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$FeNi_3$ Modified Fe_2O_3/NiO/MoO_2 Heterogeneous Nanoparticles Immobilized N, P co-doped CNTs as Efficient and Stable Electrocatalyst for Water Oxidation

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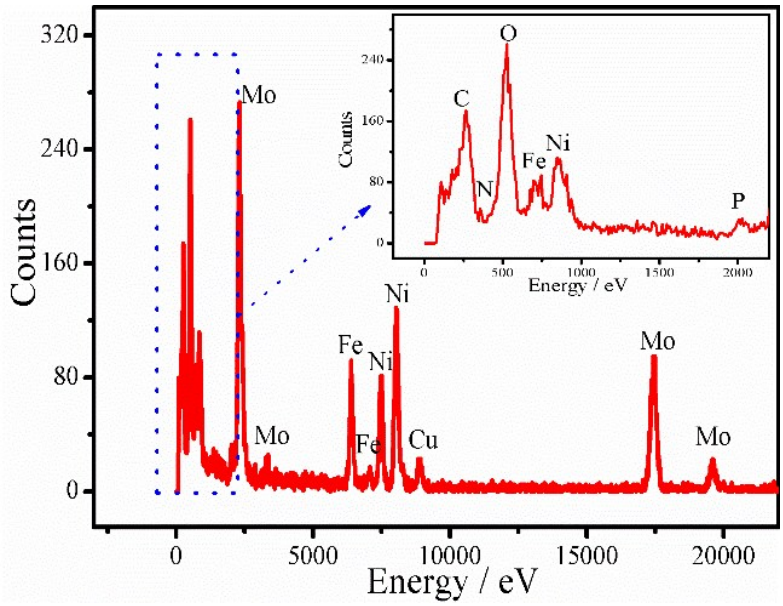

Fig. S1 EDX spectrum of the as-prepared FNM/NPCNT-40 electrocatalyst

Preparation FNM/NC hybrid

FNM/NC was prepared under the same conditions (preparation of FNM/NPCNT-x sample) without the presence of CNT.

Preparation FN/NCNT hybrid

FN/NCNT was prepared under the same conditions (preparation of FNM/NPCNT-x sample) without the presence of $H_3[P(Mo_3O_{10})_4]$.

Preparation M/NPCNT hybrid

M/NPCNT was prepared under the same conditions (preparation of FNM/NPCNT-x sample) without the presence of NiHCF.

Preparation M/P hybrid

M/P was prepared under the same conditions (preparation of FNM/NPCNT-x sample) without the presence of NiHCF and CNT.

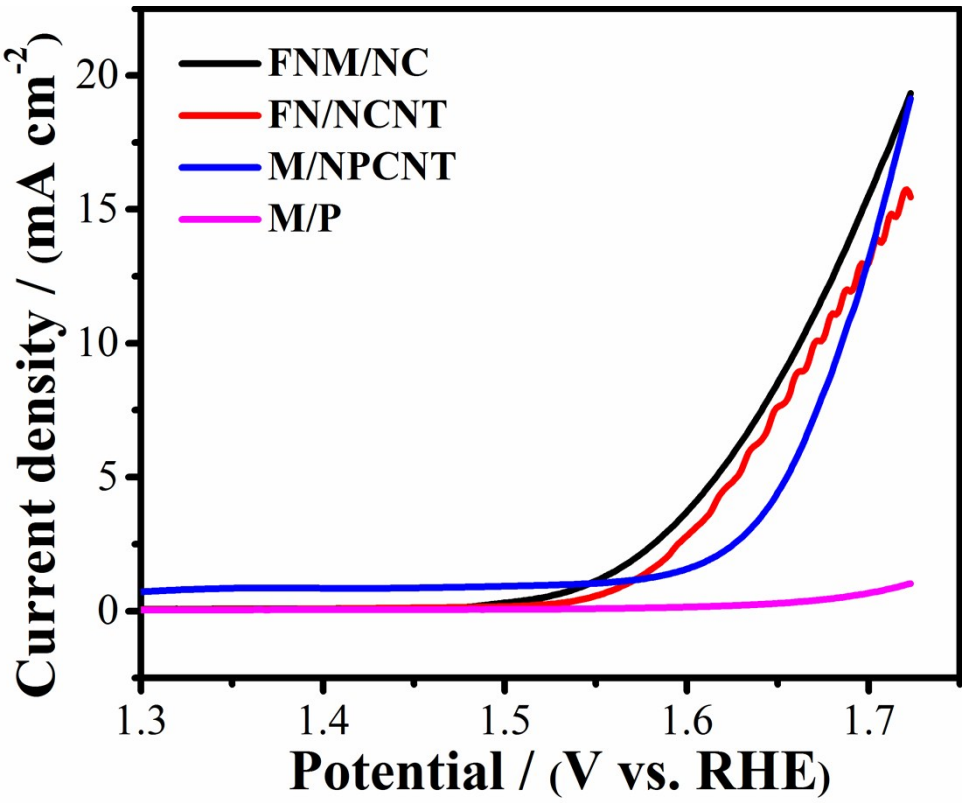

Fig. S2 LSV curves of as-prepared electrocatalyst at a scan rate of 5 mV s^{-1}

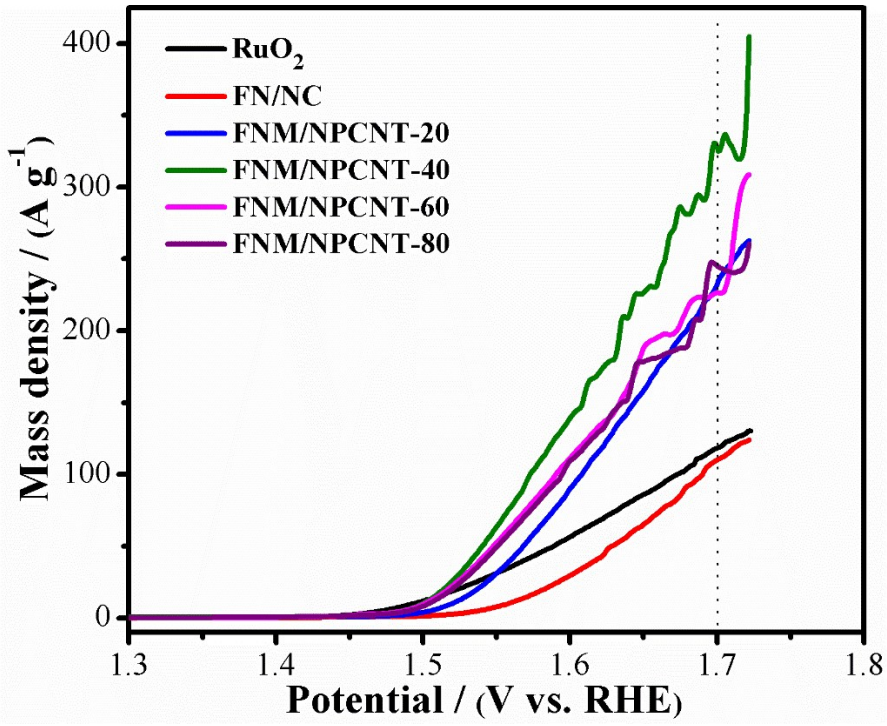

Fig. S3 Mass activity of the commercial RuO_2 and as-prepared FN/NC, FNM/NPCNT-20, FNM/NPCNT-40, FNM/NPCNT-60 and FNM/NPCNT-80 electrocatalyst

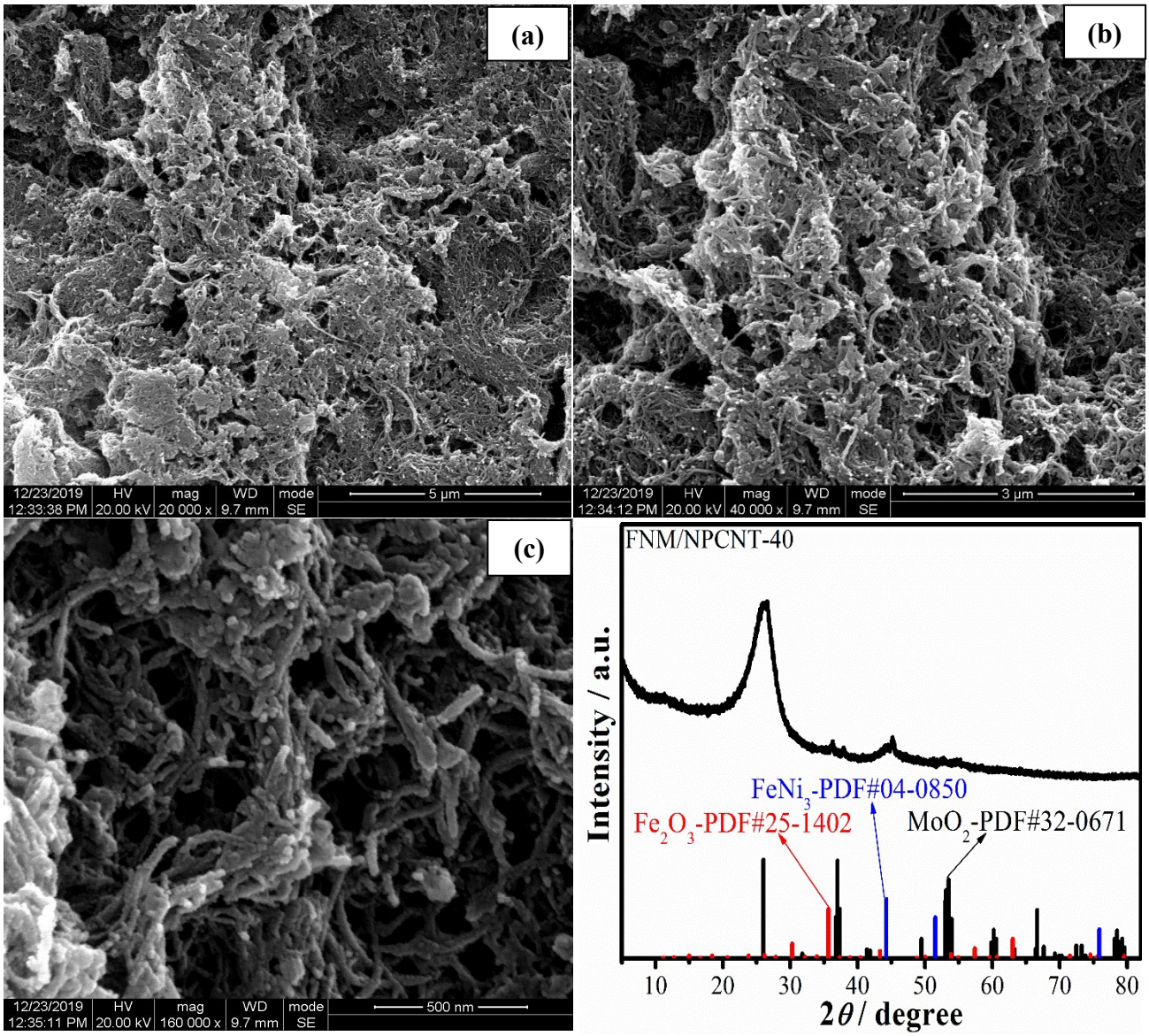

Fig. S4 SEM (a, b, c) and XRD (d) of FNM/NPCNT-40 hybrid after 2000 CV treatment in KOH medium.

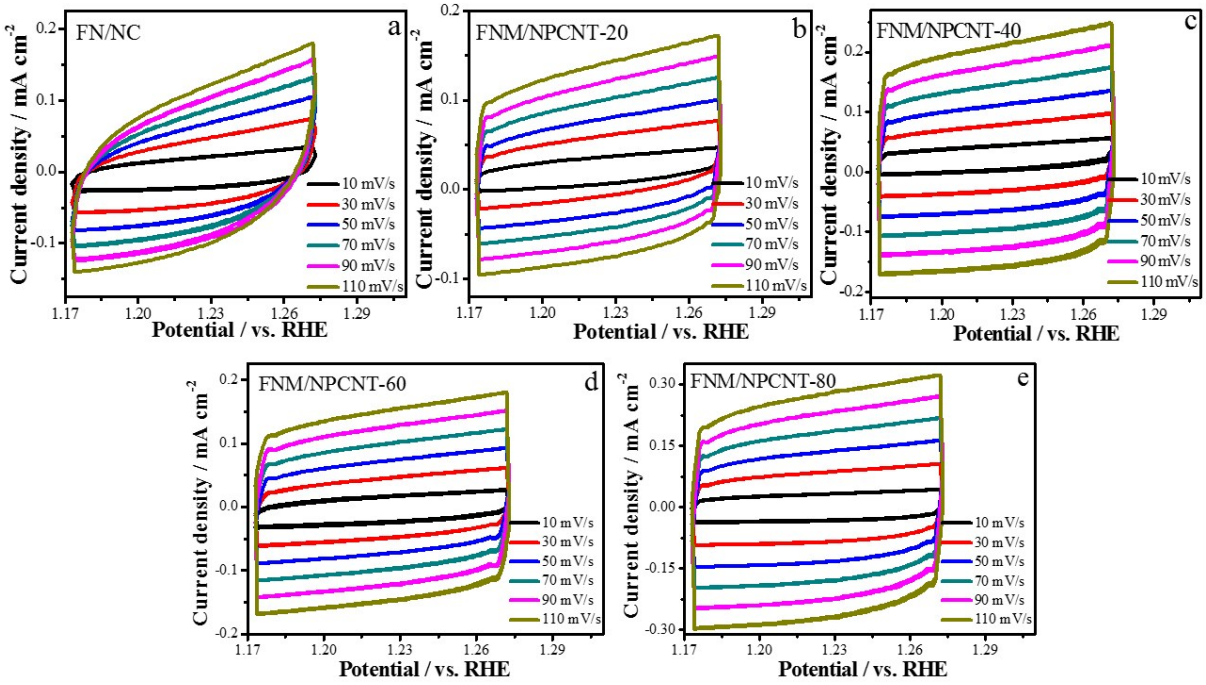

Fig. S5 CV curves of the as-prepared FN/NC (a), FNM/NPCNT-20 (b), FNM/NPCNT-40 (c), FNM/NPCNT-60 (d), and FNM/NPCNT-80 (e) electrocatalyst at different scan rates.

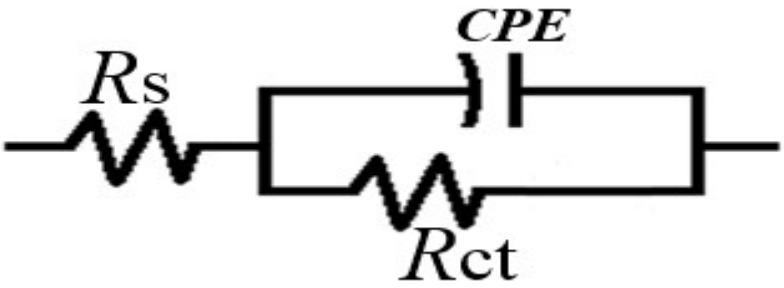

Fig. S6 EIS equivalent circuit fitting diagram of the as-prepared electrocatalyst

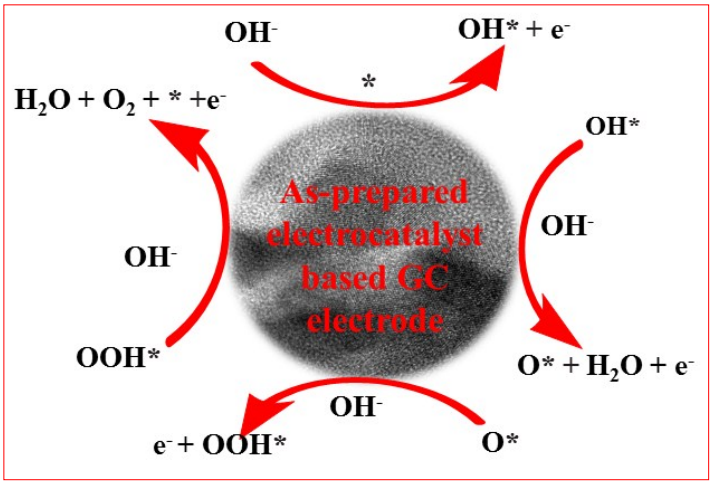

Fig. S7 Possible OER electrocatalytic mechanisms

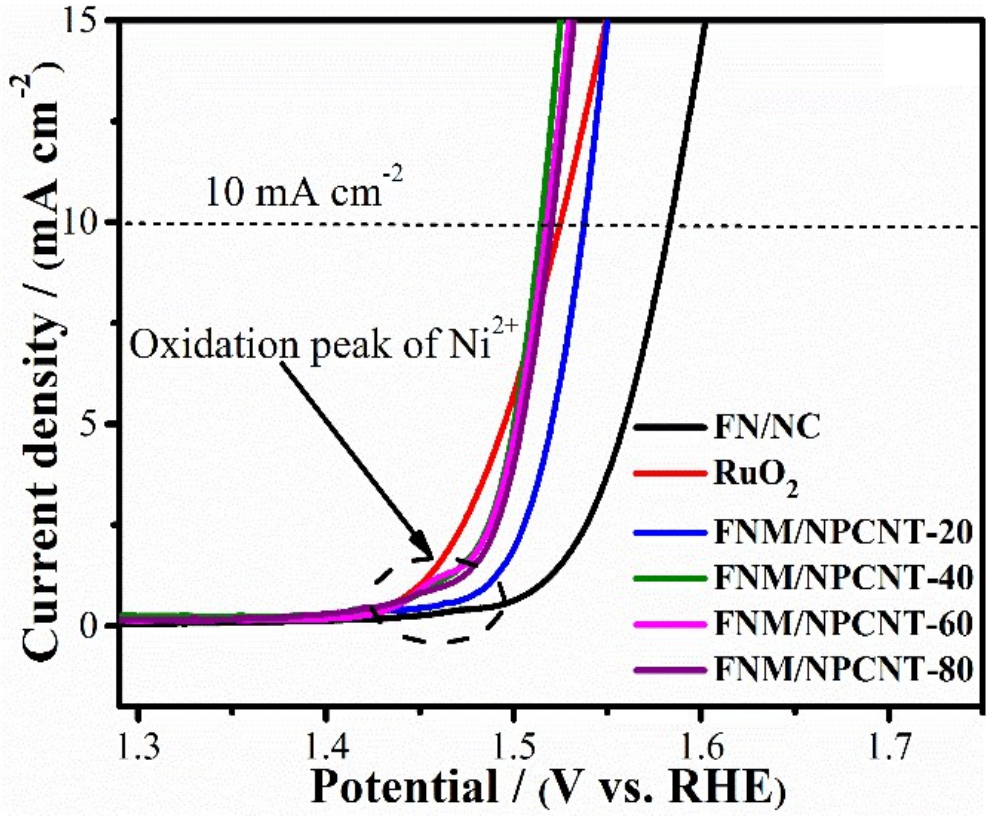

Fig. S8 Enlarged image of LSV curves of commercial RuO_2 and as-prepared electrocatalyst at a scan rate of 5 mV s^{-1}

The electrochemical active surface area (ECSA) was assessed by the double-layer capacitance (C_{dl}) acquired from the CV test, so the linear plots have been ploted by fitting (Fig. 6a) and the corresponding R^2 of the fitted line are as follows.

R^2 of the fitted line

FN/NC sample: $R^2 = 0.9865$

FNM/NPCNT-20 sample: $R^2 = 0.9974$

FNM/NPCNT-40 sample: $R^2 = 0.9997$

FNM/NPCNT-60 sample: $R^2 = 0.9998$

FNM/NPCNT-80 sample: $R^2 = 0.9991$

Table S1. ICP-OES results of FNM/NPCNT-40 hybrid.

sample	Content of Ni ($mg\ L^{-1}$)	Content of Fe ($mg\ L^{-1}$)	Content of Mo ($mg\ L^{-1}$)	The ratio of Fe: Ni: Mo
FNM/NPCNT-40	2.0	1.3	11.3	1.5 : 1 : 8.7

Table S2 Summary of recently reported non-precious Fe/Ni/Mo-based catalysts for OER

Catalysts	Overpotential (mV) at 10 mA cm^{-2}	Tafel slope (mV dec^{-1})	Reference
Fe_2O_3/CNT	410	76	[1]
γ-Fe_2O_3/CNTs	340	45	[2]
MoO_2-$Co_2Mo_3O_8$@C nanorods	320	88	[3]
CoO-MoO_2 Nanocages	312	69	[4]
Co/β-Mo_2C@N-CNTs	356	67	[5]
FeNiCo alloy	400	72	[6]
Ni-Fe@rGO	350	38	[7]
CoP(MoP)-$CoMoO_3$@CNT	296	105	[8]
FeNi@NC	298	48.4	[9]
P-$Ni_{0.5}$Fe@C	256	65	[10]
FeNiP/NC	270	61.5	[11]
Fe-Ni_3S_2/FeNi	282	54	[12]
FNM/NPCNT	**282**	**46.2**	**This work**

Table S3 The fitting data of EIS equivalent circuit diagram

Sample	R_s (Ω)	R_{ct} (Ω)	CPE (S sec^n)
FN/NC	20.62	361.9	0.0002721
FNM/NPCNT-20	17.44	193.1	0.0003134
FNM/NPCNT-40	11.52	32.02	0.001436
FNM/NPCNT-60	11.37	44.12	0.001952
FNM/NPCNT-80	12.50	41.46	0.001383

Reference

[1] H.A. Bandal, A.R. Jadhav, A.A. Chaugule, W-J. Chung, H. Kim, Electrochimica Acta., 2016, 222, 1316-1325

[2] M. Tavakkoli, T. Kallio, O. Reynaud, A.G. Nasibulin, J. Sainio, H. Jiang, E.I. Kauppinen, K. Laasonen, J. Mater. Chem. A, 2016, 4, 5216-5222.

[3] Y.Q. Li, H.B. Xu, H.Y. Huang, C. Wang, L.G. Gao, T.L. Ma, Chem. Commun., 2018, 54, 2739.

[4] F.L. Lyu, Y.C. Bai, Z.W. Li, W.J. Xu, Q.F. Wang, J. Mao, L. Wang, X.W. Zhang, Y.D. Yin, Adv. Funct. Mater. 2017, 27, 1702324.

[5] T. Ouyang, Y.Q. Ye, C.Y. Wu, K. Xiao, Z.Q. Liu, Angew. Chem. Int. Ed. 2019, 58, 4923-4928.

[6] S. Saha, A.K. G. li, ChemistrySelect, 2017, 2, 1630-1636.

[7] N. Chandrasekaran, S. Muthusamy, Langmuir 2017, 33, 2-10.

[8] L. Yu, Y. Xiao, C.L. Luan, J.T. Yang, H.Y. Qiao, Y. Wang, X. Zhang, X.P. Dai, Y. Yang, H.H. Zha, ACS Applied Materials & Interfaces, 2019, 7, 6890-6899.

[9] X.J. Zhang, Y.F. Chen, B. Wang, M.L. Chen, B. Yu, X.Q. Wang, W.L. Zhang, D.X. Yang, Electrochimica Acta, 2019, 321, 134720.

[10] A.X. Fan, C.L. Qin, X. Zhang, X.P. Dai, Z. Dong, C.L. Luan, L. Yu, J.Q. Ge, F. Gao, ACS Sustainable Chem. Eng. 2019, 7, 2285-2295.

[11] Y.M. Du, Y. Han, X.D. Huai, Y.R. Liu, C.Y. Wu, Y.Y., L. Wang, International Journal of Hydrogen Energy, 2018, 43, 22226-22234.

[12] C.Z. Yuan, Z.T. Sun, Y.F. Jiang, Z.K. Yang, N. Jiang, Z.W. Zhao, U.Y. Qazi, W.H. Zhang, A.W. Xu, small 2017, 13, 1604161