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Electronic Supplementary Information

Performance-improved Li-O_2 Battery by Tailoring Phases of Mo_xC Porous Nanorods as An Efficient Cathode

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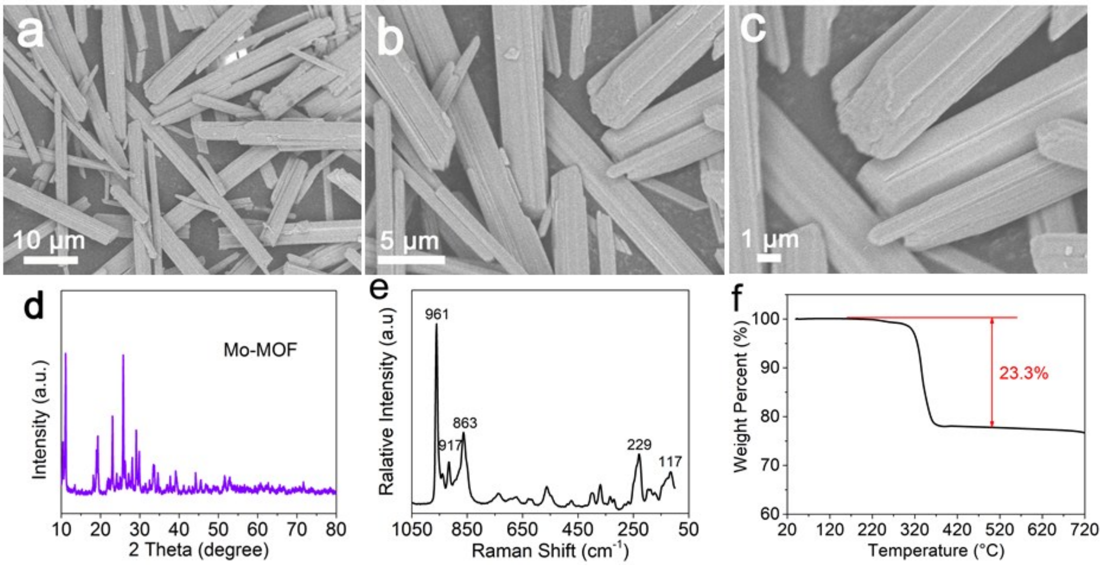

Fig. S1 (a-c) FESEM images, (d) XRD patterns, (e) Raman spectra and (f) thermogravimetric analysis (TGA) of Mo-based MOF.

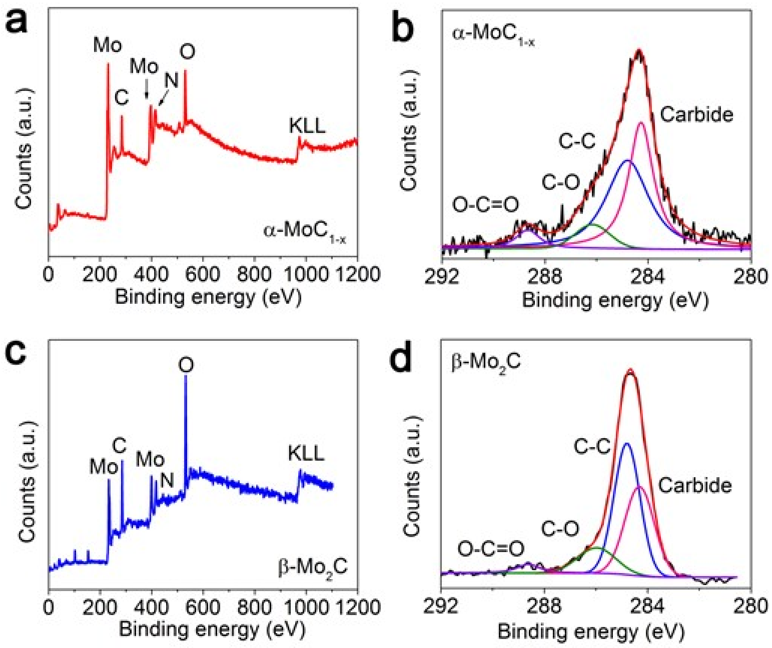

Fig. S2 XPS survey spectrum of (a) α-MoC_{1-x} and (c) β-Mo_2C. XPS high resolution scans of C 1s electrons of (b) α-MoC_{1-x} and (d) β-Mo_2C.

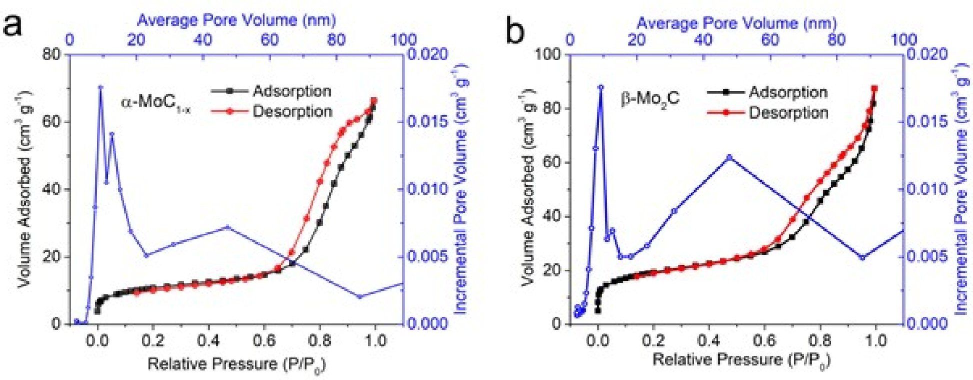

Fig. S3 Nitrogen physisorption (adsorption/desorption) isotherms and BJH adsorption pore distribution curves of (a) α-MoC_{1-x} and (b) β-Mo_2C.

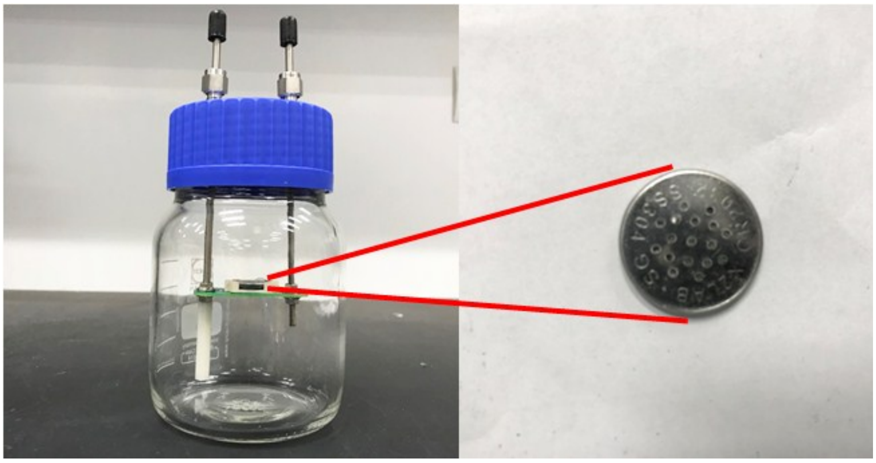

Fig. S4 Set up of Li-O_2 batteries. The batteries are assembled with coin-type of cell.

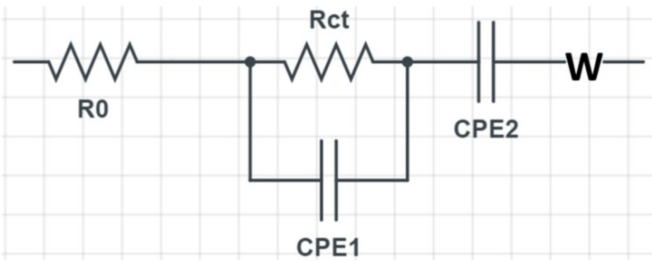

Fig. S5 The equivalent electrical circuit for impedance analysis.

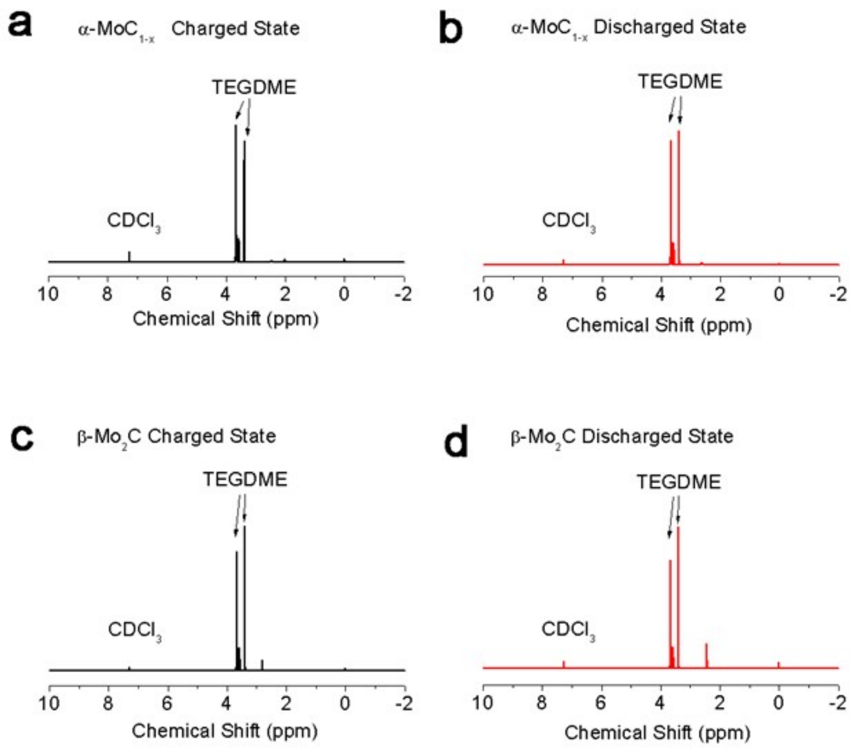

Fig. S6 ^{1}H NMR spectra of α-MoC_{1-x} charged state (a) and (b) discharged state. ^{1}H NMR spectra of β-Mo_2C charged state (a) and (b) discharged state.

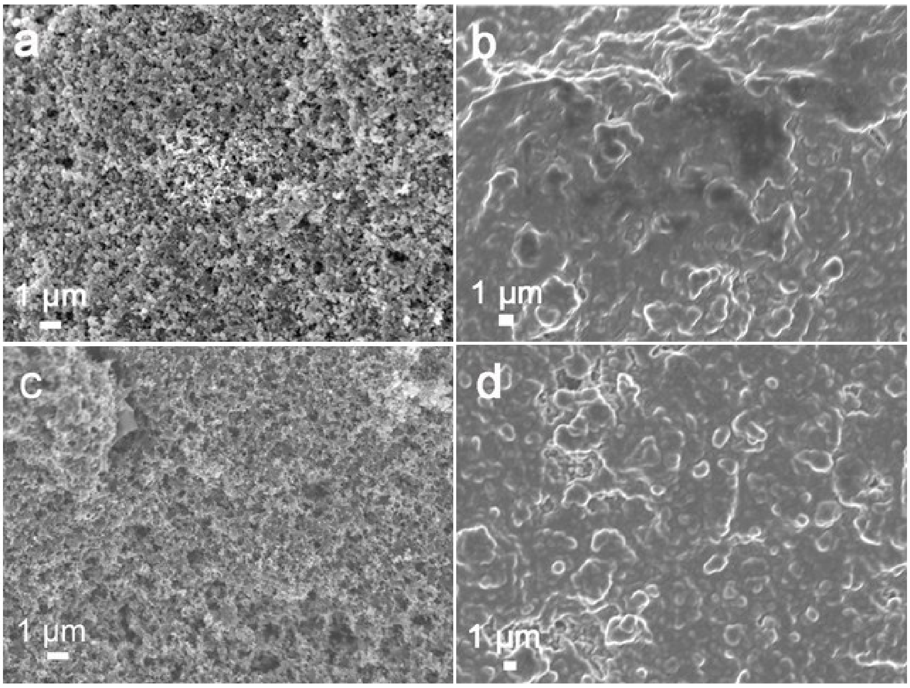

Fig. S7 FESEM images of pristine and discharged α-MoC_{1-x} (a and b) andβ-Mo_2C (c and d).

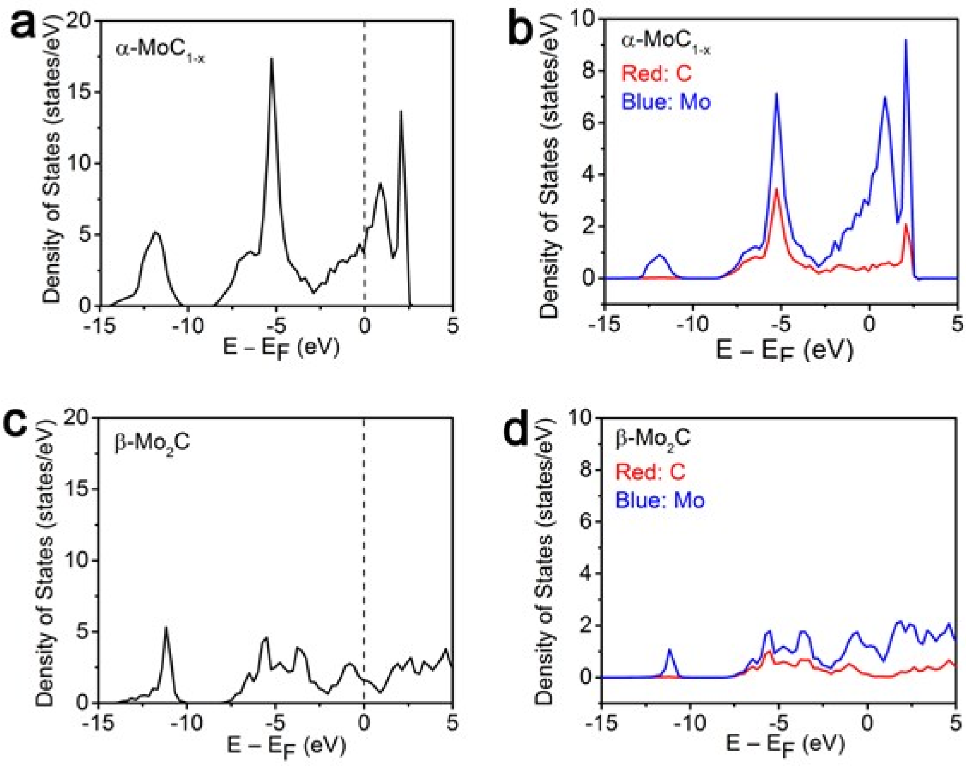

Fig. S8 The total and projected density of states (TDOS and PDOS) of bulk crystal α-MoC_{1-x} (a and b) and β-Mo_2C (c and d).

Table S1 Comparison of cyclibility of α-MoC_{1-x} with other well-performed electrocatalysts for Li-O_2 batteries.

	Electrolyte	Cut-off capacity (mA h g^{-1})	Number of cycles before dead	Charge voltage at 500 mA h g^{-1} (V)	References
TiC-C		500	80 cycles		Chem. Commun., 2016, 52, 2713
Carbon black		500	23	> 4.5	Chem. Commun., 2016, 52, 2713
TiC	TEGDME	500	25	Die at ~530 mAh g^{-1}	Nat. Mater., 2013, 12, 1050
TiC	DMSO	350	100	N.A	Nat. Mater., 2013, 12, 1050
$NiCo_2O_4$	TEGDME	500	50	~ 4.5	J. Mater. Chem. A, 2014, 2, 12053
Graphitic Porous Carbon−Co_3O_4	TEGDME	500	50	4.4	ACS Appl. Mater. Interfaces 2016, 8, 2796
Au–Pt core–shell	TEGDME	1000	20	4.1	J. Mater. Chem. A, 2014, 2, 10676
RuO_2@RGO	TEGDME	1000	50	4.0	J. Mater. Chem. A, 2016, 4, 2403–2407
p-CNT/Co_3O_4	TEGDME	500	115	> 4.5	J. Mater. Chem. A, 2017, 5, 25501
α-MoC_{1-x}		**1000**	**100**	**4.2**	**This work**

Table S2 Fitted values for equivalent circuit elements by simulation of electrochemical impedance spectroscopy in Fig. S4.

Cathode catalyst	R_0		R_{ct}	
	Initial	After cycling	Initial	After cycling
α-MoC_{1-x}	30.96	41.26	395.8	399.4
β-Mo_2C	31.11	44.2	627.9	734.0