Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Nitrogen-doped carbon encapsulating γ-MoC/Ni heterostructures for efficient oxygen evolution electrocatalysts

Xueping Zhang,[a,b] Liang Huang,[a,b] Yujie Han,[a,b] Miao Xu,[a,b] and Shaojun Dong*[,a,b]

[a]State Key Laboratory of Electroanalytical Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P.R.China

[b]University of Chinese Academy of Sciences, Beijing 100049, P.R.China

E-mail: dongsj@ciac.ac.cn

Table S1. The preparation parameters for different samples.

Samples	Melamine (mmol)	$(NH_4)_6Mo_7O_{24}\cdot 4H_2O$ (mmol)	$NiCl_2\cdot 6H_2O$ (mmol)
$Ni_{2.0}Mo_0$@NC	6.0	0	2.0
$Ni_0Mo_{0.26}$@NC	6.0	0.26	0
$Ni_{2.0}Mo_{0.13}$@NC	6.0	0.13	2.0
$Ni_{2.0}Mo_{0.26}$@NC	6.0	0.26	2.0
$Ni_{2.0}Mo_{0.39}$@NC	6.0	0.39	2.0

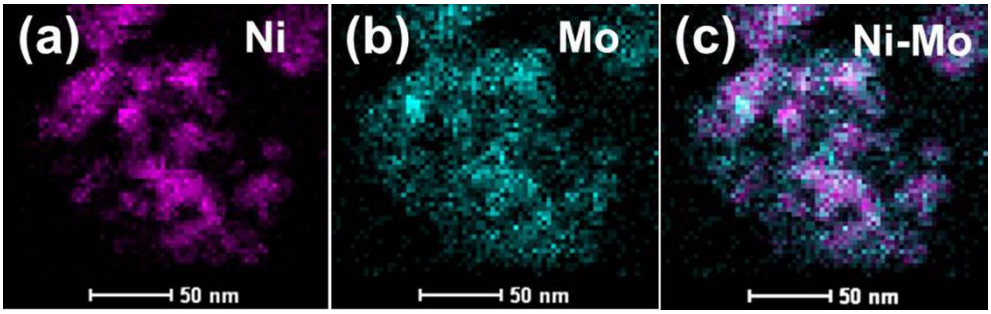

Fig. S1 The elemental mapping images for Ni (a), Mo (b), and their combined image (c).

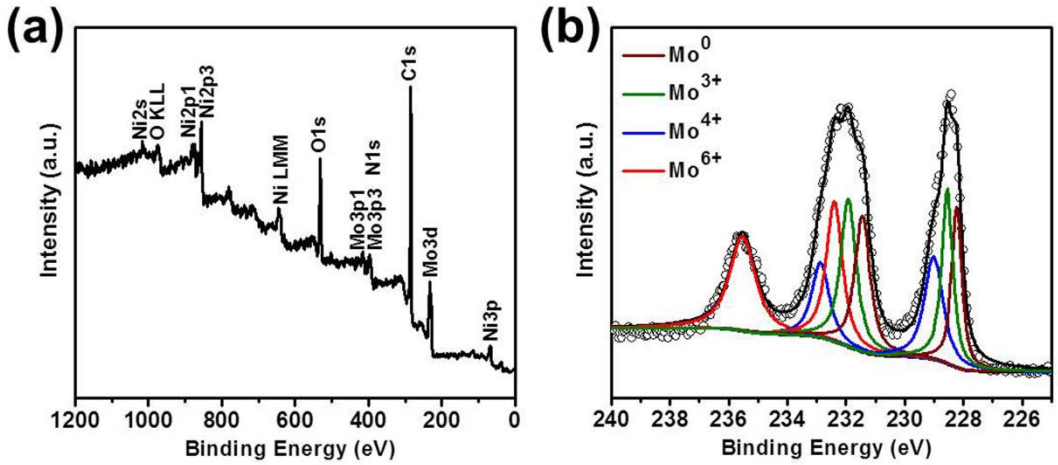

Fig. S2 (a) XPS survey spectrum and (b) high-resolution XPS spectrum of Mo 3d for sample $Ni_{2.0}Mo_{0.26}$@NC.

Table S2. Element contents (wt%) of different samples analyzed by XPS.

Sample	Mo/XPS	Ni/XPS	C/XPS	N/XPS	O/XPS
$Ni_{2.0}Mo_0$@NC	0	2.54	88.89	3.42	5.14
$Ni_0Mo_{0.26}$@NC	13.13	0	67.30	3.93	15.64
$Ni_{2.0}Mo_{0.26}$@NC	16.40	5.85	55.14	3.39	19.22
$Ni_{2.0}Mo_{0.13}$@NC	11.39	4.61	64.31	4.06	15.63
$Ni_{2.0}Mo_{0.39}$@NC	19.42	5.68	54.36	3.24	17.30

Table S3. Element contents (wt%) of different samples analyzed by ICP-AES and element analysis.

Sample	Mo/ICP	Ni/ICP	C/Element	N/Element	H/Element
$Ni_{2.0}Mo_0$@NC	0	58.76	36.04	2.01	0.495
$Ni_0Mo_{0.26}$@NC	71.14	0	11.24	1.80	0.796
$Ni_{2.0}Mo_{0.26}$@NC	43.07	30.96	21.79	2.91	0.251
$Ni_{2.0}Mo_{0.13}$@NC	34.27	33.53	32.39	3.36	0.391
$Ni_{2.0}Mo_{0.39}$@NC	48.54	28.48	18.25	2.97	0.232

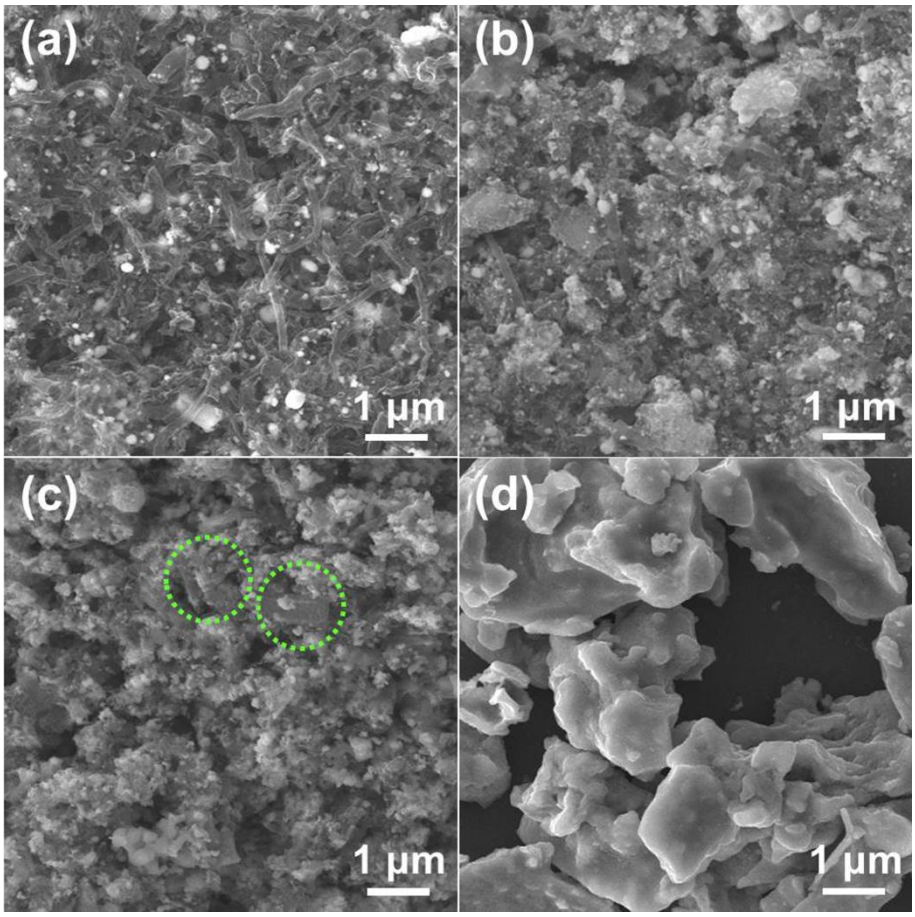

Fig. S3 SEM images of sample (a) $Ni_{2.0}Mo_0$@NC, (b) $Ni_{2.0}Mo_{0.13}$@NC, (c) $Ni_{2.0}Mo_{0.39}$@NC, and (d) $Ni_0Mo_{0.26}$@NC.

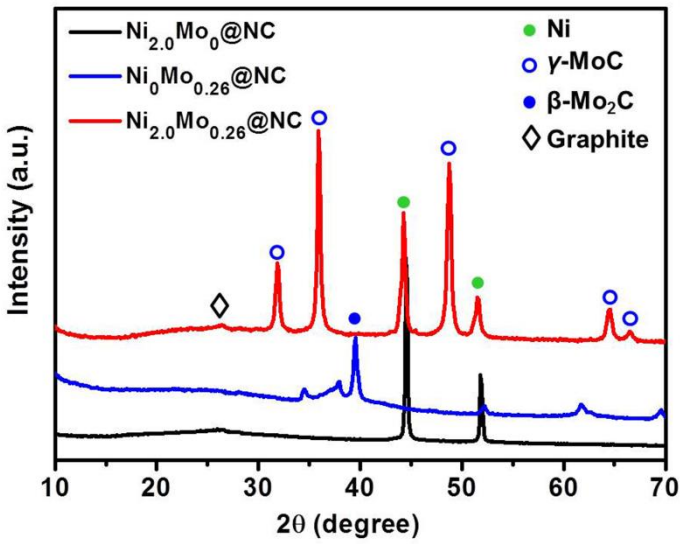

Fig. S4 XRD patterns of sample $Ni_{2.0}Mo_0$@NC, $Ni_0Mo_{0.26}$@NC and $Ni_{2.0}Mo_{0.26}$@NC.

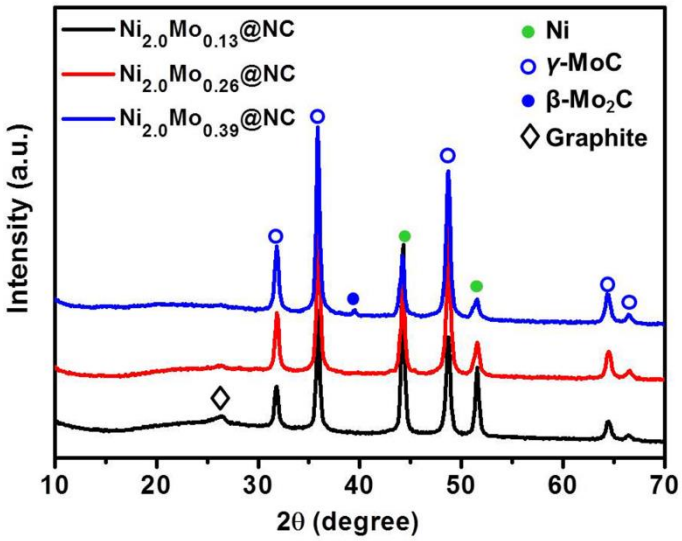

Fig. S5 XRD patterns of sample $Ni_{2.0}Mo_{0.13}$@NC, $Ni_{2.0}Mo_{0.26}$@NC and $Ni_{2.0}Mo_{0.39}$@NC.

.

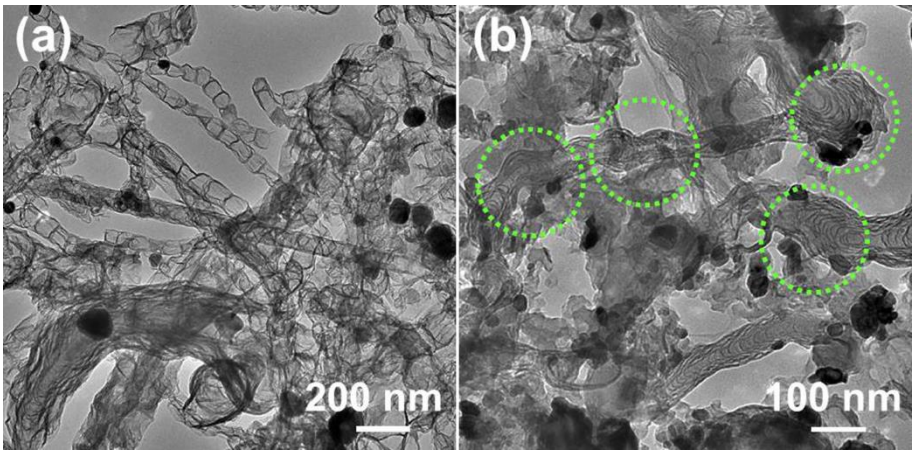

Fig. S6 TEM images of sample (a) $Ni_{2.0}Mo_0$@NC and (b) $Ni_{2.0}Mo_{0.13}$@NC.

Table S4. Comparison of the OER electrocatalytic performance for different catalysts.

Catalysts	Electrolyte	Overpotential (mV) at 10 mA/cm^2	Reference
$Ni_{2.0}Mo_{0.26}$@NC	**1 M KOH**	**310**	**This work**
Ni nanoparticles/N-doped graphene	0.1 M KOH	320	*Energy Environ. Sci.*, 2013, 6, 3693
α-$Ni(OH)_2$ nanocrystals	0.1 M KOH	331	*J. Am. Chem. Soc.*, 2014, 136, 7077
NiFe-LDH nanosheets	1 M KOH	300	*Nat. commun.*, 2014, 5, 4477
NiCo LDH nanoplates	1 M KOH	367	*Nano Lett.*, 2015, 15, 1421
NiO-TiO_2 nanosheet	1 M KOH	320	*J. Am. Chem. Soc.*, 2016, 138, 6517
Ni^{2+}/birnessite	1 M KOH	400	*Angew. Chem. Int. Ed.* 2016, 55, 10381
$FeNiS_2$ nanosheets	0.1 M KOH	310	*Nano Energy* 2016, 27, 526
$NiFe_2O_4$ nanoparticles/ α-$Ni(OH)_2$ nanosheet	0.1 M NaOH	340	*J. Power Sources* 2016, 324, 499
rGO/(Ni^{2+}/THPP/Co^{2+}/THPP)n	1 M KOH	330	*Chem. Sci.*, 2016, 7, 5640

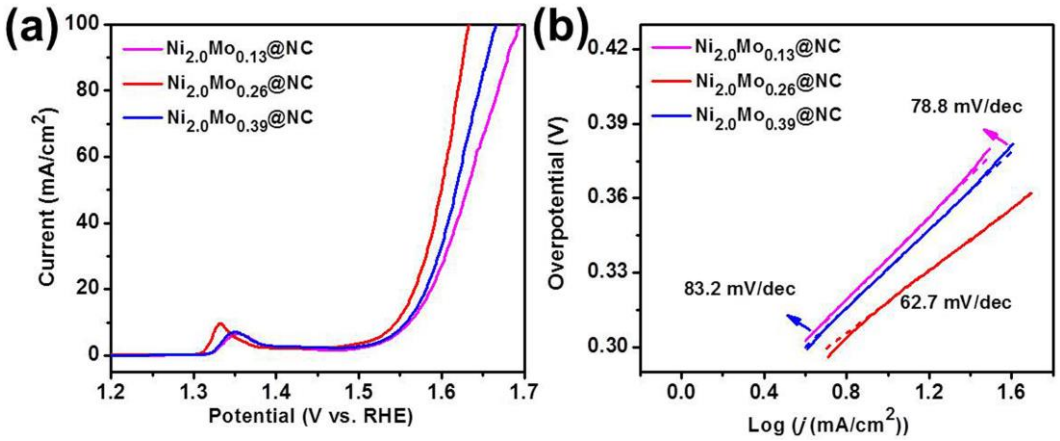

Fig. S7 (a) LSV plots for different samples after *iR* compensation in 1 M KOH at a scan rate of 5 mV s^{-1} and a rotating speed of 1600 rpm. (b) Corresponding Tafel plots.

Table S5. Comparison of the OER electrocatalytic performance for different samples.

Sample	Onset overpotential (mV)	Overpotential (mV) at 10 mA/cm^2	TOC (s^{-1})
$Ni_{2.0}Mo_{0.13}$@NC	275	332	0.0054
$Ni_{2.0}Mo_{0.26}$@NC	240	310	0.012
$Ni_{2.0}Mo_{0.39}$@NC	270	328	0.0086

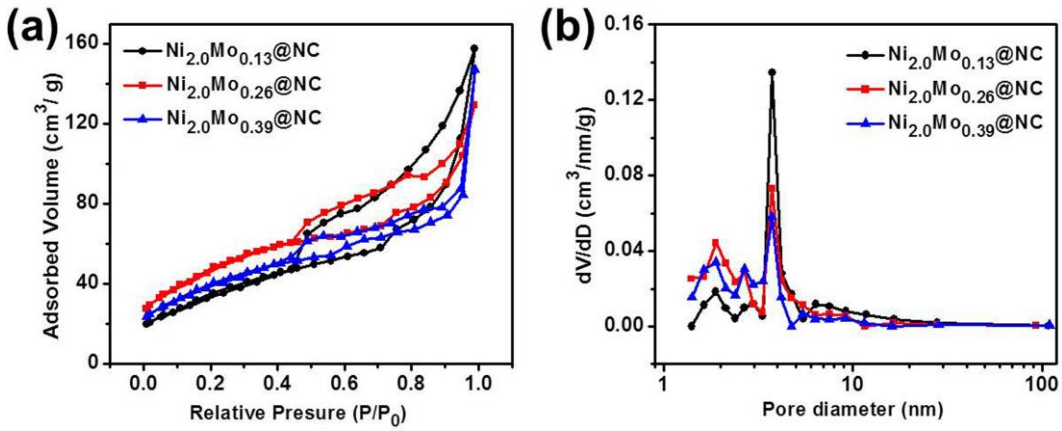

Fig. S8 (a) Nitrogen adsorption and desorption isotherm and (b) BJH pore distribution of sample $Ni_{2.0}Mo_{0.13}$@NC, $Ni_{2.0}Mo_{0.26}$@NC and $Ni_{2.0}Mo_{0.39}$@NC.

Table S6. The N_2 sorption data for different samples.

Sample	S_{BET} ($m^2\ g^{-1}$)	V_{total} ($cm^3\ g^{-1}$)	$V_{micropore}$ ($cm^3\ g^{-1}$)	$PD_{average}$ (nm)
$Ni_{2.0}Mo_{0.13}$@NC	129.7	0.23	0.009	3.75
$Ni_{2.0}Mo_{0.26}$@NC	172.0	0.29	0.032	3.74
$Ni_{2.0}Mo_{0.39}$@NC	143.2	0.25	0.023	3.74

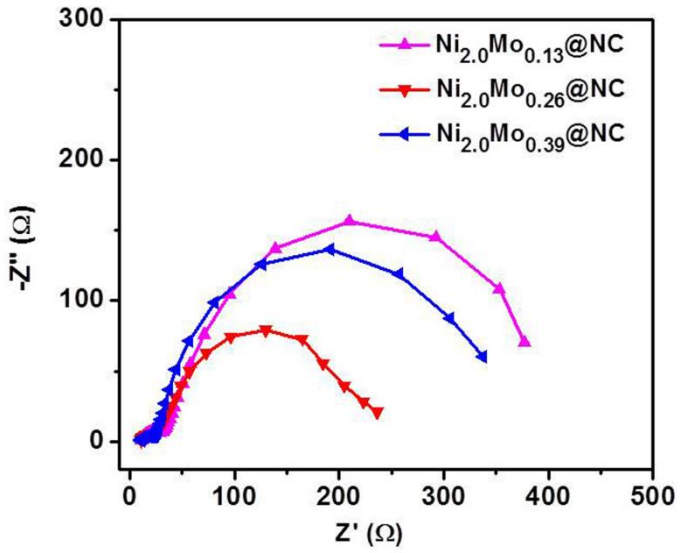

Fig. S9 EIS plots of sample $Ni_{2.0}Mo_{0.13}$@NC, $Ni_{2.0}Mo_{0.26}$@NC and $Ni_{2.0}Mo_{0.39}$@NC.