^{-1}	
	768 (1000)	1 A g^{-1}	

Table S2. Discharge capacities of the ZCS@NC/CNTs electrode in different regions of the discharge process at various cycles.

Cycle No.	Total capacity (mAh g^{-1})	Capacity in region 1 (mAh g^{-1})	Capacity in region 2 (mAh g^{-1})
1st cycle	671	225	446
10th cycle	614	216	398
50th cycle	629	183	446
100th cycle	630	152	478
200th cycle	769	174	595
300th cycle	845	198	647
500th cycle	992	243	749

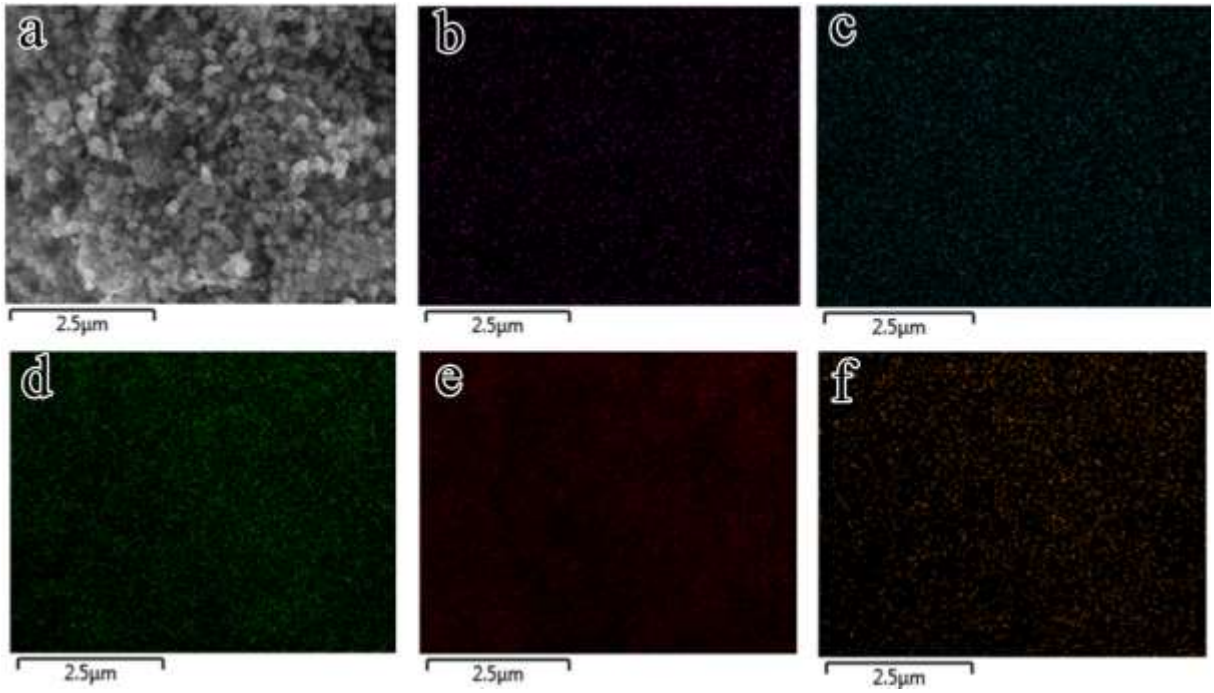

Figure S1. SEM and EDX mapping images of the ZCS@NC/CNTs electrode: (a) SEM, (b) Zn element, (c) Co element, (d) Se element, (e) C element and (f) N element.

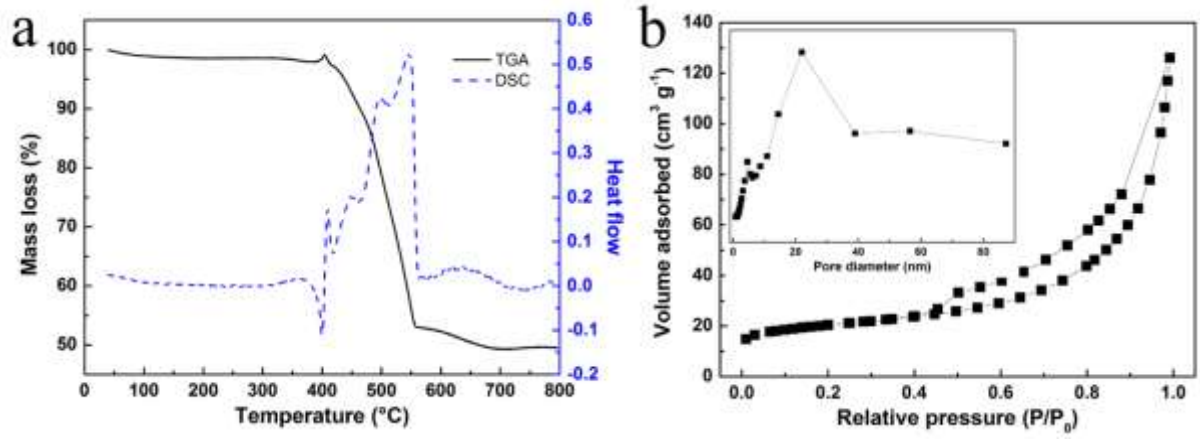

Figure S2. (a) TGA and DSC curves of the ZCS@NC/CNTs composite at a heating rate of 10 ^{o}C min^{-1} under Ar atmosphere. (b) N_2 adsorption-desorption isotherm and pore size distribution (inset) of ZCS@NC/CNTs.

The mass loss of the ZCS@NC/CNTs composite at the temperature between 50 and 500 ^{o}C is 46%. During the TGA measurement in air flow, carbon would be burned out, while ZnSe and CoSe are converted into ZnO and Co_3O_4 at 800 ^{o}C, shown as the following chemical reactions (1) and (2), respectively:[1]

$$ZnSe\ (s) + 2O_2\ (g) = ZnO\ (s) + 3Se\ (g) \quad (1)$$

$$3CoSe\ (s) + 2O_2\ (g) = Co_3O_4\ (s) + 3Se\ (g) \quad (2)$$

The ratio of Zn and Co in the ZnCoSe@NC/CNTs composite is confirmed by inductive coupled plasma (ICP) to be 1.12. The carbon content of ZCS@NC/CNTs is recalculated to be 11.7%, according to the TGA result and the Zn/Co ratio.

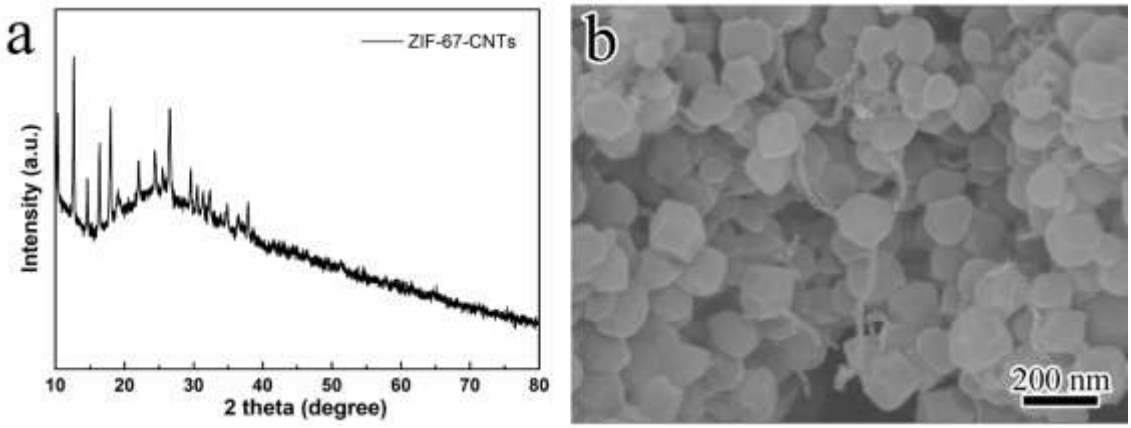

Figure S3. XRD pattern, SEM image, Raman spectrum of the ZIF-67-CNTs precursor.

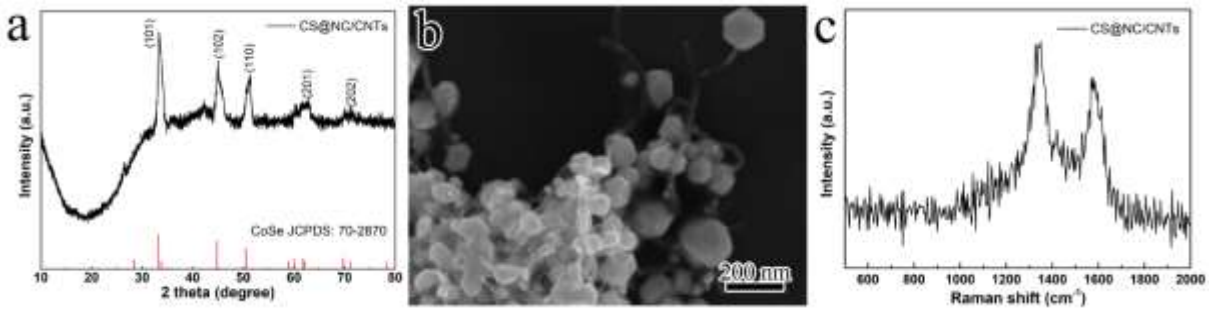

Figure S4. XRD pattern, SEM image and Raman spectrum of the CS@NC/CNTs composite. CoSe: JCPDS No. 70-2870.

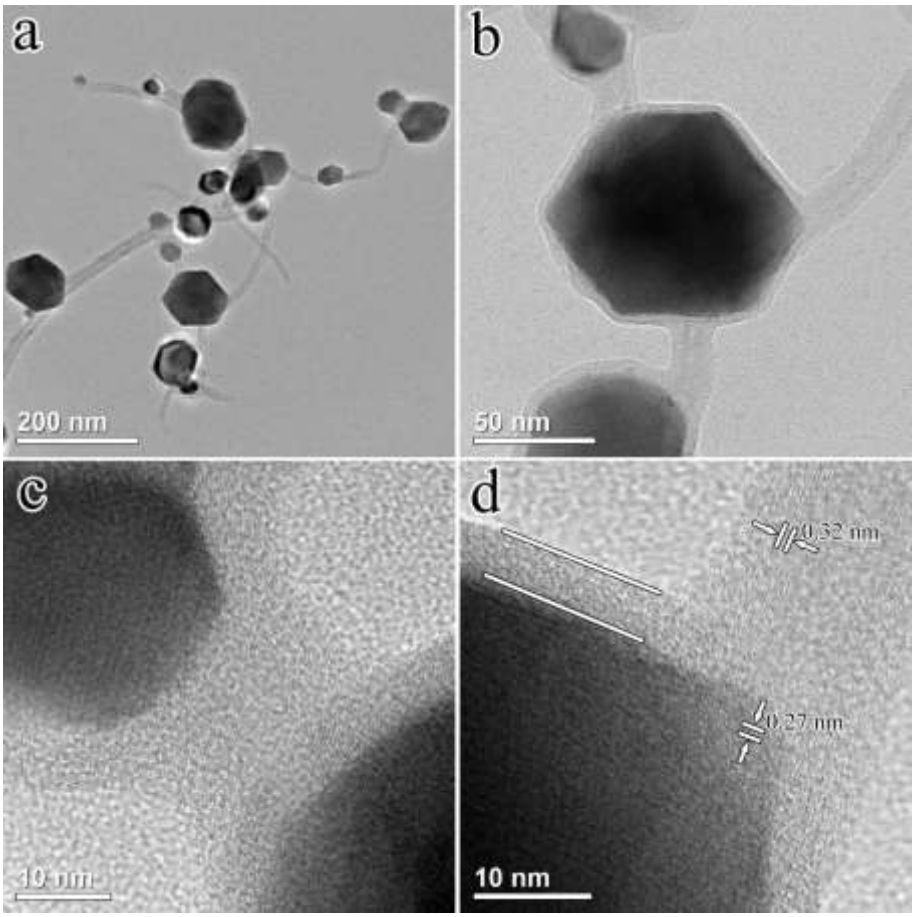

Figure S5. TEM and HRTEM images of the CS@NC/CNTs composite.

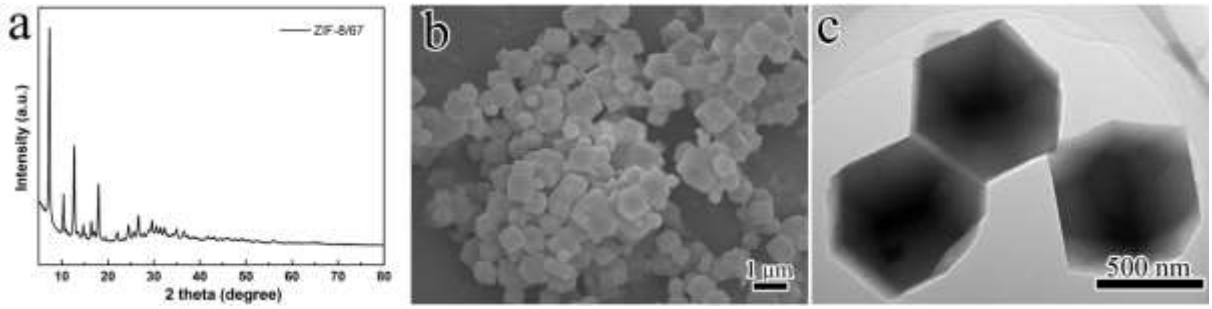

Figure S6. (a) XRD pattern, (b) SEM image, and (c) TEM image of the ZIF-8/67 precursor.

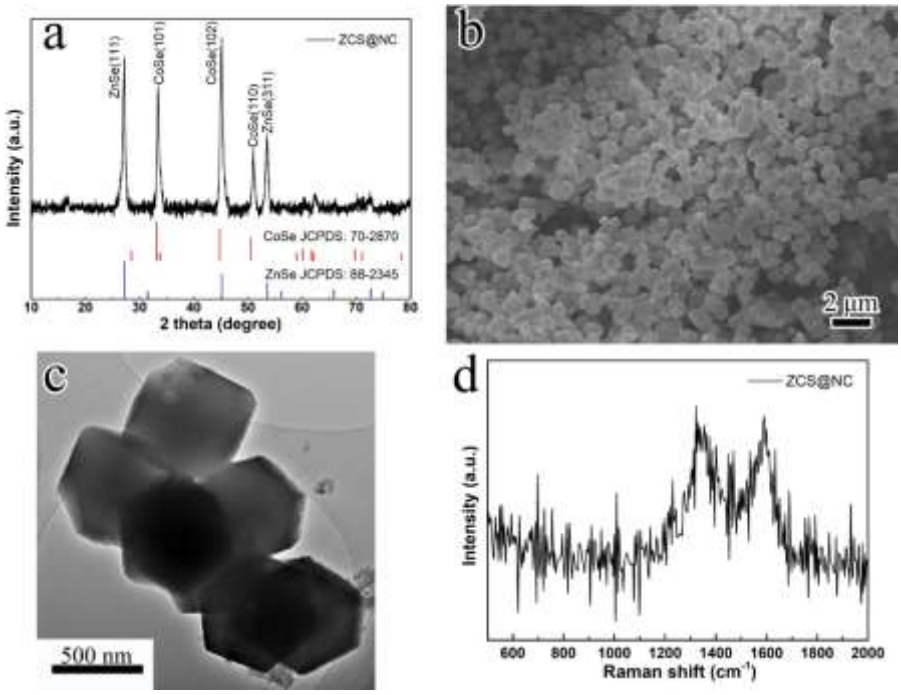

Figure S7. (a) XRD pattern, (b) SEM image, (c) TEM image and (d) Raman spectrum of the ZCS@NC composite. ZnSe: JCPDS No. 88-2345; CoSe: JCPDS No. 70-2870.

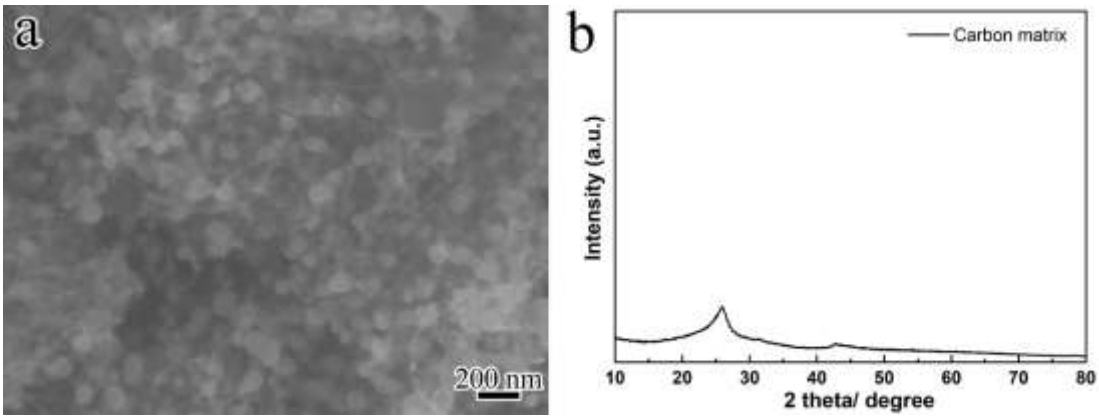

Figure S8. (a) SEM image and (b) XRD pattern of carbon matrix in ZCS@NC/CNTs.

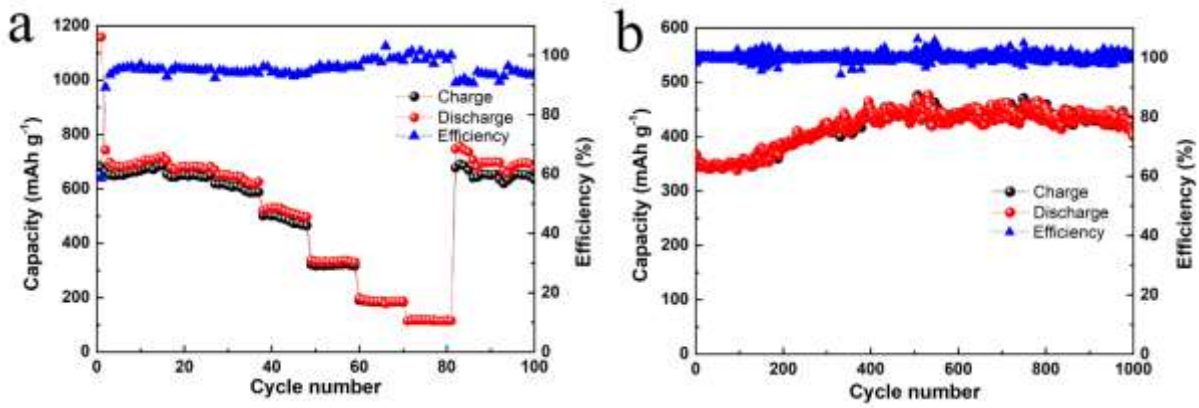

Figure S9. Electrochemical performances of the CS@NC/CNTs electrode: (a) rate performance at various current densities (0.1, 0.2, 0.3, 0.5, 1, 2 and 3 A g^{-1}) and (b) cycle performance at 1 A g^{-1}.

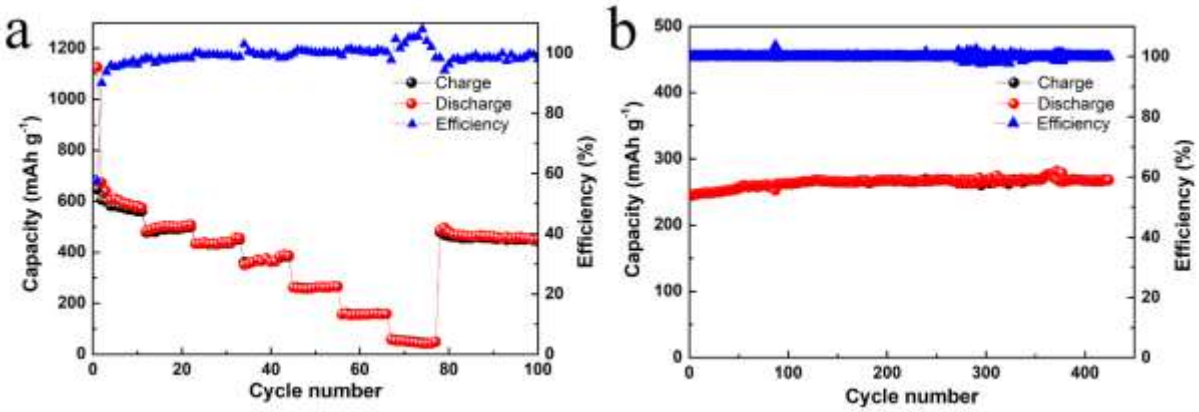

Figure S10. Electrochemical performances of the ZCS@NC electrode: (a) rate performance at various current densities (0.1, 0.2, 0.3, 0.5, 1, 2 and 3 A g^{-1}) and (b) cycle performance at 1 A g^{-1}.

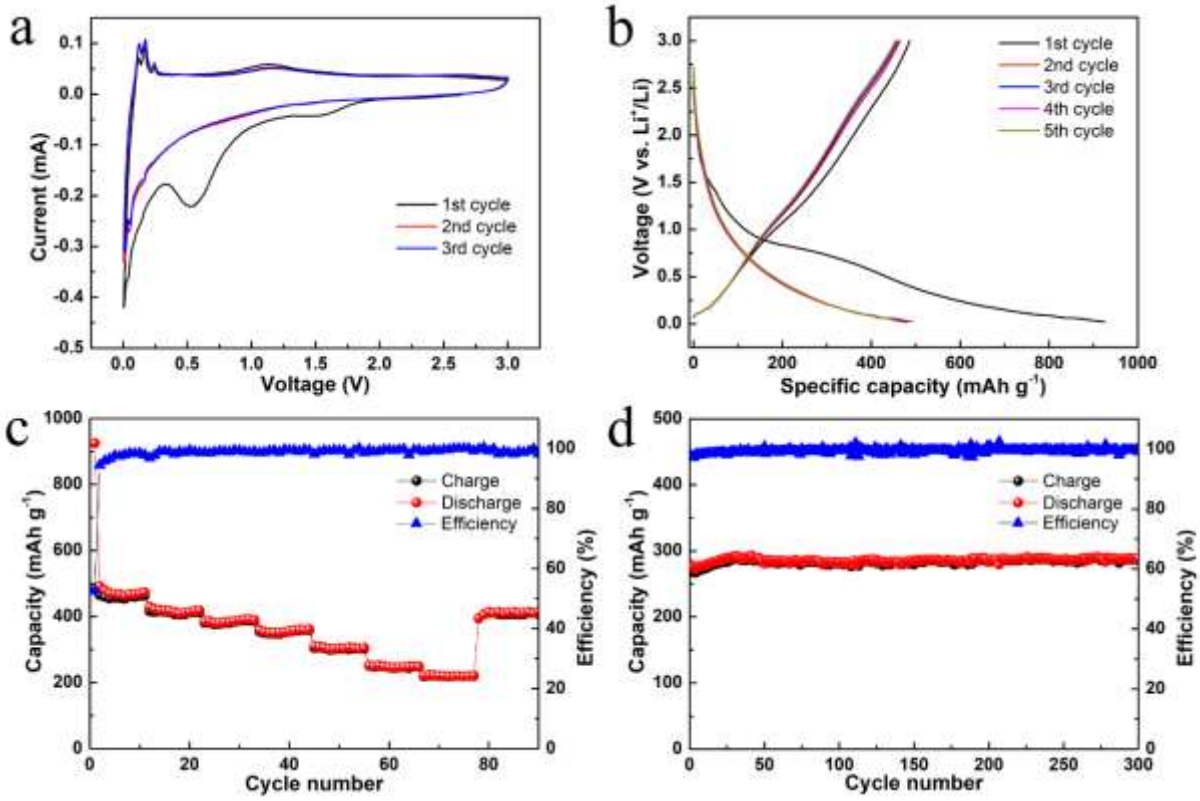

Figure S11. Electrochemical performances of the carbon matrix in ZCS@NC/CNTs: (a) CV curves at a scan rate of 0.1 mV s^{-1}, (b) discharge-charge profiles at a current density of 0.1 A g^{-1}, (c) rate performance at various rates (0.1, 0.2, 0.3, 0.5, 1, 2, and 3 A g^{-1}) and (d) cycle performance at 1 A g^{-1}.

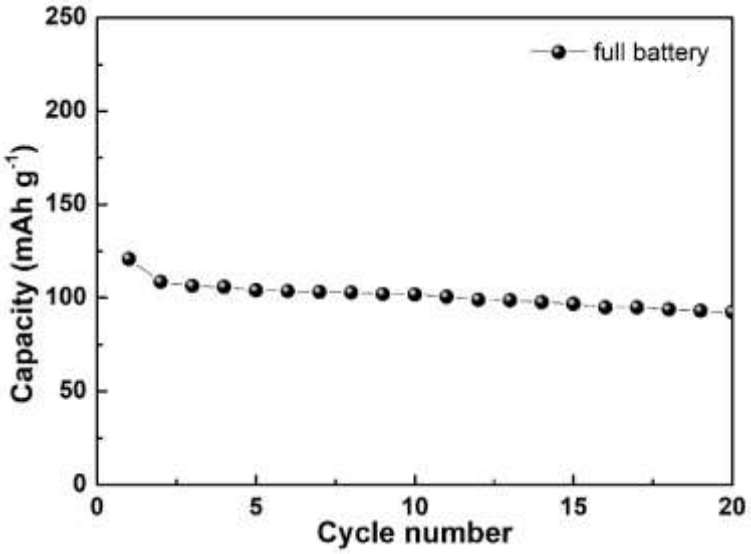

Figure S12. Cycle performance of the ZCS@NC/CNTs//$LiFePO_4$ full battery at 0.2 C (1 C=170 mA g^{-1} vs. $LiFePO_4$).

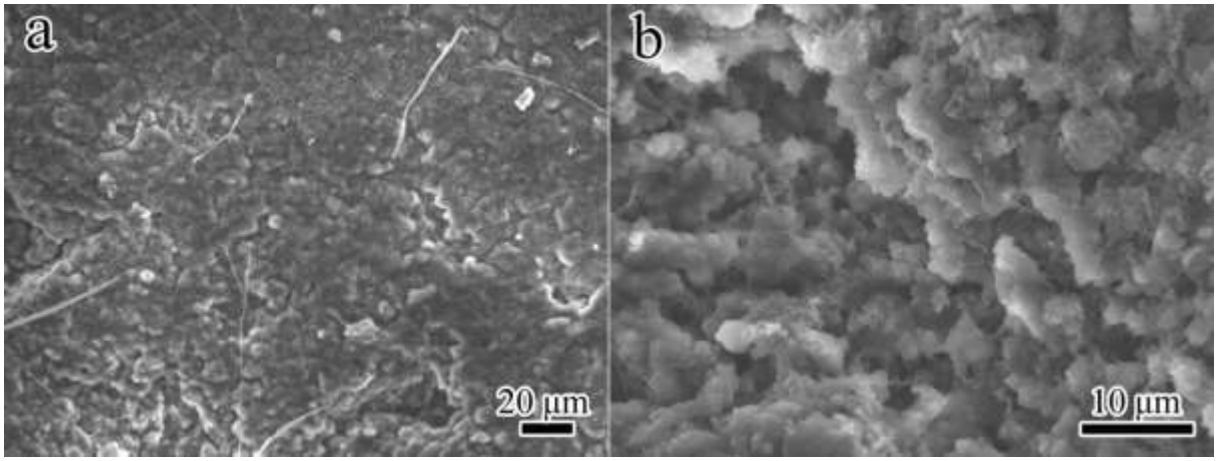

Figure S13. SEM images of the ZCS@NC/CNTs electrode after 100 cycles.

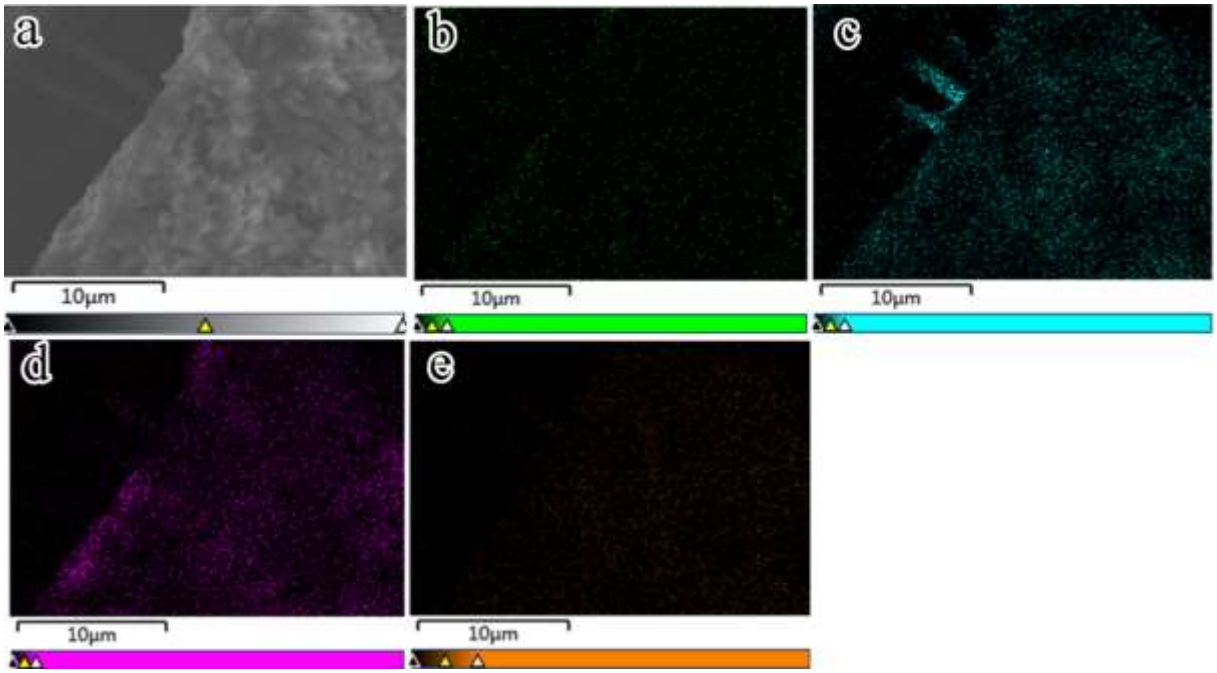

Figure S14. SEM and EDS images of the ZCS@NC/CNTs electrode after 100 cycles: (a) SEM image, (b) Zn element, (c) Co element, (d) Se element and (e) N element.

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