Supporting Information

Oxygen Vacancy Enhanced Catalytic Oxidation of H_2S Based on ZnO Incoperated N-doped Hollow Carbon Nanofibers for Cathodes Construction of High-performance Li-S Batteries

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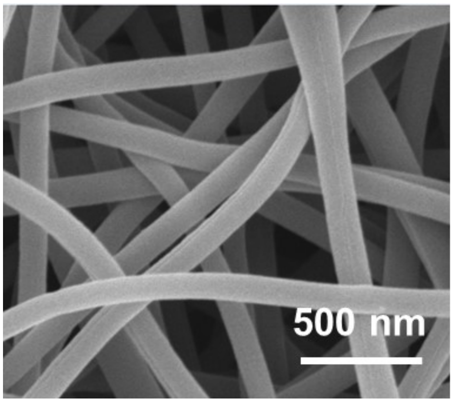

Figure S1. SEM image of precursor PMMA/Zn(Ac)$_2$ composites.

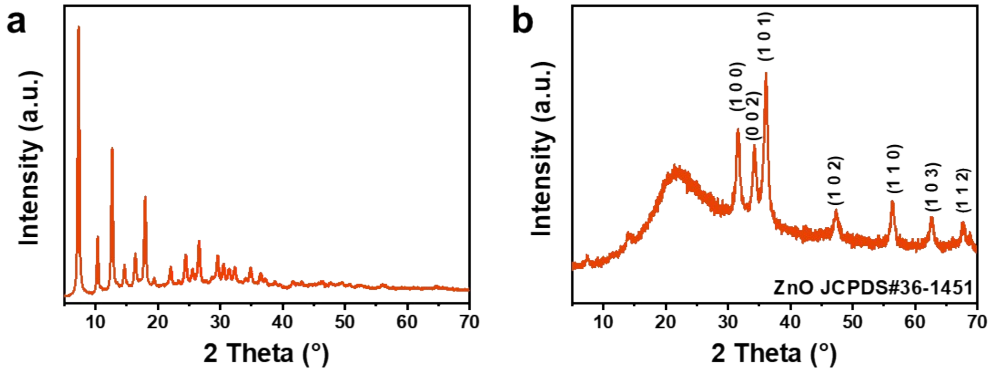

Figure S2. XRD patterns of (a) PMMA@Zn-ZIF and (b) O$_d$-ZnO/NHCFs samples.

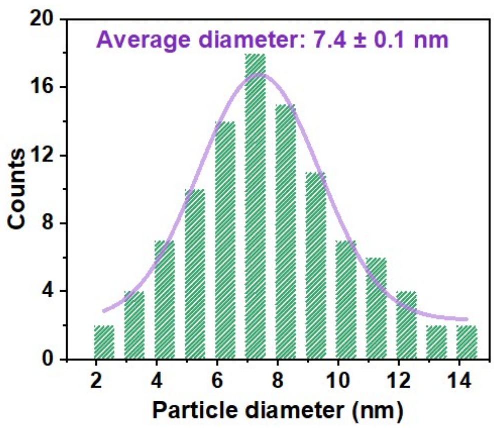

Figure S3. The statistical graph of ZnO nanoparticle size distribution in O$_d$-ZnO/NHCFs.

Table S1. Zn content (by ICP determination) in the samples after treated with different concentration of HCl solutions and the calculated ZnO loading amount in the materials.

Content (wt%)	Acid treatment condition				
	0.1 M	0.2 M	0.5 M	1 M	1 M (12 h)
Zn	40.32	28.52	20.29	9.69	\
ZnO	50.24	35.54	25.28	12.06	\

Table S2. Modulation of VOs in O_d-ZnO/NHCFs by changing the flow rate of H_2 and their corresponding saturated capacity of H_2S (Q_S).

Sample	Flow rate of H_2 (sccm)	VOs (%) (XPS)	Q_S (g H_2S/ g cat.)
ZnO/NHCFs	-	23.9	2.66
O_{d3}-ZnO/NHCFs	5	37.2	3.70
O_{d2}-ZnO/NHCFs	10	40.6	4.15
O_{d1}-ZnO/NHCFs	**20**	**50.3**	**4.64**
O_{d4}-ZnO/NHCFs	50	31.6	3.08

Table S3. Results from UPS spectra in the cutoff (E_{cutoff}), and the onset (E_i) energy regions of different samples. The ionization energy values (numerically equal to the work function (Φ) of materials) of ZnO before and after desulfurization were determined by the equation of $\Phi = 21.20\ \text{eV}-(E_{cutoff}-E_i)$.

Sample	E_{cutoff} /eV	E_i /eV	Φ/eV
ZnO	18.34	1.34	4.20
ZnO after desulfurization	18.57	1.69	4.32
ZnS	18.83	2.03	4.40

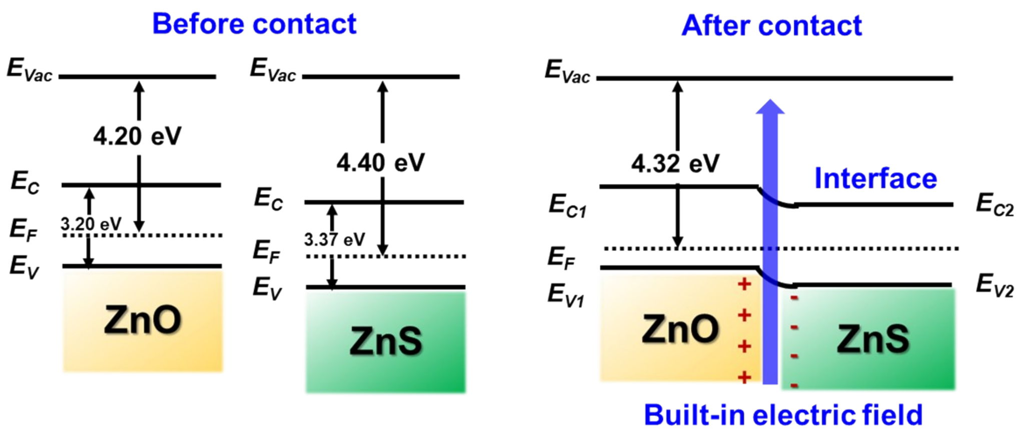

Figure S4. Schematic diagram of the difference in value of Φ between ZnO and ZnS due to the construction of heterostructure.

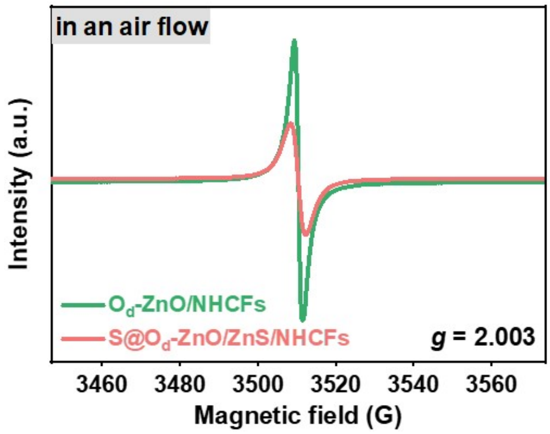

Figure S5. EPR spectra of fresh O_d-ZnO/NHCFs and the spent S@O_d-ZnO/ZnS/NHCFs.

Table S4. Elemental contents in various spent catalysts after elemental S removal.

Sample	Elemental content (wt%)		Sulfidation degree (%)	ZnO/ZnS
	S	Zn (ICP)		
ZnO/ZnS/NHCFs	1.63	28.43	11.65	7.58
O_{d3}-ZnO/ZnS/NHCFs	5.09	27.21	38.00	1.63
O_{d2}-ZnO/ZnS/NHCFs	6.45	26.78	48.92	1.04
O_{d1}-ZnO/ZnS/NHCFs	**7.18**	**25.99**	**56.12**	**0.78**
O_{d4}-ZnO/ZnS/NHCFs	3.38	27.69	24.79	3.03

Table S5. Elemental contents in spent catalysts with different desulfurization duration after elemental S removal.

Sample	Desulfurization reaction time (h)	ZnO/ZnS
O_{d1}-ZnO/ZnS/NHCFs	20	2.19
	25	1.46
	30	**0.92**
	36	0.78

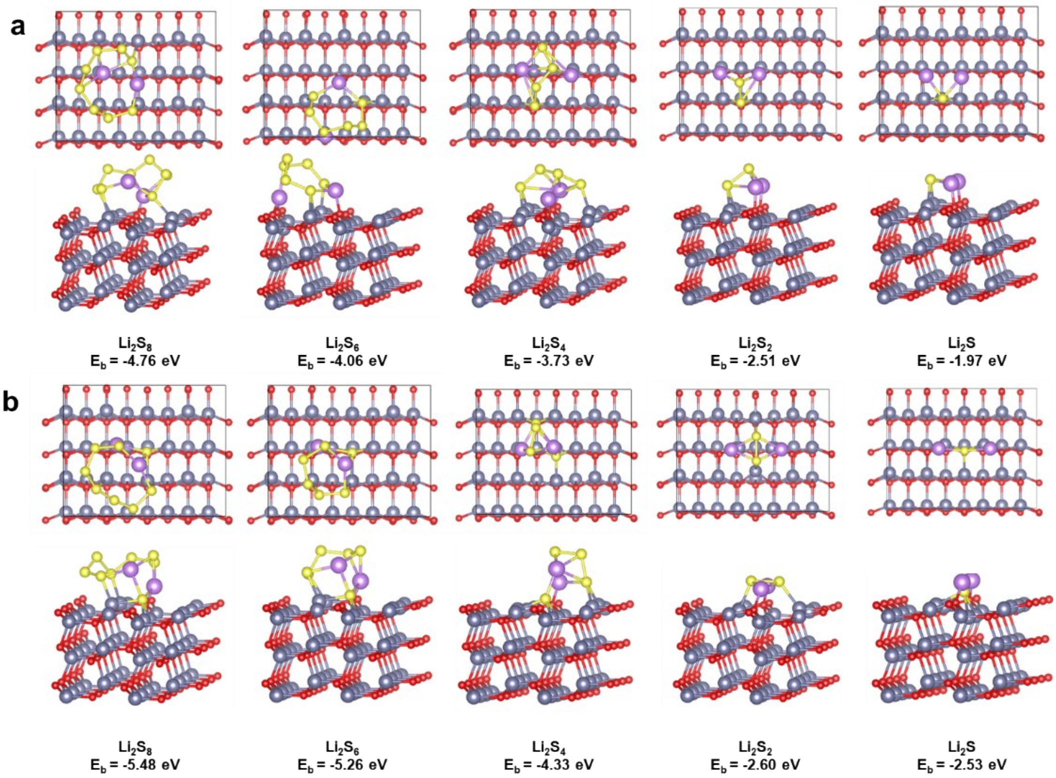

Figure S6. Atomic structures of Li_2S, Li_2S_2, Li_2S_4, Li_2S_6 and Li_2S_8 adsorbed on (a) ZnO (1 0 0) and (b) O_d-ZnO (1 0 0) facets (top panels: top view; bottom panels: side view), the Zn, O, Li, S atoms are shown as spheres in grey, red, purple and yellow, respectively.