Supporting Information

Heteroatoms (P, B, S) incorporated NiFe-based nanocubes as efficient electrocatalysts for oxygen evolution reaction

*Cuijuan Xuan[a], Jie Wang[a], Weiwei Xia[b,c], Jing Zhu[a], Zongkai Peng[a], Kedong Xia[a], Weiping Xiao[a], Huolin L. Xin[b], Deli Wang[a]**

[a] Key laboratory of Material Chemistry for Energy Conversion and Storage (Huazhong University of Science and Technology), Ministry of Education, Hubei Key Laboratory of Material Chemistry and Service Failure, School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology.

[b] Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, USA

[c] SEU-FEI Nano-Pico Center, Key Laboratory of MEMS of the Ministry of Education, Southeast University, Nanjing 210096, China

E-mail: wangdl81125@hust.edu.cn

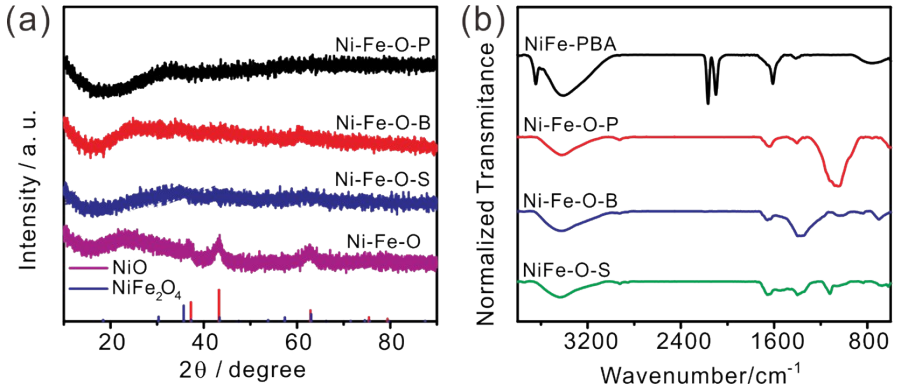

Figure S1 (a) XRD patterns of Ni-Fe-O-P, Ni-Fe-O-B, Ni-Fe-O-S, and Ni-Fe-O. (b) FT-IR spectra of NiFe-PBA, Ni-Fe-O-P, Ni-Fe-O-B, and Ni-Fe-O-S.

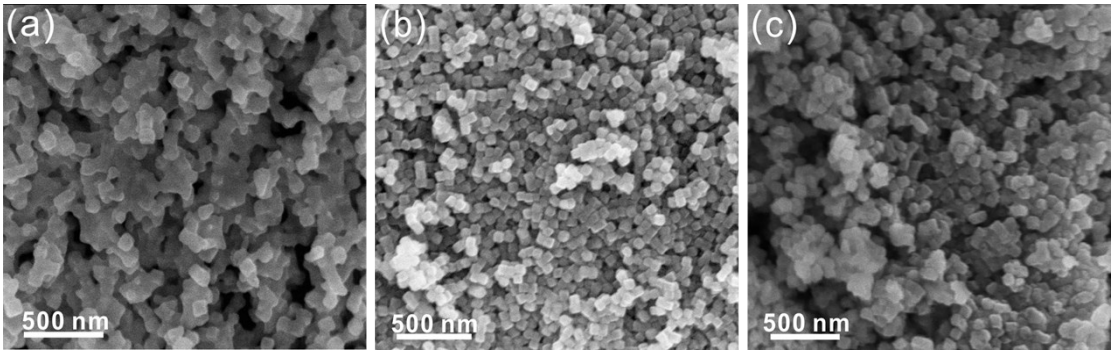

Figure S2 SEM images of Ni-Fe-O-P, Ni-Fe-O-B, and Ni-Fe-O-S.

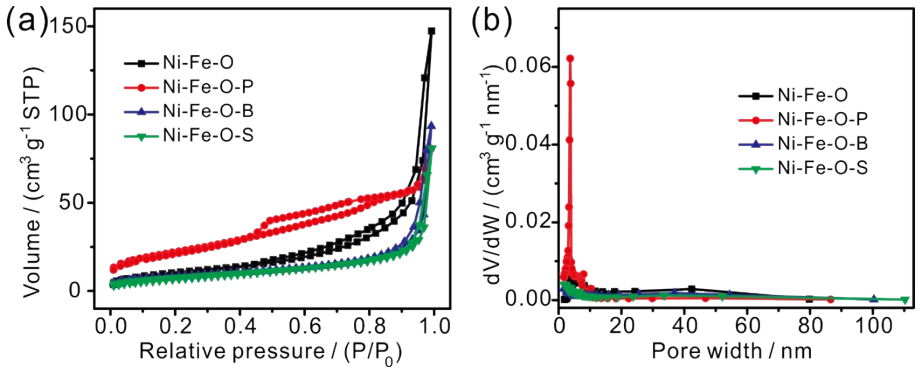

Figure S3 (a) Nitrogen adsorption/desorption isotherms of Ni-Fe-O-P, Ni-Fe-O-B, Ni-Fe-O-S, and Ni-Fe-O, and (b) the corresponding pore size distribution.

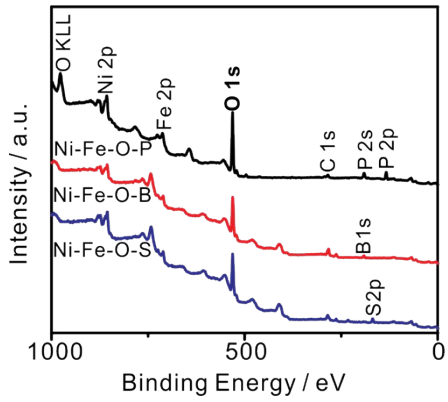

Figure S4 XPS survey spectra of Ni-Fe-O-P, Ni-Fe-O-B, and Ni-Fe-O-S.

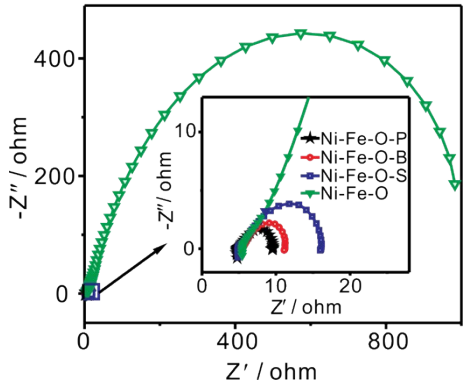

Figure S5 Nyquist plots of Ni-Fe-O-P, Ni-Fe-O-B, Ni-Fe-O-S, and Ni-Fe-O at the potential of 1.5 V.

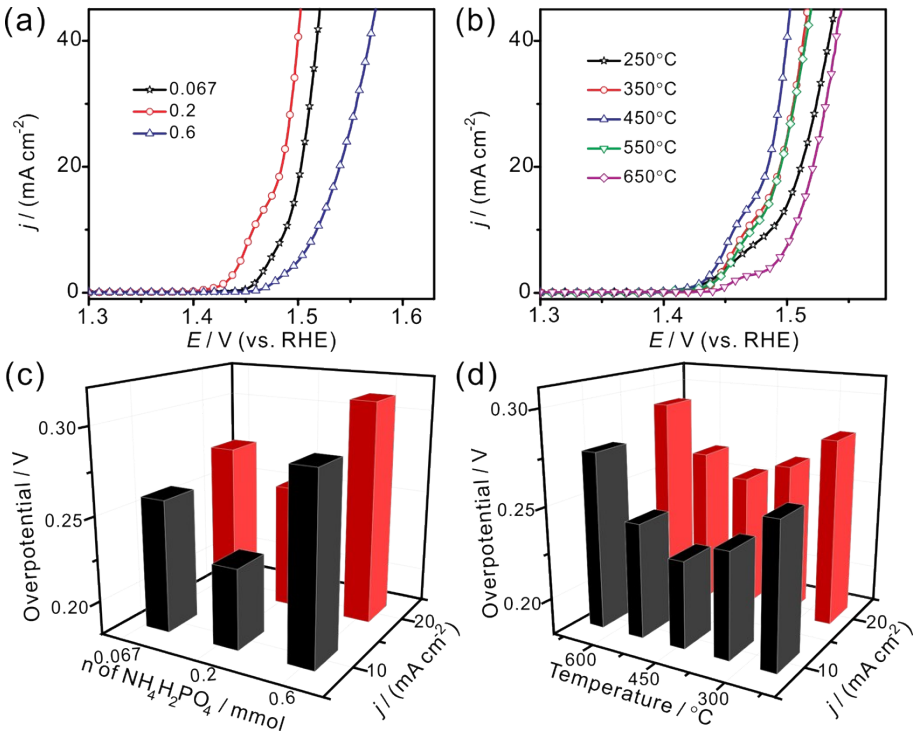

Figure S6 LSV curves of Ni-Fe-O-P prepared at different amount of $NH_4H_2PO_4$ (a) and at different temperatures (b), and (c, d) the corresponding overpotential at current densities of 10 mA cm^{-2} and 20 mA cm^{-2}.

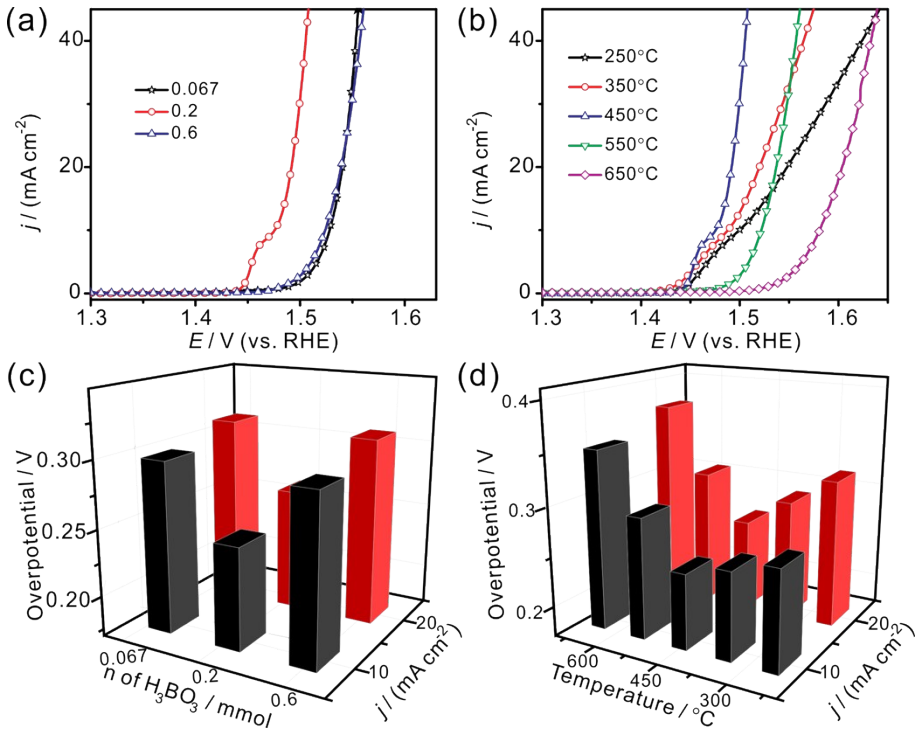

Figure S7 LSV curves of Ni-Fe-O-B prepared at different amount of H_3BO_3 (a) and at different temperatures (b), and (c, d) the corresponding overpotential at current densities of 10 mA cm^{-2} and 20 mA cm^{-2}.

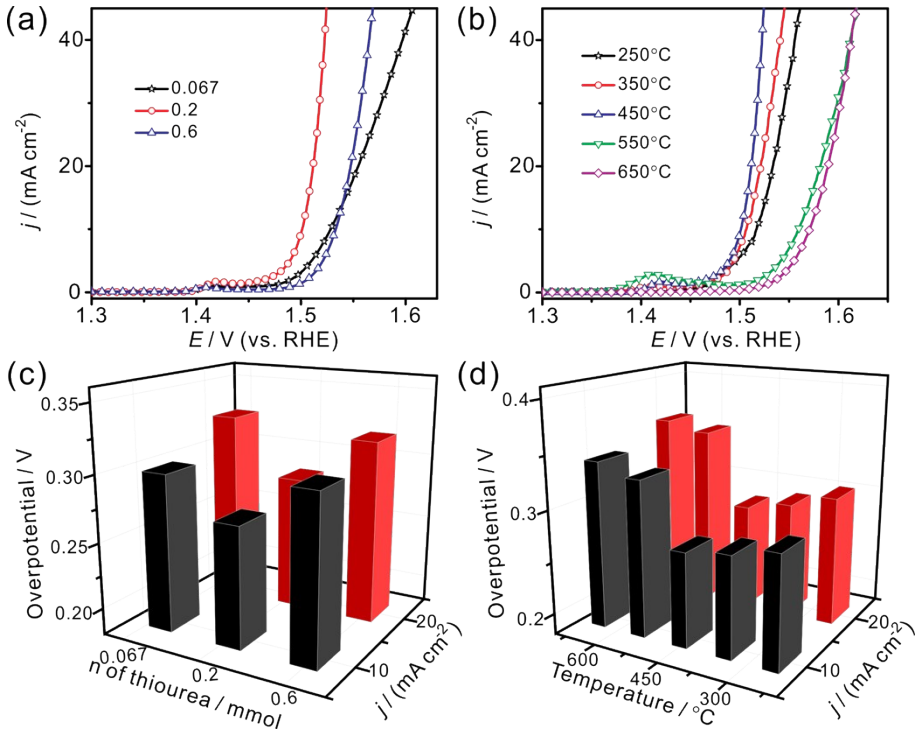

Figure S8 LSV curves of Ni-Fe-O-S prepared at different amount of thiourea (a) and at different temperatures (b), and (c, d) the corresponding overpotential at current densities of 10 mA cm^{-2} and 20 mA cm^{-2}.

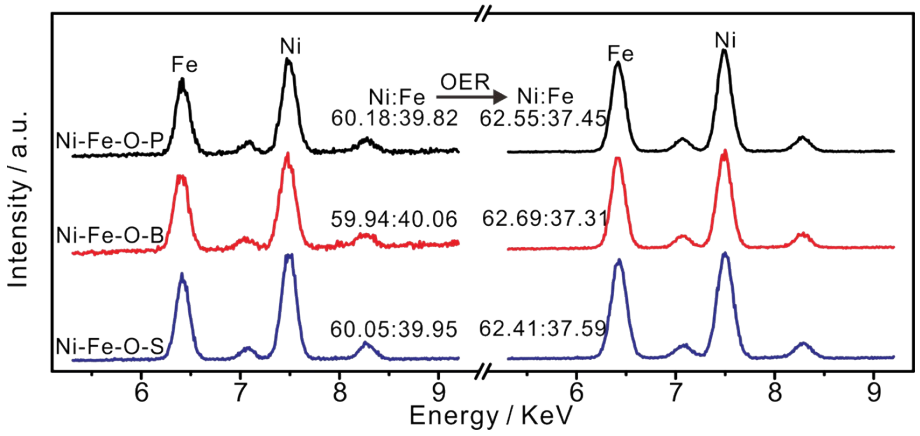

Figure S9 XRF patterns of Ni-Fe-O-P, Ni-Fe-O-B, and Ni-Fe-O-S before and after stability test.

Table S1 Comparison of OER catalytic performance of NiFe-based catalysts reported in literature.

Catalyst	Electrolyte	Loading amount (mg cm^{-2})	*j* / (mA cm^{-2})	η / mV	Refs
$NiFeO_x$ film	1.0 M KOH	$(1.17\pm0.14)\times10^{-3}$	10	336	[1]
NiFe LDH	1.0 M KOH	0.071	10	300	[2]
$NiFeO_x$	1.0 M NaOH	—	10	350	[3]
$Fe_{0.1}Ni_{0.9}O$	1.0 M KOH	0.09	10	297	[4]
flower-like Ni-Fe layered double hydroxide	1.0 M KOH	0.14	10	344	[5]
Nickel-iron binary oxide nanorods	1.0 M KOH	0.12	10	302	[6]
bimetallic iron-nickel nanoparticles	1.0 M NaOH	0.029	10	311	[7]
nanoamorphous ($Ni_{0.8}$, $Fe_{0.2}$) oxide	1.0 M NaOH	0.06±0.02	10	286	[8]
NiO-$NiFe_2O_4$/Reduced Graphene Oxide	1.0 M KOH	0.2	10	296	[9]
$NiFe_2O_x$ Spinels	1.0 M KOH	0.04	10	356	[10]
NiFe/$NiFeO_x$ core/shell electrocatalysts	0.1 M KOH	0.25	10	340	[11]
NiFe LDH/C (Vulcan XC-72R)	0.1 M KOH	0.1	10	360	[12]
NiFe LDH/O-decorated graphene/single-walled CNT hybrids	0.1 M KOH	0.26	10	350	[13]
$Ni_{0.5}Fe_{0.5}Ox$	0.1 M KOH	0.35	10	584	[14]
Ni_3FeN	0.1 M KOH	0.13	10	355	[15]
$FeNiS_2$	0.1 M KOH	0.10	10	310	[16]
Ni-Fe-O-P	1.0 M KOH	0.42	10	227	This work
			20	254	
Ni-Fe-O-B			10	243	
			20	261	
Ni-Fe-O-S			10	272	
			20	287	

References

1 L. Trotochaud, J. K. Ranney, K. N. Williams and S. W. Boettcher, *J. Am. Chem. Soc.*, 2012, **134**, 17253-17261.

2 F. Song and X. Hu, *Nat. Commun.*, 2014, **5**, 4477.

3 C. C. McCrory, S. Jung, J. C. Peters and T. F. Jaramillo, *J. Am. Chem. Soc.*, 2013, **135**, 16977-16987.

4 K. Fominykh, P. Chernev, I. Zaharieva, J. Sicklinger, G. Stefanic, M. Döblinger, A. Müller, A. Pokharel, S. Böcklein and C. Scheu, *ACS nano*, 2015, **9**, 5180-5188.

5 L.-J. Zhou, X. Huang, H. Chen, P. Jin, G.-D. Li and X. Zou, *Dalton Trans.*, 2015, **44**, 11592-11600.

6 G. Liu, X. Gao, K. Wang, D. He and J. Li, *Nano Res.*, 2017, **10**, 2096-2105.

7 S. L. Candelaria, N. M. Bedford, T. J. Woehl, N. S. Rentz, A. R. Showalter, S. Pylypenko, B. A. Bunker, S. Lee, B. Reinhart and Y. Ren, *ACS Catal.*, 2017, **7**, 365-379.

8 J. M. Barforoush, D. T. Jantz, T. E. Seuferling, K. R. Song, L. C. Cummings and K. C. Leonard, *J. Mater. Chem. A*, 2017, **5**, 11661-11670.

9 G. Zhang, Y. Li, Y. Zhou and F. Yang, *ChemElectroChem*, 2016, **3**, 1927-1936.

10 C. N. Chervin, P. A. DeSario, J. F. Parker, E. S. Nelson, B. W. Miller, D. R. Rolison and J. W. Long, *ChemElectroChem*, 2016, **3**, 1369-1375.

11 K. Zhu, M. Li, X. Li, X. Zhu, J. Wang and W. Yang, *Chem. Commun.*, 2016, **52**, 11803-11806.

12 F. Dionigi, T. Reier, Z. Pawolek, M. Gliech and P. Strasser, *ChemSusChem*, 2016, **9**, 962-972.

13 X. Zhu, C. Tang, H.-F. Wang, Q. Zhang, C. Yang and F. Wei, *J. Mater. Chem. A*, 2015, **3**, 24540-24546.

14 J. Jiang, C. Zhang and L. Ai, *Electrochim. Acta*, 2016, **208**, 17-24.

15 G. Fu, Z. Cui, Y. Chen, L. Xu, Y. Tang and J. B. Goodenough, *Nano Energy*, 2017, **39**, 77-85.

16 J. Jiang, S. Lu, H. Gao, X. Zhang and H.-Q. Yu, Nano Energy, 2016, **27**, 56-534.