Supporting information for

Molybdenum Oxynitride Nanoparticles on Nitrogen-Doped CNT Architectures for Oxygen Evolution Reaction

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Density functional theory (DFT) calcualtion

The atomic simulation environment (ASE) software package with GPAW calculator and Perdew-Burke-Ernzerhof (PBE) functional were utilized to compute the exchange-correlation energy[1-3]. The cell parameters of MoO_2 were obtained from the inorganic crystal structure database (ICSD)[4]. From the initial cell parameters, the model of N-MoO_2 (100) was constructed with the surface layer of Mo_4O_8 and atomic locking on the lower layer. The model was set up in a 15 Å vacuum atmosphere without interference. The K point was established in the Brillouin region by using the 4*4*1 monkhorst-pack mesh and the cutoff energy of plane wave was set to 400 eV.[5] The final structure was confirmed when the maximum atomic force was lower than 0.05 eV/A. The Gibbs free energy of the catalysts was calculated following $\Delta G = \Delta E + \Delta ZPE - T\Delta S$ including zero-point energies (ZPE) and entropy contribution adsorbates. The simulated temperature was 298.15 K, and the Gibbs free energy near N and Mo atoms of the same model was calculated and compared.

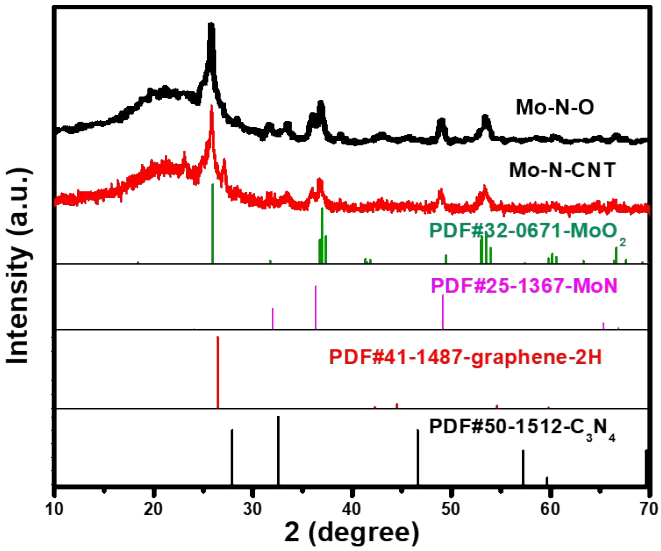

Fig. S1 XRD spectra of Mo-N-O and Mo-N-CNT; the standard PDF card of MoO_2, MoN, graphene-2H and C_3N_4.

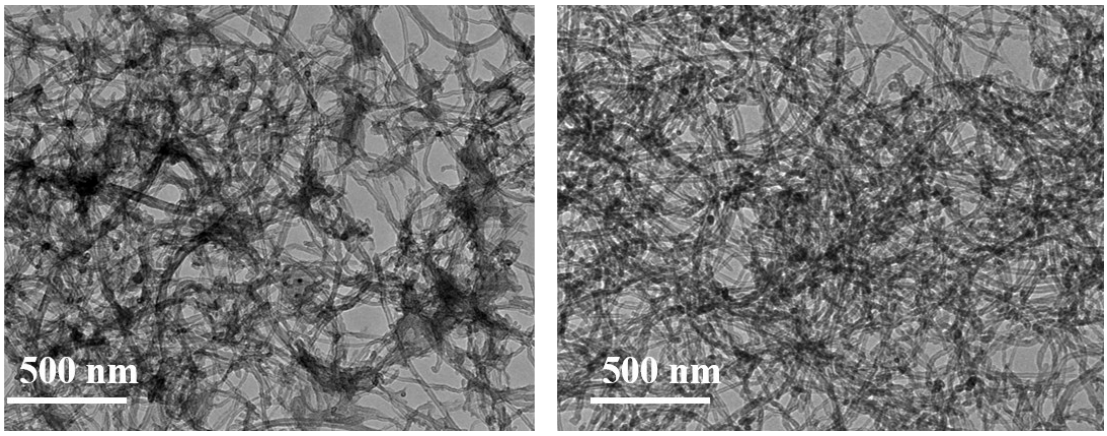

Fig. S2 TEM image of Mo-N-CNT.

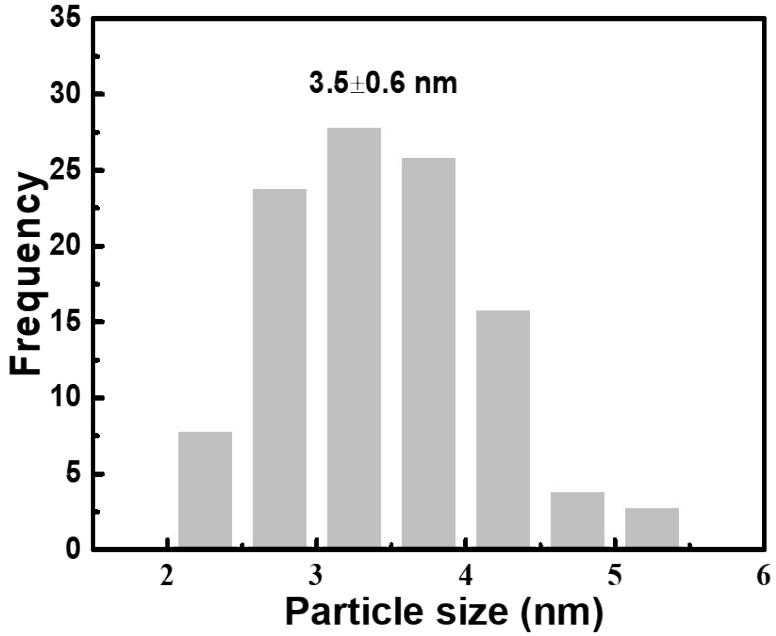

Fig. S3 The size distribution of MoN nanoparticles.

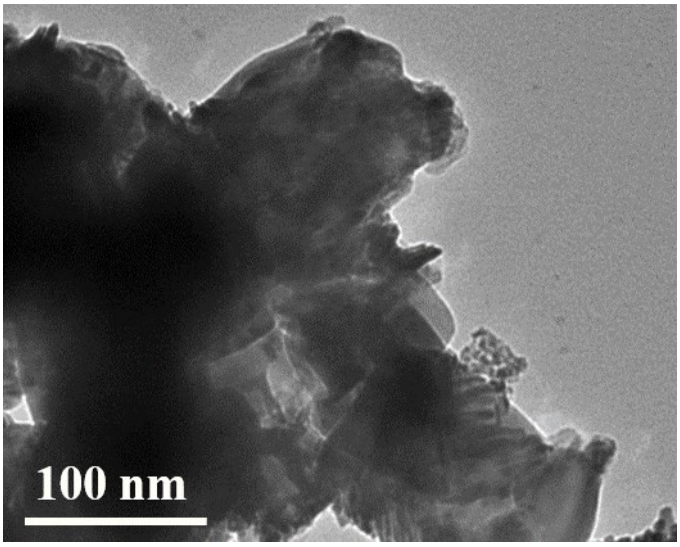

Fig. S4 TEM image of Mo-N-O.

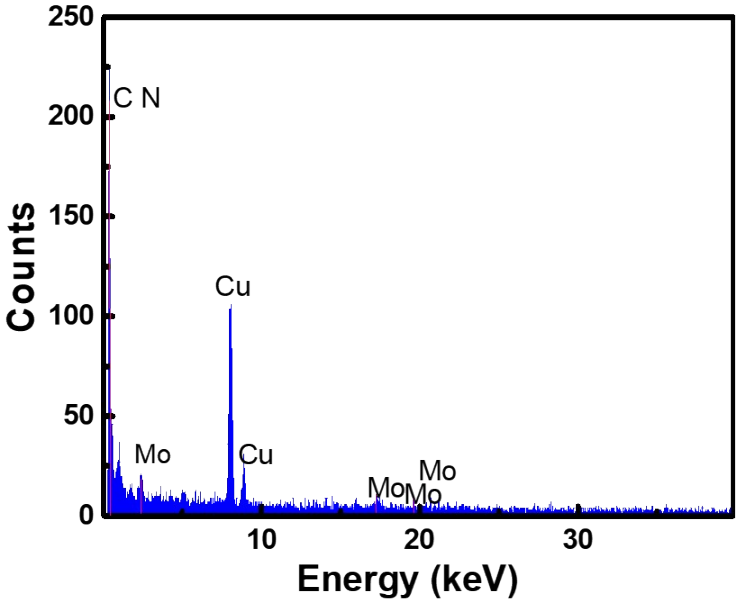

Fig. S5 The overview EDX of Mo-N-CNT.

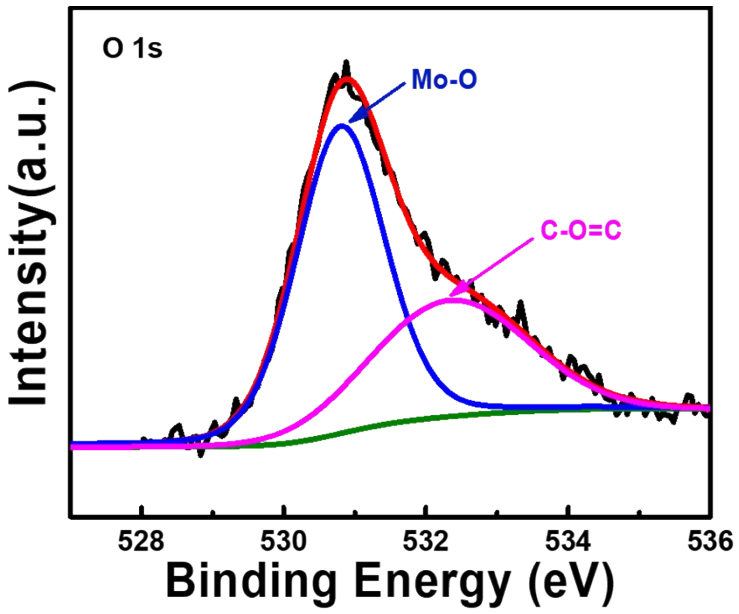

Fig. S6 The XPS of O 1s for Mo-N-CNT.

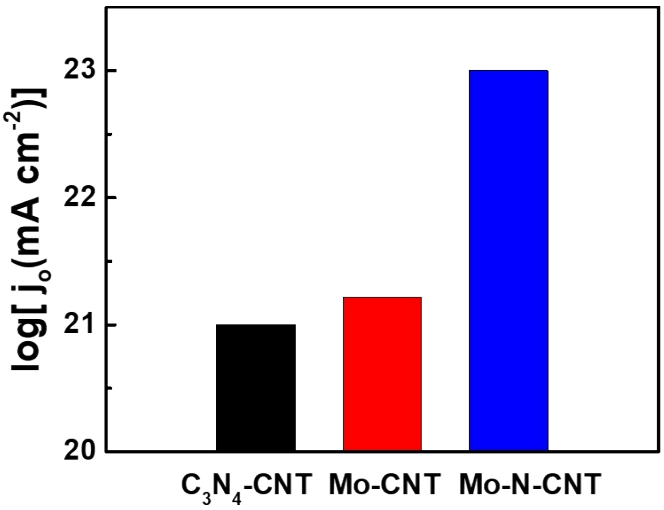

Fig. S7 The exchange current density of C_3N_4-CNT, Mo-CNT and Mo-N-CNT.

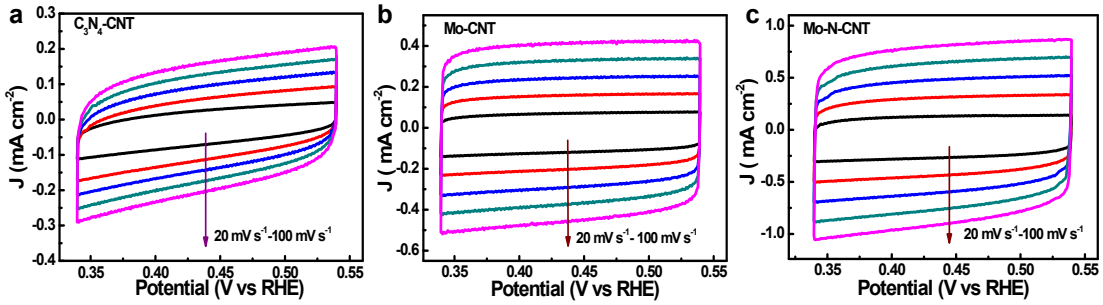

Fig. S8 Cyclic voltammetry (CV) curves of (a) C_3N_4-CNT (b) Mo-CNT and (c) Mo-N-CNT with various scan rates (20-100 mV s^{-1}) in the region of 0.35 to 0.55V vs RHE.

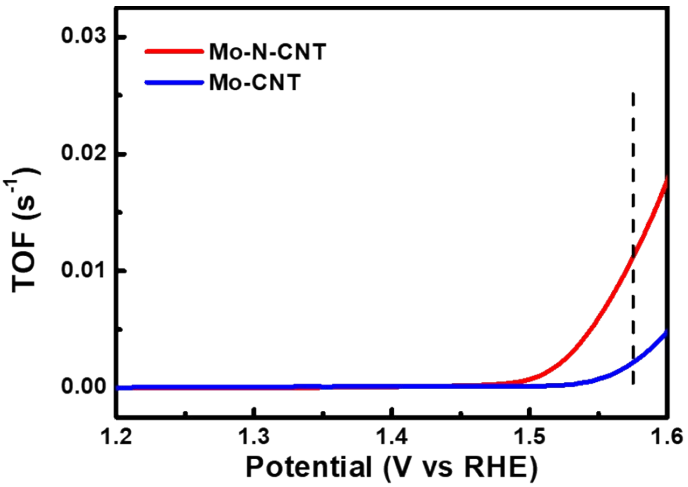

Fig. S9 The turnover frequency value of Mo-N-CNT and Mo-CNT as a function of potential.

The TOF values were calculated from the equation of TOF= (j*A)/(4*F*m). Where j is the current density at overpotential of 0.3 V, A is the surface area of the electrode, F is the Faraday constant (96485 C mol^{-1}), and m is the number of moles of active materials that are deposited onto the electrodes. [6,7]

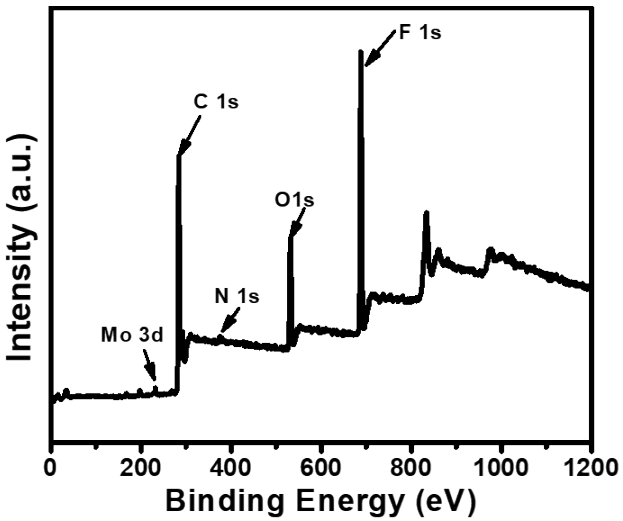

Fig. S10 Full scan XPS spectra of Mo-N-CNT after OER test.

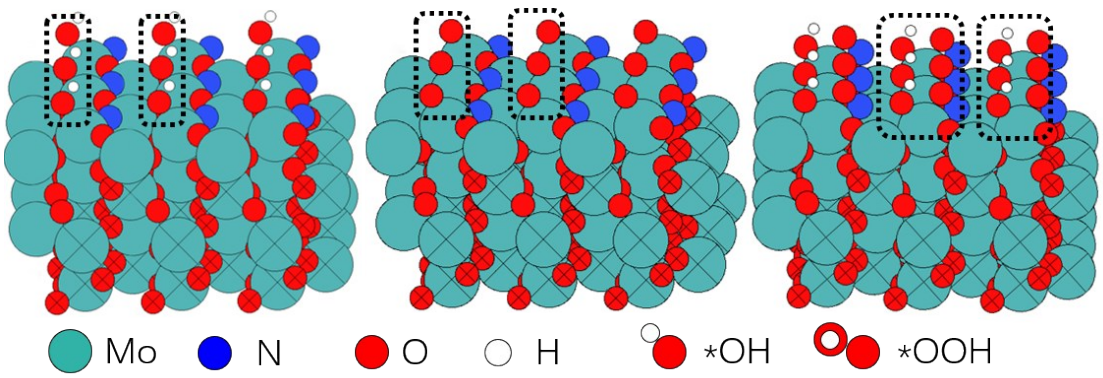

Fig. 11 The calculation modeling of Mo-N-CNT with the adsorption of *OH, *O, *OOH at the N sites.

Table S1. The atomic ratio of Mo-N-CNT.

	C	O	Mo	N
at%	93.71	4.46	1.02	0.8

Table S2. A comparison of the electrocatalytic performance of Mo-N-CNT with recently reported similar highly active materials in alkaline media.

Electrocatalyst	Electrolyte	OER η(mV) at 10 mA cm^{-2}	Ref.
Mo-N-CNT	1 M KOH	350	This work
Mo–N/C@MoS_2	1 M KOH	390	[8]
Co-N/C/CNT	1 M KOH	372	[9]
Co_4Mo_2@NC	10 M KOH	330	[10]
g-C_3N_4@carbon	0.1 M KOH	365	[11]
TCCN	0.1 M KOH	365	[12]
3D g-C_3N_4 NS–CNT	0.1M KOH	360	[13]
$CoFe_2O4$/graphene	0.1 M KOH	464	[14]
Co_3O_4 /mMWCNT	0.1 M KOH	390	[15]
Co_3S_4/NCNTs	0.1 M KOH	430	[16]
plasma-engraved Co_3O_4	0.1 M KOH	353	[17]
Co_4N/carbon cloth	1 M KOH	257	[18]

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