Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting information

Plasma-Enhanced Cycling Durability of a Mo_2C Decorated N-doped Carbon Nanofiber Electrocatalyst for Li-O_2 Battery Cathode

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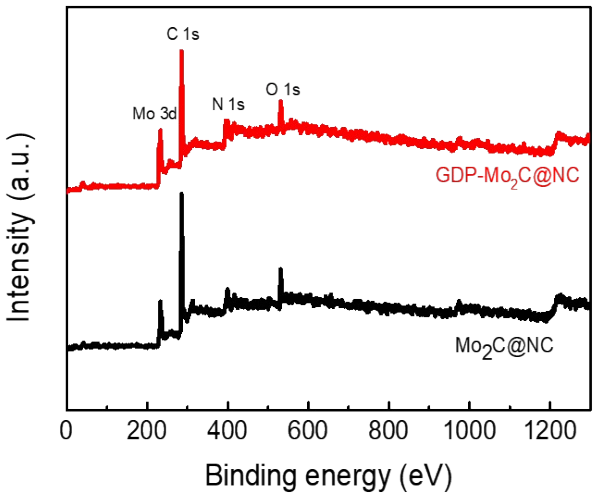

Figure S1. The survey XPS profiles of GDP-Mo_2C@NCF and Mo_2C@NCF

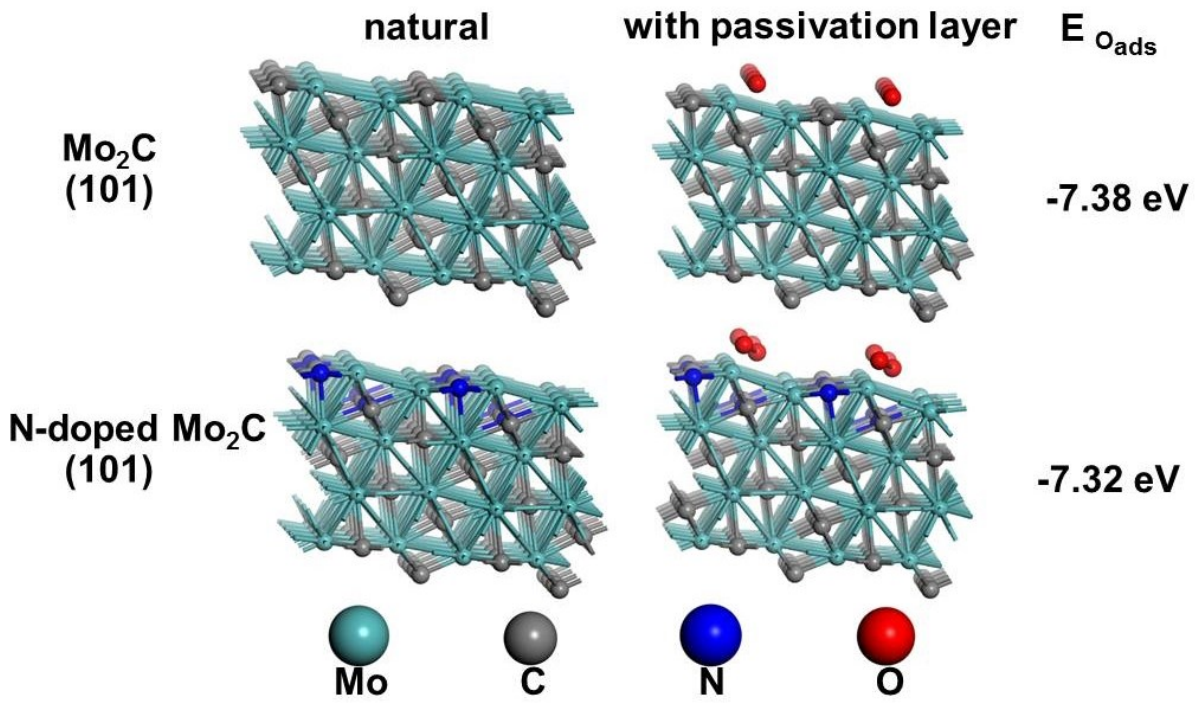

Figure S2. Optimized structure and E_{Oads} of O_2 adsorption to generate passivation layer on (101) surface of both Mo_2C and N-doped Mo_2C.

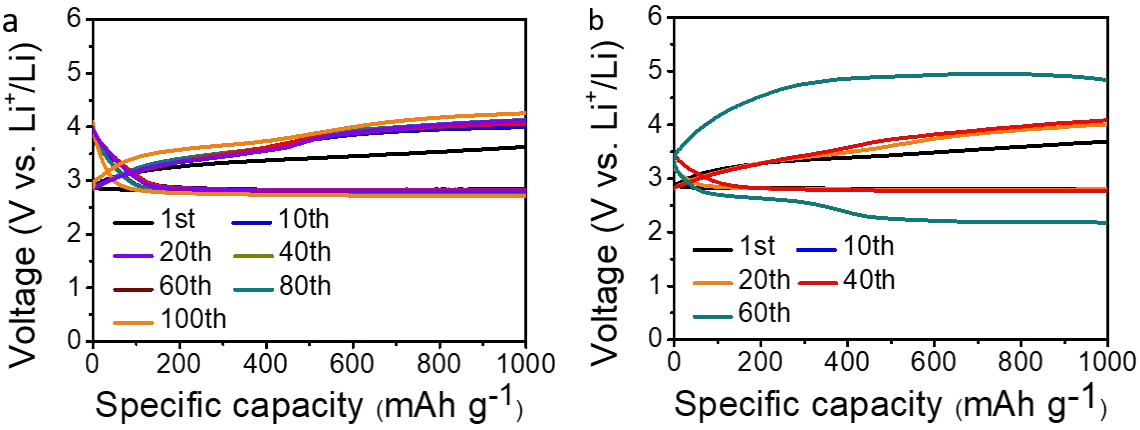

Figure S3. Cycling satbility of GDP-Mo_2C@NCF (a) and Mo_2C@NCF (b) -based LOBs.

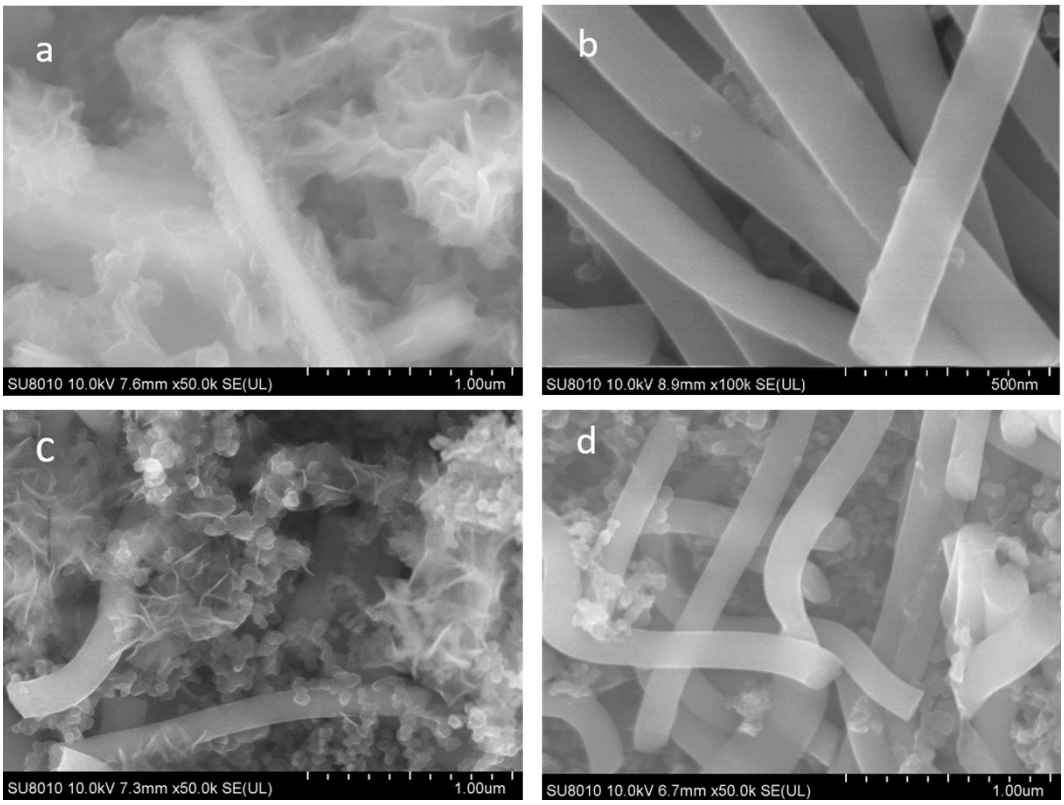

Figure S4. SEM images of GDP-Mo_2C@NCF-based cathode at (a) 10^{th} discharge state, (b) 10^{th} charge state, SEM images of Mo_2C@NCF-based cathode (c) 10^{th} discharge state, (d) 10^{th} charge state.

Table S1. Summary of calculated parameters of energy of forming native passivation layer on different lattic planes of Mo_2C and N-doped Mo_2C.

Lattice plane	E1 (eV)	E2 (eV)	E3 (eV)	E_{Oads} (eV)
Mo_2C (001)	-25089.25809	-25966.92036	-868.046429	-9.615841
N-doped Mo_2C (001)	-25322.54341	-26198.69060	-868.046429	-8.100761
Mo_2C (101)	-33460.99523	-34336.42657	-868.046429	-7.384911
N-doped Mo_2C (101)	-33694.38875	-34569.75360	-868.046429	-7.318421

Notes:

E1: energy of lattice plane before O_2 adsorption

E2: energy of lattice plane after O_2 adsorption

E3: energy of O_2 molecule

E_{Oads}: energy of forming native passivation layer

Table S2. Comparison of battery performance of GDP-Mo_2C@NCF with other reported electrodes.

Catalyst	Current density ($mA\ g^{-1}$)	Fixed capacity ($mAh\ g^{-1}$)	Voltage gap at 1st cycle (V)	Cycle times	Discharge capacity ($mAh\ g^{-1}$)	Rf.
Co-N-CNT/CNF	200	500	1.5	130+	11512.4	[1]
Fe /FeC_3 /NC	0.1 mA cm^{-1}	800	0.65	30+	7150.0	[2]
MoN/N-C	0.1 mA cm^{-1}	400	1.3	30+	1400.0	[3]
TiC-C	100	500	1.25	90+	3460.0	[4]
α-MoC_{1-X}	100	1000	1.43	100+	20212.0	[5]
W_2C@NC	200	500	1.6	55+	10976.0	[6]
MoS_2 /AuNP	300	1000	1.7	50+	3576.0	[7]
HMCN	200	600	1.55	161+	3100.0	[8]
GDP-Mo_2C@NCF	100	1000	0.61	105+	7468.3	this work

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