Supporting Information for

Sulfur, phosphorus and iron codoped nickel oxide as efficient catalyst for oxygen evolution reaction

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Part I

The detailed position coordinates of the optimized structure of S,P-NiO(Fe)/CC in form of fractional coordinates.

S,P-NiO(Fe)/CC

1.0

8.9447965622	0.0000000000	0.0000000000
0.0000000000	8.9447965622	0.0000000000
0.0000000000	0.0000000000	18.3249282837

O	P	S	Fe	Ni
33	2	1	1	35

Direct

0.334059000	0.000038000	0.026110999
0.998816013	0.332670003	0.246610999
0.169551998	0.165876999	0.139504999
0.155638993	0.142157003	0.364196986
0.669275999	0.996227026	0.026393000
0.338248998	0.334654003	0.242799997
0.502976000	0.164605007	0.139203995
0.998696983	0.995806992	0.025504000
0.670969009	0.336041987	0.240618005
0.839899004	0.162696004	0.138827994
0.852518976	0.149902001	0.366712004
0.333476990	0.331034005	0.026303001
0.995151997	0.662419975	0.243395001
0.172172993	0.500586987	0.138786003
0.165821001	0.510258019	0.368901998
0.663815022	0.331261992	0.024394000
0.325046986	0.676060975	0.249640003
0.503292978	0.500248015	0.138358995
0.998392999	0.331735998	0.026699999
0.664466023	0.664273977	0.241693005

0.841261029	0.503261983	0.139090002
0.334500015	0.664550006	0.025796000
0.001333000	0.996353984	0.240908995
0.160722002	0.832893014	0.139575005
0.153871998	0.841077983	0.361981004
0.670261979	0.666599989	0.026611000
0.334760994	0.002198000	0.242081001
0.493443012	0.832791984	0.138808995
0.479847997	0.839399993	0.367911994
0.998220980	0.667864025	0.025645999
0.664337993	0.001877000	0.245938003
0.830614984	0.833140016	0.142699003
0.843289971	0.843815029	0.363368988
0.532238007	0.482098997	0.379909992
0.825201988	0.512214005	0.378870010
0.477394015	0.167830005	0.378834993
0.347775996	0.658315003	0.359717995
0.997501016	0.333404005	0.137895003
0.996037006	0.330745995	0.375512004
0.165637001	0.164704993	0.022304000
0.165384993	0.169138998	0.255739003
0.333359003	0.332682014	0.137406006
0.321498007	0.361472994	0.388348013
0.499599010	0.164767995	0.020637000
0.496749997	0.167705998	0.253919005
0.664162993	0.332439989	0.136953995
0.697947979	0.309338987	0.395166010
0.831743002	0.165101007	0.021203000
0.834053993	0.166628003	0.255602002
0.001201000	0.666751981	0.137529999

0.999481022	0.676307976	0.378555000
0.165089995	0.498522997	0.022430999
0.166547999	0.496302009	0.255843997
0.334632009	0.664844990	0.137391999
0.499273986	0.497752994	0.020771001
0.507185996	0.493743986	0.257212996
0.668404996	0.666674972	0.137399003
0.654972017	0.687918007	0.387403995
0.831071973	0.497350991	0.021271000
0.831339002	0.502121985	0.255741000
0.000246000	0.998652995	0.137562007
0.000544000	0.995905995	0.370660007
0.166215003	0.831377029	0.021697000
0.163059995	0.835058987	0.252099991
0.334217012	0.000685000	0.137204006
0.315176010	0.990350008	0.374386996
0.500261009	0.830857992	0.021516001
0.501465023	0.834789991	0.254736006
0.667577028	0.998687983	0.137248993
0.675152004	0.008275000	0.375611007
0.832889020	0.831416011	0.019479999
0.831268013	0.833796024	0.253901005

Part II Complementary results

Fig. S1

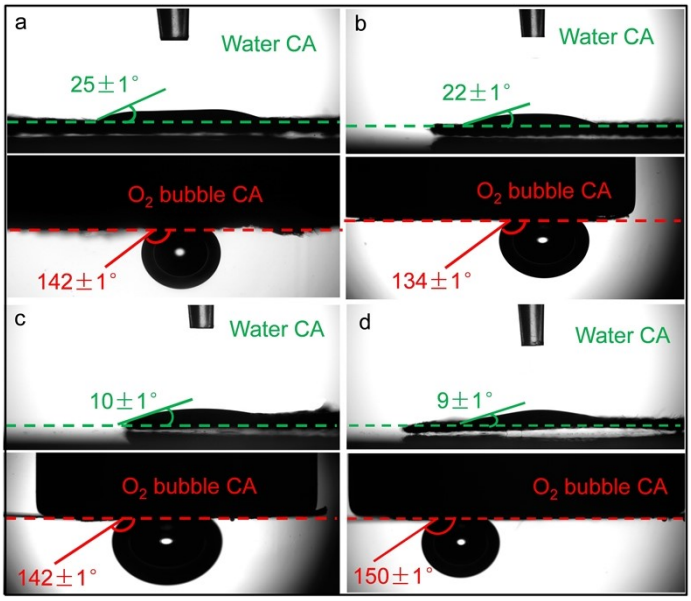

Fig. S1 Water droplet (top) and O_2 bubble (bottom) CAs of (a) S-NiO/CC, (b) S,P-NiO/CC,(c) S-NiO(Fe)/CC, (d) S,P-NiO(Fe)/CC (Measured by three parallel trials, and the CAs were the average value including deviation).

Fig. S2

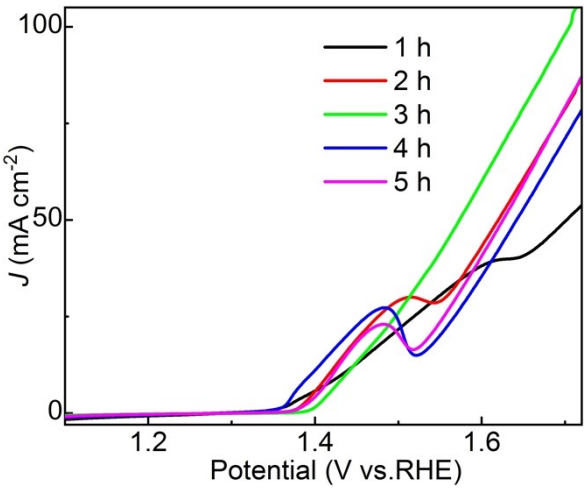

Fig. S2 The LSV of S,P-NiO(Fe)/CC electrodes prepared at different impregnation time in 0.1 M $Fe(NO_3)_3$ solution.

Fig. S3

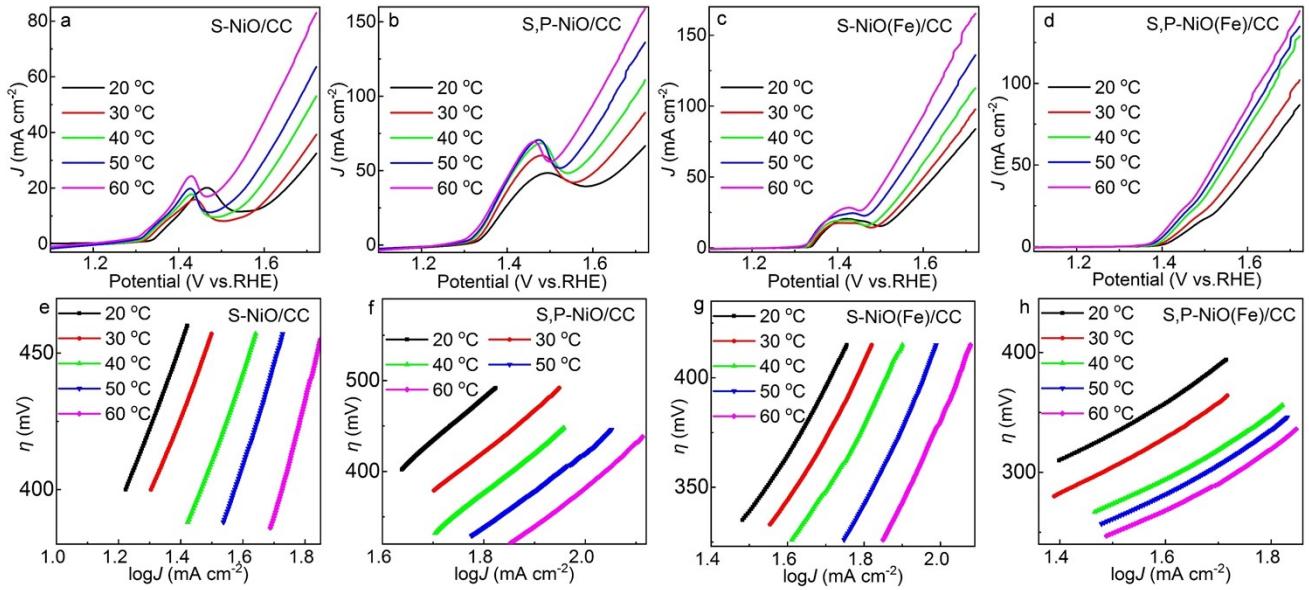

Fig. S3 (a~d) LSVs at 5 mV s^{-1} and (e~h) Tafel slopes of (a,e) S-NiO/CC, (b,f) S,P-NiO/CC, (c,g) S-NiO(Fe)/CC and (d,h) S,P-NiO(Fe)/CC electrodes at different temperatures in 1.0 M KOH.

Fig. S4

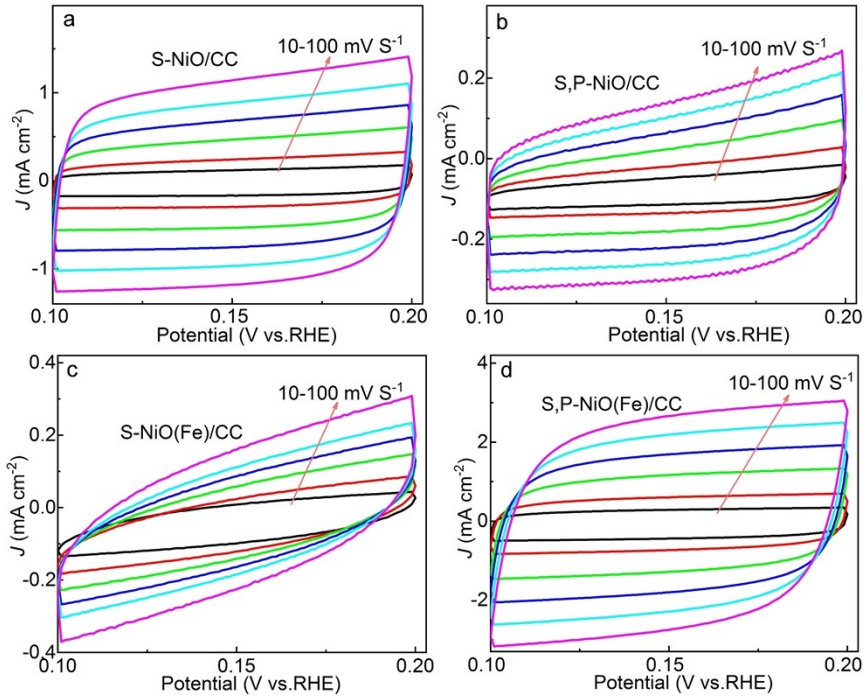

Fig. S4 CV curves of (a) S-NiO/CC, (b) S/P-NiO/CC, (c) S-NiO(Fe)/CC and (d) S/P-NiO(Fe)/CC in non-faradaic region at scan rates of 10~100 mV s^{-1} in 1 M KOH.

Fig. S5

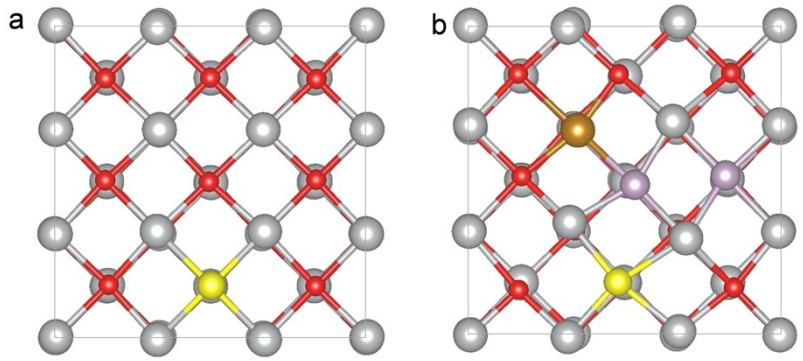

Fig. S5 The optimized crystal structures of (a) S-NiO/CC and (b) S/P-NiO (Fe)/CC.

Fig. S6

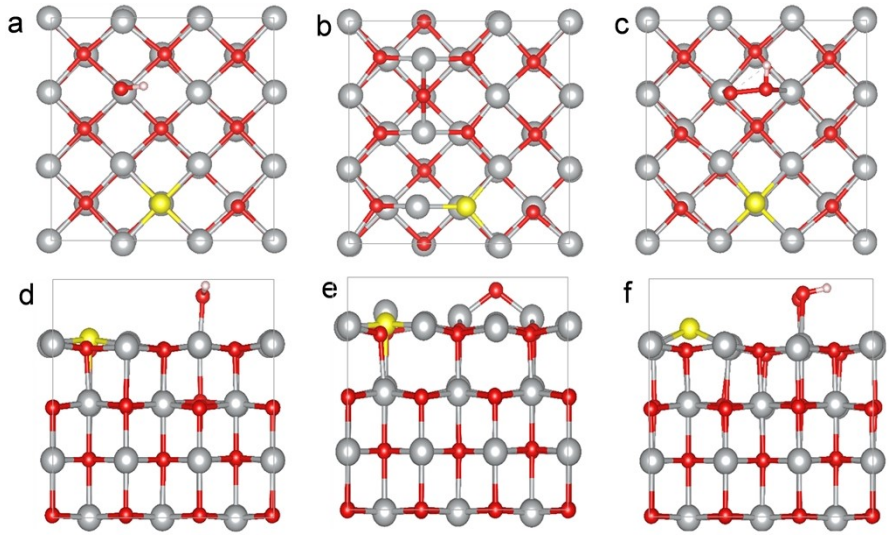

Fig. S6 The optimized structures of S-NiO/CC models for *OH, *O, and *OOH adsorption.

Fig. S7

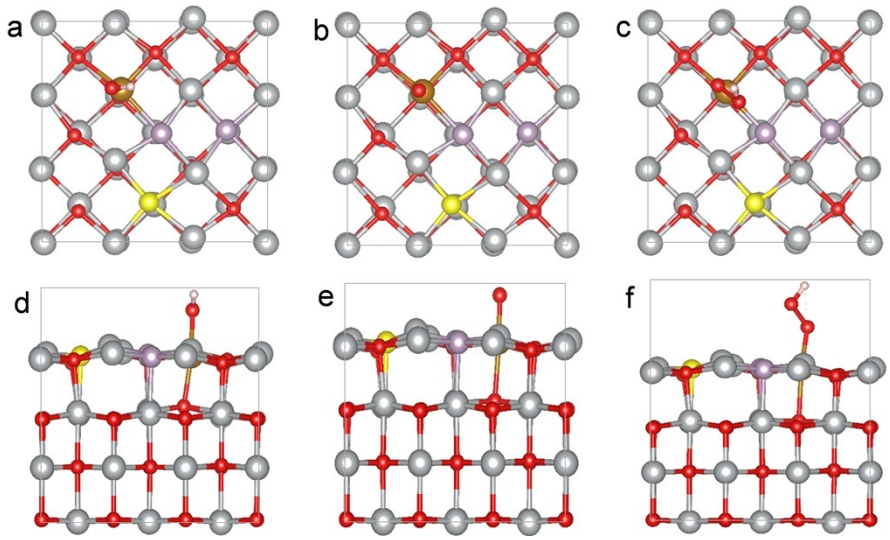

Fig. S7 The optimized structures of S,P-NiO(Fe)/CC models for *OH, *O, and *OOH adsorption.

Fig. S8

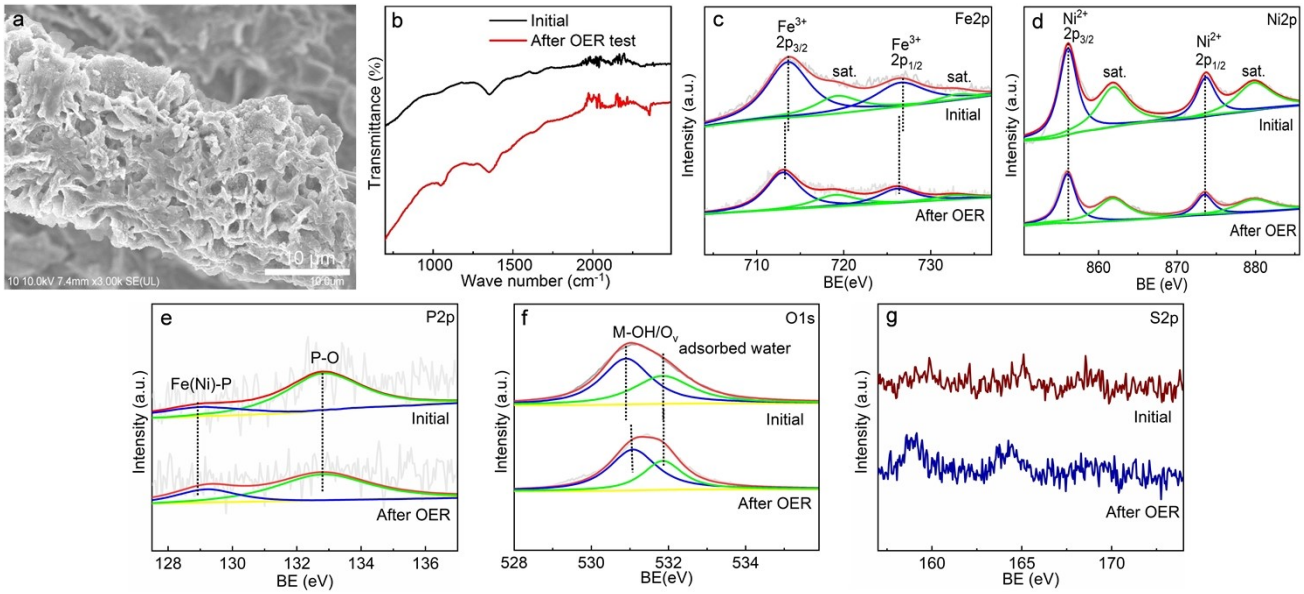

Fig. S8 Post *V-t* (a) SEM, (b) FTIR, (c~g) Fe2p, Ni2p, P2p, O1s and S2p XPS of S/P-NiO(Fe)/CC.

From Fig. S8a, the post *V-t* SEM of S/P-NiO(Fe)/CC exhibits fused flakes and nanoparticles with rough surface, which resembles to its initial morphology, showing the morphological stability undergoes long-term OER operation. In addition, the bending vibration of surface -OH groups at 1354 cm^{-1} maintains unvaried from FTIR (Fig. S8b), also roughly evidencing the unvaried chemical composition of S,P-NiO(Fe)/CC at high potential. The post *V-t* XPS (Figs. S8 c~g) reveal that the BEs of $Fe2p_{3/2}$, $Fe2p_{1/2}$ spin orbitals downshift faintly, while the BEs of Ni2p spin orbitals maintain

unvaried, these outcomes evidence the oxidation values of metal elements are rather stable. From these characterizations, the stable structure of S,P-NiO(Fe)/CC contributes partially to the long-term durabilities for OER and water electrolysis.