Supplementary Materials

Rare-earth-based strategies for lithium-sulfur batteries: enhancing multi-electron conversion reaction kinetics

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Supplementary Table 1. Adsorption energies (ΔE, eV) of sulfur species on rare-earth-containing hosts/coatings/binders and carbon benchmarks

RE active sites	Adsorption energies (ΔE, eV)						Ref.
	S_8	Li_2S_8	Li_2S_6	Li_2S_4	Li_2S_2	Li_2S	
N-doped carbon	-1.47	-2.10	-1.90	-1.76	-1.95	-1.97	[S1]
CNTs	—	-0.35	-0.28	-0.13	-0.26	-0.42	[S2]
La_2O_3	-2.18	-4.06	-4.48	-4.13	-4.73	-5.11	[S1]
Gd_2O_3	—	—	—	-2.71	—	—	[S3]
Sc_2O_3	-0.71	-3.26	-2.75	-2.31	-3.31	-4.52	[S4]

$ScO_{0.95}$	-1.15	-4.70	-4.57	-4.50	-4.49	-5.51	[S4]
Y_2O_3	—	—	—	-2.15	—	—	[S5]
$LaNiO_3$	—	-0.91	-0.70	-1.67	-3.44	-2.90	[S2]
$LaNiO_{3-x}$	—	-1.55	-3.25	-3.33	-4.29	-3.61	[S2]
CeO_2	—	—	-2.73	—	—	—	[S6]
$CeO_{2-x}S_x$	—	—	-3.85	—	—	—	[S6]
CeF_3	—	—	-2.37	-4.47	—	—	[S7]
Single atom Ce/N_4	—	—	-2.71	—	—	—	[S8]
LaOCl	—	-1.85	-2.17	-2.35	-2.51	-2.17	[S9]
$LaCO_3OH$	—	—	-1.40	-2.12	-3.95	-3.94	[S10]
La_2O_2S	-0.82	-2.03	-2.03	-2.33	-3.34	-3.16	[S11]
La_2S_3	-6.84	-8.75	-8.57	-7.42	-8.08	-7.21	[S11]
Y-pyridine complex	—	—	—	-4.17	—	—	[S12]
CMC-Ce	-0.15	-1.34	-1.31	-1.66	-2.52	-2.07	[S13]

Supplementary Table 2. Li-ion transport descriptors for rare-earth-enabled systems in LSB

RE-based materials	**Li ion diffusion coefficient ($Li_2S_4 \rightarrow Li_2S$, cm^2/S)**	**Ionic conductivity (S/cm)**	**T (K)**	**Ref.**
2% $Y(NO_3)_3$ + 1% $LiNO_3$	0.1×10^{-8}	—	298	[S14]
$Nd(OTf)_3$	9.2×10^{-7}	—	298	[S15]
$Li_{0.34}La_{0.56}TiO_3$	—	2.0×10^{-5}	338	[S16]
$Li_7La_3Zr_2O_{12}$	—	4.0×10^{-4}	298	[S17]
$Li_7P_{2.9}Y_{0.1}S_{10.8}I_{0.2}$	—	3.1×10^{-3}	303	[S18]
Li_3HoBr_6	—	1.1×10^{-3}	298	[S19]
$Li_7P_{2.9}Ce_{0.1}S_{11}$	—	7.7×10^{-4}	298	[S20]

Supplementary Table 3. Summary of RE oxides as composite sulfur electrode host for LSB

Material	**Loading (mg**	**Rate (C)**	**Initial**	**Retention (n^{th})**	**Ref.**

	cm^{-2})		capacity (mAh g^{-1})		
La_2O_3-Mxene/CNF	1.0	0.2	1165.3	85% (400th)	[S21]
CeO_{2-x}/CNT	0.88	0.5	1233.9	85% (600th)	[S22]
Ga_2O_3/KB	3.1	0.5	817.2	48% (500th)	[S3]
ScO_2/N-PGC	0.5-1.0	0.5	1046.0	61% (1000th)	[S4]
Y_2O_3/KB	3.01	0.5	828.0	47% (500th)	[S5]
Nd_2O_3/CA	2.2-3.0	0.2	1327.0	82% (100th)	[S23]
Sm_2O_3/CA	1.5-1.8	0.5	1175.0	73% (300th)	[S24]
Cu-CeO_{2-X}@N/C	5.4	0.1	871.2	74% (100th)	[S25]
$LaFeO_3$	1.2-1.4	1.0	~750.0	87% (220th)	[S26]
$LaNiO_{3-x}$/CNT	4.4	0.5	714.0	~99% (1000th)	[2]
MoS_2-CeO_2/CNT	——	0.2	1250.0	75% (200th)	[S27]
La_2MoO_6/CNF	——	0.1	1097.8	73% (100th)	[S28]
LaOCl/CNF	1.8	1.0	~600.0	94% (1000th)	[S9]
$LaCO_3OH$	1.0-1.2	1.0	900.0	52% (1000th)	[S10]

Supplementary Table 4. Performance comparison of various rare-earth elements used in different parts of Li-S batteries

RE-based LSB	Sulfur loading (mg/cm^2)	Electrolyte to sulfur ratio (μL/mg)	Areal capacity (mAh/cm^2)	Rate (C, 1C = 1675 mAh/g)	Retention (%, nth)	Ref.
			Cathode catalyst			
La_2O_2S	1.5	20	1.5	1	66.4 (300)	[S11]
$LaNiO_{3-x}$	11.6	4	8.5	0.05	100 (250)	[S2]
$ScO_{0.95}$	4.5	30	3.5	0.1	85.5 (50)	[S4]
CeF_3	3.5	10	~2.4	1 A g^{-1}	63.2 (200)	[S7]
Cu–CeO_{2-x}	5.4	5	4.5	0.3	86.0 (60)	[S25]
			Binder			
Y-pyridine complex	6.6	10	5.0	0.1	72 (150)	[S12]
CMC-Ce	7.86	9	7.1	0.1	60.8 (80)	[S13]
			Additive			
2% $Y(NO_3)_3$ +	1.5	-	1.3	0.5	78.1 (250)	[S14]

1% $LiNO_3$ $Nd(OTf)_3$ (Li_2S)	8 (Li_2S)	8 (Li_2S)	7.0	116.6 mAh/g	78.0 (60)	[S15]
Solid electrolyte						
LATP+LLZO (25 °C)	12	-	~14.1 (7Ah Pouch cell)	0.1	~100 (30)	[S29]
$Li_7P_{2.9}Y_{0.1}S_{10.8}I_{0.2}$ (60 °C)	~1.9	-	~2.7	0.05	98.2 (50)	[S18]

*When not explicitly reported, areal capacities were recalculated from specific capacity × loading, and entries are normalized to the first stable cycle

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