Supporting Information

KB-templated, *in situ* synthesis of highly dispersed bimetallic NiFe phosphides as efficient oxygen evolution catalysts

Yunheng Li,^[a] Lin Ge,^[b] Yajun Zhou,^{*[a]} Liang Li,^[a] Wei Li,^[a] Jieyu Xu,^[a] and

Yongsheng Li^{*[a]}

^a Lab of Low-Dimensional Materials Chemistry, Key Laboratory for Ultrafine Materials of Ministry of Education, Shanghai Engineering Research Center of Hierarchical Nanomaterials, School of Materials Science and Engineering, East China University of Science and Technology, Shanghai 200237, China

^b State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan 030001, China

* Corresponding author. E-mail: zhouyj@ecust.edu.cn (YJ Zhou), ysli@ecust.edu.cn (YS Li)



Fig. S1 XRD patterns of (a) (Ni_{0.5}Fe_{0.5})₂P/C-KB-*T* (*T*=800, 900, 1000), (b) (Ni_{0.5}Fe_{0.5})₂P/C-900 and (c) Ni₂P/C-KB-800 and Fe₂P/C-KB-800.



Fig. S2 (a) SEM and (b) TEM images of $(Ni_{0.5}Fe_{0.5})_2P/C$ -900-KB.



Fig. S3 TEM images of (a) Ni_2P/C -KB-900, (c) Fe_2P/C -KB-900 and (e) $(Ni_{0.5}Fe_{0.5})_2P/C$ -900.

HRTEM images of (b) Ni₂P/C-KB-900 and (d) Fe₂P/C-KB-900.

Catalyst	Fe (wt%)	Ni (wt%)	$S_{BET}\left(m^2~g^{1}\right)$
Ni ₂ P/C-KB-900	-	18.19	688
(Ni _{0.8} Fe _{0.2}) ₂ P/C-KB-900	3.91	15.26	609
(Ni _{0.5} Fe _{0.5}) ₂ P/C-KB-900	8.94	8.22	684
(Ni _{0.2} Fe _{0.8}) ₂ P/C-KB-900	13.96	3.52	581
Fe ₂ P/C-KB-900	15.08	-	660
$(Ni_{0.5}Fe_{0.5})_2P/C-900$	20.11	27.00	121

900 and (Ni_{1-x}Fe_x)₂P/C-KB-900 (x=0, 0.2, 0.5, 0.8, 1).

Tab. S1 Ni, Fe contents detected by ICP-OES and BET specific surface area of $(Ni_{0.5}Fe_{0.5})_2P/C$ -



Fig. S4 (a) XPS survey spectrum and (b) C 1s, (c) P 2p and (d) Ni 2p high-resolution XPS spectra of Ni₂P/C-KB-900.



Fig. S5 (a) XPS survey spectrum and (b) C 1s, (c) P 2p and (d) Fe 2p high-resolution XPS spectra of the $Fe_2P/C-KB-900$

Sample	η_{10}	η_{20}	Tafel Slope	R _{ct}	C _{dl}	TOF*
Sampie	[mV]	[mV]	[mV dec ⁻¹]	[Ω]	[mF cm ⁻²]	[s ⁻¹]
Ni ₂ P/C-KB-900	350	379	110	36.2	15.3	0.029
(Ni _{0.8} Fe _{0.2}) ₂ P/C-KB-900	285	308	89	5.8	16.3	0.123
(Ni _{0.5} Fe _{0.5}) ₂ P/C-KB-900	272	296	77	4.2	23.1	0.162
(Ni _{0.2} Fe _{0.8}) ₂ P/C-KB-900	307	333	94	14.9	18.8	0.085
Fe ₂ P/C-KB-900	343	373	107	67.0	10.7	0.042
$(Ni_{0.5}Fe_{0.5})_2P/C-900$	365	398	165	128.5	3.0	0.008

Tab. S2 Summary of OER performance in 1 M KOH solution of the as-prepared $(Ni_{0.5}Fe_{0.5})_2P/C$ -

900 and (Ni_{1-x}Fe_x)₂P/C-KB-900 (*x*=0, 0.2, 0.5, 0.8, 1).

*The turn-over frequencies (TOFs) values have been calculated according to the equation of TOFs= (J*A)/(4*F*n). Here J is the geometrical current density at a given overpotential (0.35 V), and A is the surface area of the electrode (0.2827 cm⁻²). The number 4 represents four-electron transfer per mole of O₂. F is the Faraday constant (96485 C mol⁻¹), and n is the number of moles of the active sites on the electrode. It is assumed that only the phosphides as the active sites, which can be calculated through the formula of (n(Ni)+n(Fe))/2. The Ni, Fe contents were obtained from ICP-OES results.



Fig. S6 The OER polarization curves of (Ni_{0.5}Fe_{0.5})₂P/C-KB-*T* (*T*=800, 900, 1000).



Fig. S7 CV curves in the potential region of 1.123-1.223 V with various scan rates (20-200 mV s⁻¹) in 1 M KOH solution for (a) Ni₂P/C-KB-900, (b) (Ni_{0.8}Fe_{0.2})₂P/C-KB-900, (c) (Ni_{0.5}Fe_{0.5})₂P/C-KB-900, (d) (Ni_{0.2}Fe_{0.8})₂P/C-KB-900, (e) Fe₂P/C-KB-900 and (f) (Ni_{0.5}Fe_{0.5})₂P/C-900.