

Electronic Supplementary Information (ESI)

MoCl₅ as a Dual-Function Redox Mediator for Li-O₂ Batteries

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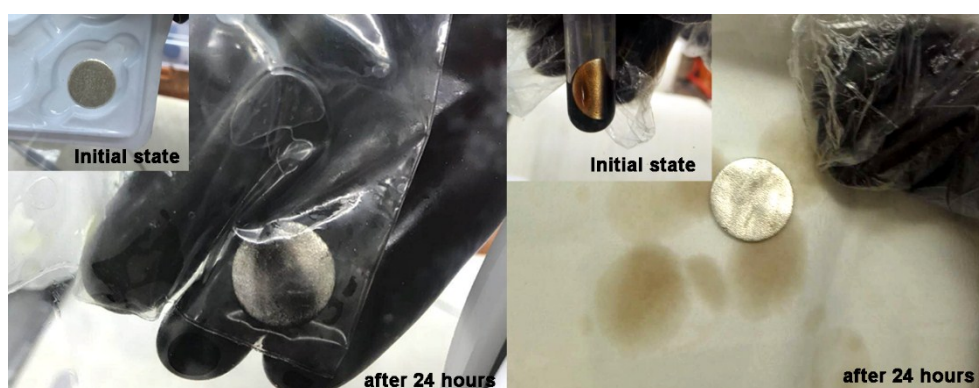


Fig. S1. Different states of lithium soaked in the electrolyte containing (left) FeCl₃ or (right) MoCl₅.

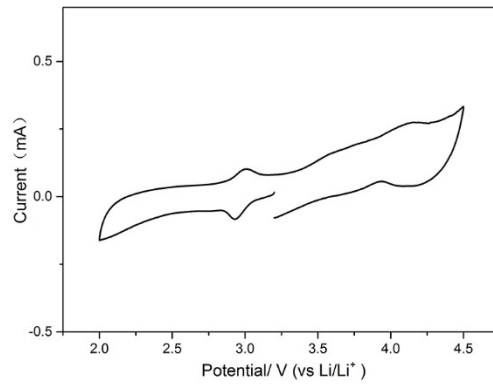


Fig. S2. CV curves of Li-O₂ batteries with MoCl₅ under Ar at a scan rate of 0.1 mV/s.

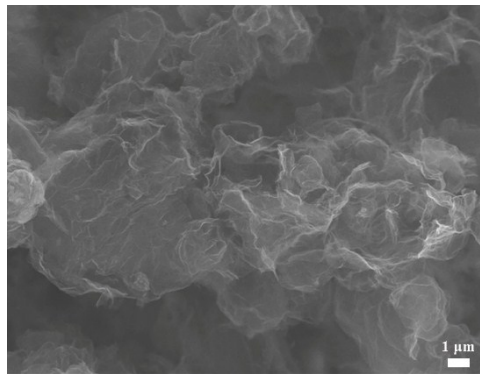


Fig. S3. SEM image of graphene cathodes at the initial stage.

Table S1. Summary of redox mediators used in Li-O₂ batteries.

Redox Mediator	Concentration (M)	Electrolyte	Cathode			Discharge capacity			Cycle Performance		Note	Reference		
			Material	Weight	Diameter	Discharge capacity	Current	Cycles	Current density	Cutoff capacity				
Organic redox Mediator	TTF	0.01	1 M LiClO ₄ /DMSO	Nano porous gold	0.15 to 5 mg cm ⁻²	Unknown	—	—	100	0.078 to 1mA cm ⁻²	300 mAh g _{gold} ⁻¹	OER	1	
	TEMPO	0.01	0.1 M LiTFSI/DME	Ketjen black	0.3-0.5 mg	10 mm	—	—	50	0.1 mA g ⁻¹	500 mA h g ⁻¹	OER	2	
	MPT	0.1	1.0 M LiCF ₃ SO ₃ /TEGDME	Super P and SWCNT	0.11–0.15 mg	Unknown	—	—	50	150 mA g ⁻¹	1000 mA h g ⁻¹	OER	3	
	DMPZ	0.2	1.0 M LiTFSI/TEGDME	dried gas diffusion layer	Unknown	Unknown	—	—	25	0.052 mA cm ⁻²	0.5 mA h cm ⁻²	OER	4	
	DBBQ	0.01	1.0 M LiTFSI/TEGDME or DME	gas diffusion layers	—	4*4 mm	~ 400 mA h m ⁻² ~ 440 mA h m ⁻²	0.2 mA cm _{real} ⁻² 0.1 mA cm _{real} ⁻²	—	—	—	—	ORR	5
	CoQ ₁₀	0.01	1.0 M LiTFSI/TEGDME	Super P	0.7 mg	12 mm	570 mA h m ⁻²	0.1 mA cm ⁻²	—	—	—	—	ORR	6

Metal Complex												
FePc	0.002	0.1 M LiTFSI/DMSO	Carbon fiber with Fe-N/C Graphene	0.25 mg cm ⁻²	Unknown	~ 3600 mAh g ⁻¹ (Carbon fiber with Fe-N/C)	0.5 mA cm ⁻¹	135 cycles (graphene)	0.5 mA cm ⁻²	1000 mA h g ⁻¹	ORR and OER	7
Heme	0.0023	1 M LiClO ₄ /TEGDME	MWCNT	Unknown	12.7 mm	2,871 mA h g ⁻¹	100 mA g ⁻¹	50 cycles	200 mA g ⁻¹	600 mA h g ⁻¹	ORR and OER	8
Co(Terp) ₂	0.05	1.0 M LiTFSI/DME: Pyr ₁₄ TFSI	CNTs	0.4-1.2 mg	10*10 mm	8200 mA h g ⁻¹	200 mA g ⁻¹	—	—	—	OER	9
Dual mediators												
DBBQ+ TEMPO	0.025+0.025	0.3 M LiClO ₄ /DME	gas diffusion layers	Unknown	4mm	40mA h cm ⁻²	1.0 mA cm ⁻² _{real}	50 cycles	1.0 mA cm ⁻²	2 mA h cm ⁻²	ORR and OER	10
DBBQ+ H ₂ O	0.01+ 20000ppm	0.25 M LiTFSI/DME	Super P rGO	1 mg cm ⁻² 0.1 mg	4 mm	~16 mA h cm ⁻² ~18 mA h cm ⁻²	0.1 mA cm ⁻²	—	—	—	ORR	11
Inorganic Redox mediator												
LiI	0.05	1.0 M LiTFSI/TEGDME	CNTs	Unknown	12.7 mm	—	—	900 cycles	2 A g ⁻¹	1000	OER	12
	0.05	0.2 M LiTFSI/TEGDME	Carbon paper	Unknown	Unknown	4.2 mA h cm ⁻²	0.13 mA cm ⁻²	300 cycles 30 cycles	0.052 mA cm ⁻²	0.052 mA h cm ⁻²	OER	13
LiBr	0.05	0.2 M LiTFSI/DME	Carbon paper	Unknown	Unknown	~6.5 mA h cm ⁻²	0.13 mA cm ⁻²	30 cycles	0.052 mA cm ⁻²	0.52 mA h cm ⁻²	OER	13
RuBr ₃	0.1	1 M LiTFSI/DMSO	Carbon paper	Unknown	Unknown	—	—	~50 cycles	0.052 to 0.208 mA cm ⁻²	0.5 mA h cm ⁻²	OER	14

H₂O	Hydrate-melt	LiTFSI LiBETI/H ₂ O	Ketjen Black	0.38 or 0.12 mg	7 mm	38000 mA h g ⁻¹	100 mA g ⁻¹	50	500 mA g ⁻¹	1000 mA h g ⁻¹	ORR and OER	15
IL-TEMPO	1%	0.5 M LiTFSI/DEGDME	Carbon Paper	—	10 mm	3 25 mA h cm ⁻²	0.1 mA cm ⁻²	100	0.1 mA cm ⁻²	0.25 mA h cm ⁻²	ORR and OER	16
Anthraquinone	10 mM	1M LiTFSI/TEGDME	Ketjen Black	0.7 ± 0.2 mg cm ⁻²	—	11000 mA h g ⁻¹	0.1 mA cm ⁻²	—	—	—	ORR	17
MoCl₅	0.05	1.0 M LiTFSI/TEGDME	Graphene	0.1~0.2 mg	12 mm	27530 mA h g ⁻¹	400 mA g ⁻¹	45 cycles 25 cycles	400 mA g ⁻¹ 800 mA g ⁻¹	1000 mA h g ⁻¹	ORR and OER	This work

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