

Supporting Information

Hierarchical carbon-supported iron carbide derived from zinc-iron bimetallic coordination polymer as an efficient electrocatalyst for alkaline oxygen evolution

Tianlong Cao^{a,b,c,d,1,*}, Yanfang Li^{a,1}, Jianguo Zhao^{a,d}, Qihui Jiao^a, Wenjie Chuai^e,
Xuefei Zhang^f, Zuopeng Li^e, Mingjun Pang^{a,d,*}

a Engineering Research Center of Coal-Based Ecological Carbon Sequestration Technology of the Ministry of Education, Shanxi Datong University, Datong 037009, China.

b Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan 030001, China.

c Northwest Yongxin Coating Limited Company, Lanzhou 730046, China.

d Key Laboratory of Graphene Forestry Application of National Forest and Grass Administration, Shanxi Datong University, Datong 037009, China.

e School of Chemistry and Chemical Engineering, Shanxi Datong University, Datong 037009, China.

f Qingyuan Innovation Laboratory, Quanzhou 362801, China.

¹ These authors contributed equally to this work.

* Correspondence: tianlong230228@163.com; pangmingjun3714@163.com.

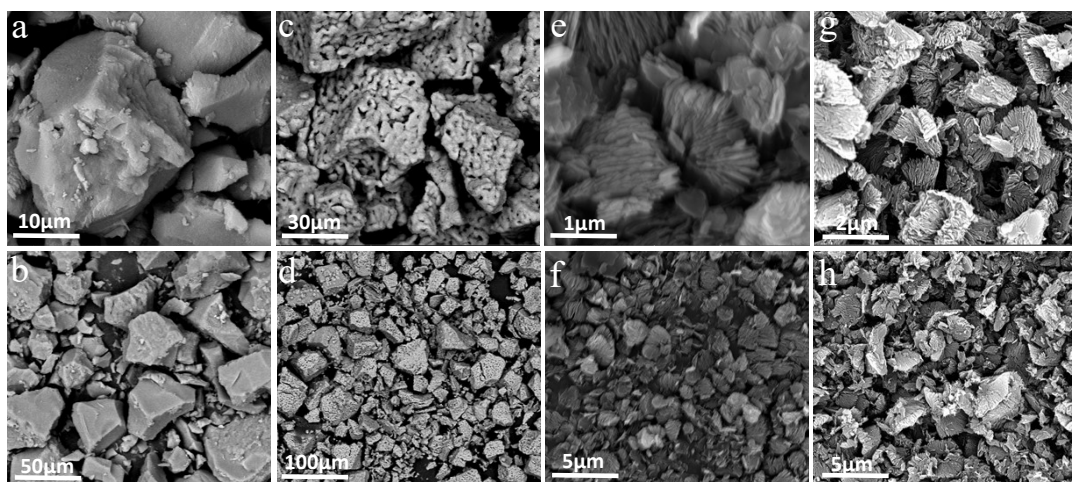


Figure S1 SEM images of (a-b) Fe-CP, (c-d) Fe/C-900, (e-f) Zn-CP and (g-h) Zn/C-900.

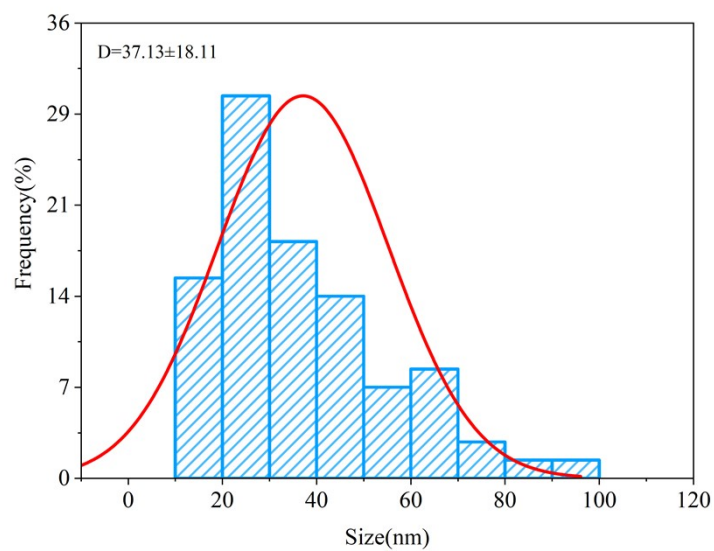


Figure S2 Particle size distribution of Fe_3C on $\text{ZnFe}(3:1)/\text{C-900}$ catalyst.

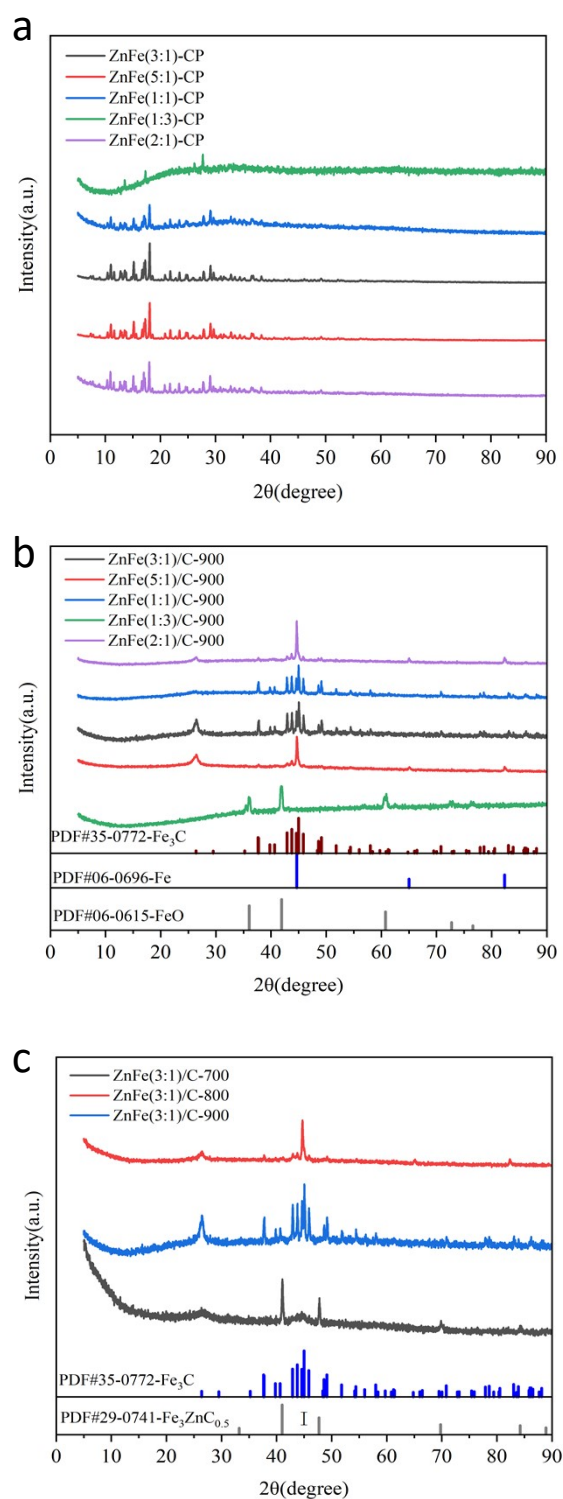


Figure S3 (a) XRD patterns of ZnFe(3:1)-CP, ZnFe(5:1)-CP, ZnFe(1:1)-CP, ZnFe(1:3)-CP and ZnFe(2:1)-CP; (b) XRD patterns of ZnFe(3:1)/C-900, ZnFe(5:1)/C-900, ZnFe(1:1)/C-900, ZnFe(1:3)/C-900 and ZnFe(2:1)/C-900; (c) XRD patterns of ZnFe(3:1)/C-700, ZnFe(3:1)/C-800 and ZnFe(3:1)/C-900.

Table S1 Atomic percentage content and mass percentage content of ZnFe(3:1)/C-900 catalyst surface elements.

Elements	Atom/%	Mass/%
C	91.25	86.28
N	2.86	3.15
O	4.93	6.22
Fe	0.8	3.53
Zn	0.16	0.82

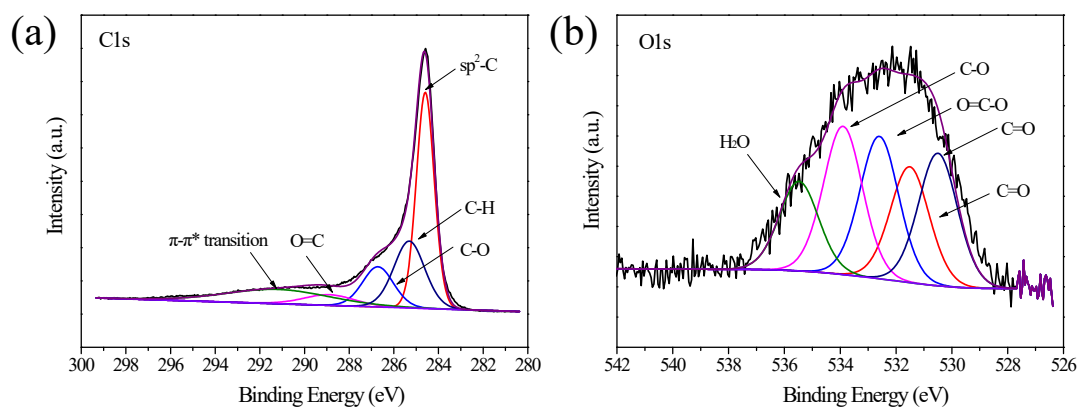


Figure S4 Deconvolution curves of (a) C1s and (b) O1s XPS fine spectra for ZnFe(3:1)/C-900 catalyst.

Table S2 Performance comparison of commercial RuO₂ and IrO₂ catalysts versus several carbon supported iron-based catalysts for alkaline OER.

Sample	Overpotential (mV)	Tafel slope (mV/dec)	Stability (h)	Electrolyte	Ref.
Commercial RuO ₂	310 mV@10mA/cm ²	49.2	<1	1.0 M KOH	[1]
Commercial IrO ₂	320 mV@10mA/cm ²	70	<3	0.1 M KOH	[2]
B-C ₃ N ₄ @Fe ₃ C	243 mV@10mA/cm ²	38.2	32	1.0 M KOH	[3]
FeSAs-PFN-CNTs	310 mV@10mA/cm ²	63.8	24	1.0 M KOH	[4]
Fe/Ni_3.0h	310 mV@10mA/cm ²	37	10	1.0 M KOH	[5]
Fe ₃ C@CNF/NC-950	311 mV@10mA/cm ²	63	16	1.0 M KOH	[6]
Co/FeC@NHC-1	380 mV@10mA/cm ²	70	11	1.0 M KOH	[7]
Fe ₃ C/CoFe ₂ O ₄ @CNFs-1.5	340 mV@10mA/cm ²	128.4	8	0.1 M KOH	[8]
Fe ₃ C@CNTs	375 mV@20mA/cm ²	120	4	1.0 M KOH	[9]
Fe ₃ C@NG800-0.2	361 mV@10mA/cm ²	62	20	0.1 M KOH	[10]
NiFe ₃ @NGHS-NCNTs	383 mV@10mA/cm ²	136.13	15	0.1 M KOH	[11]
Fe ₃ S ₄ /NF	257 mV@10mA/cm ²	45.9	12	1.0 M KOH	[12]
FNC@PANi NCs	219 mV@10mA/cm ²	108.7	10	1.0 M KOH	[13]
ZnFe(3:1)/C-900	408 mV@10mA/cm ²	76.1	15	1.0 M KOH	This work

Reference

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Table S3 Elemental reaction pathway of the Krasil'shchikov mechanism model for Metal Catalysts in the OER (M: Metal; *: Transition state).

Equation	Tafel slope (mV/dec)	Number
$M^* + OH^- \leftrightarrow M^*O-H + e^-$	120	1
$M^*O-H + OH^- \leftrightarrow M^*O^- + H_2O$	60	2
$M^*O^- \rightarrow M^*O + e^-$	45	3
$2 M^*O \rightarrow M^* + O_2$	15	4

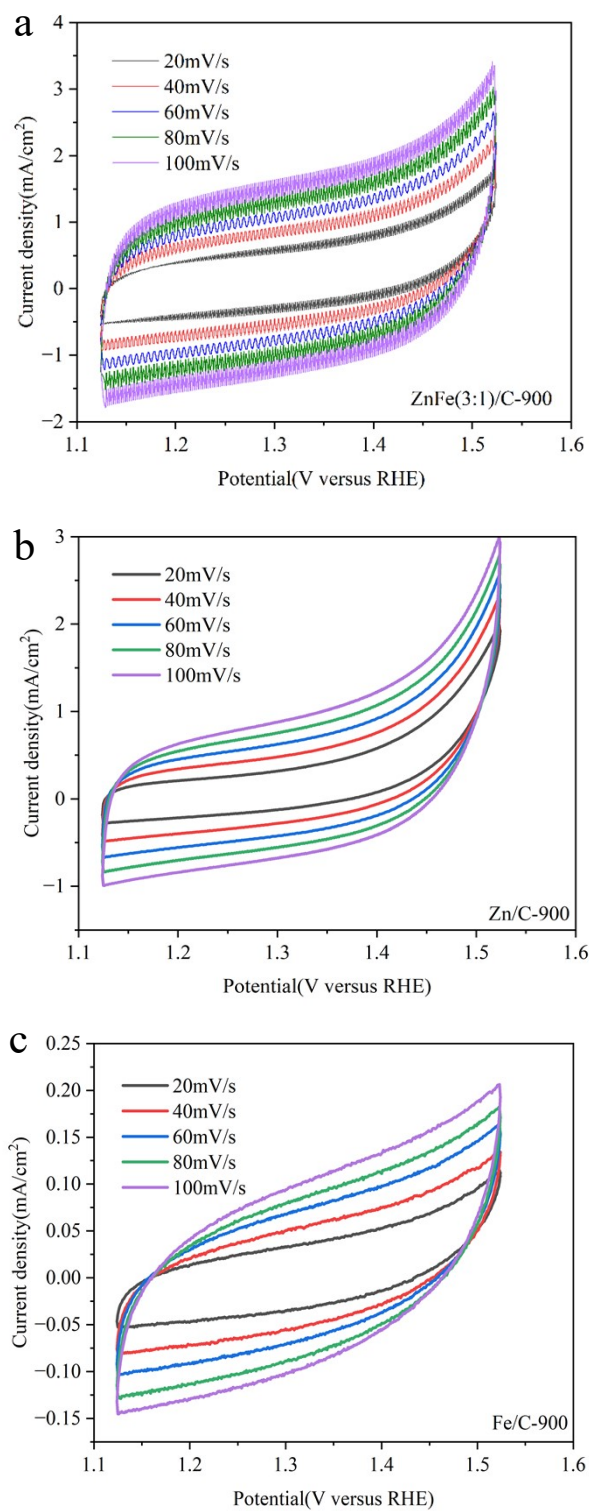


Figure S5 CV curves at different scan rates (Range: 20 mV/s-100 mV/s, Step length: 20 mV/s) for (a) ZnFe(3:1)/C-900, (b) Zn/C-900 and (c) Fe/C-900 samples.

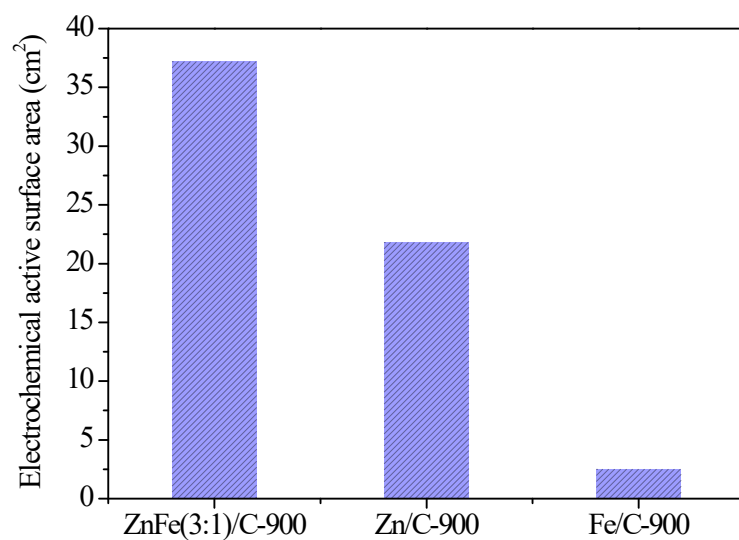


Figure S6 ECSA comparison of ZnFe(3:1)/C-900, Zn/C-900, and Fe/C-900 catalysts.

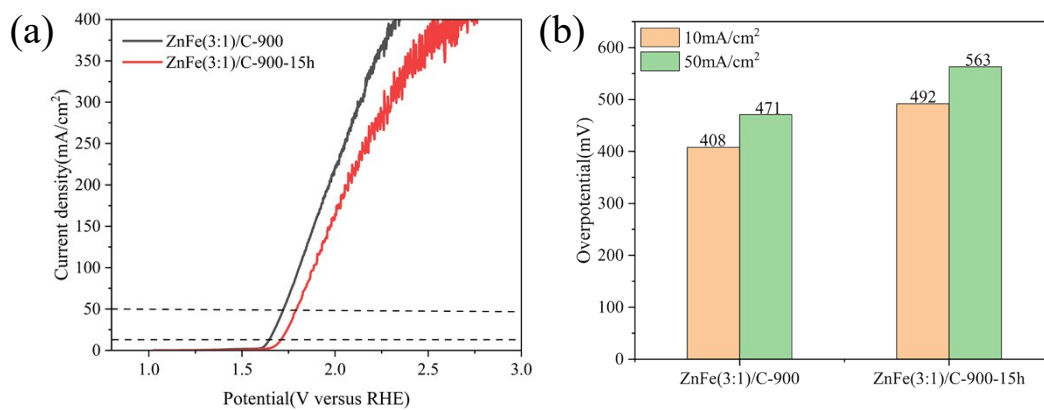


Figure S7 LSV comparison and overpotential values of ZnFe(3:1)/C-900 catalyst at 10 mA/cm² and 50 mA/cm² before and after stability testing.

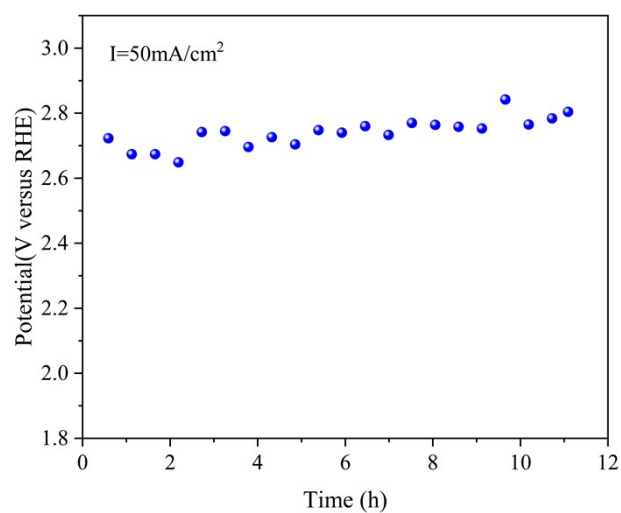


Figure S8 Durability test of ZnFe(3:1)/C-900 at 50 mA cm⁻².

Table S4 XPS elemental comparison of catalysts before and after reaction.

Sample	Elemental content (at.%)				
	C	N	O	Fe	Zn
ZnFe(3:1)/C-900-before OER	91.25	2.86	4.93	0.8	0.16
ZnFe(3:1)/C-900-after OER	86.94	0.82	10.09	1.98	0.18
ZnFe(3:1)/C-900- after 15h stability	62.09	2.15	32.66	2.73	0.37

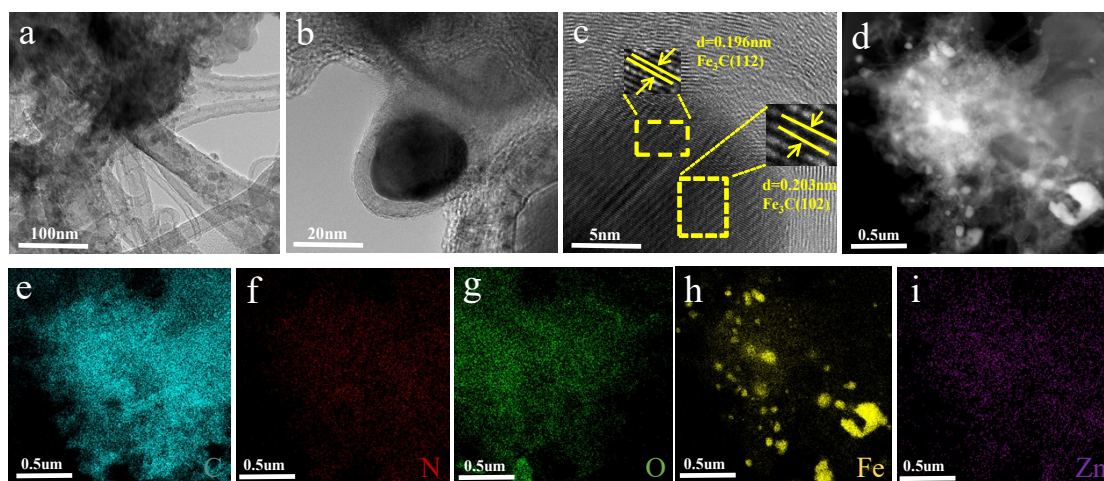


Figure S9 (a-b) TEM images and (c) HR-TEM image of ZnFe(3:1)/C-900-after stability. (d) HAADF-STEM image and (e-i) TEM elemental mappings of the ZnFe(3:1)/C-900-after 15 h stability.

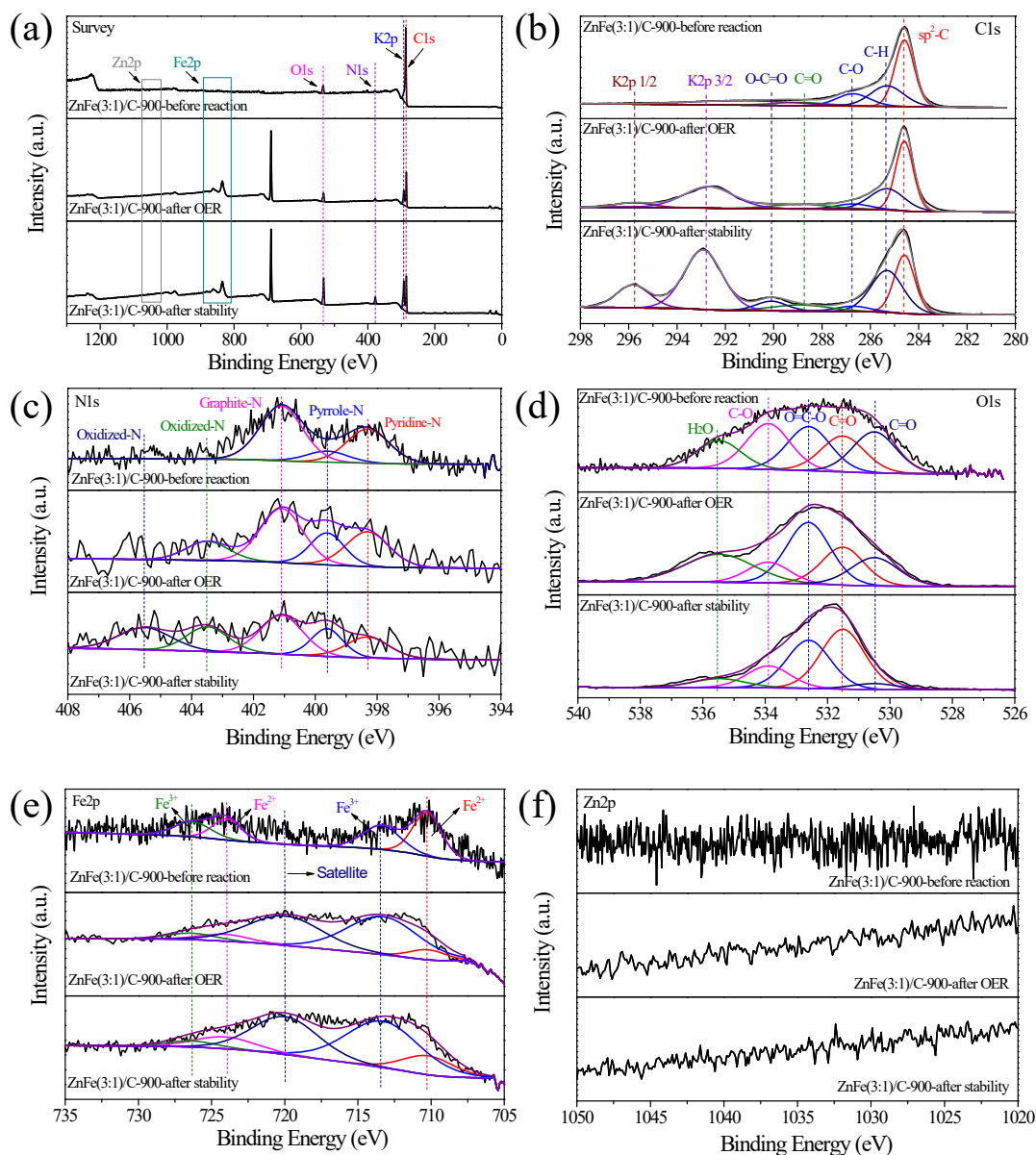


Figure S10 Comparison of XPS survey spectra (a) and high-resolution core-level spectra (C 1s (b), N 1s (c), O 1s (d), Fe 2p (e), Zn 2p (f)) of the ZnFe(3:1)/C-900 catalyst in pre-OER, post-OER, and post-stability testing states.