

## Supporting Information

### **Novel Fe<sub>2.55</sub>Sb<sub>2</sub> Alloy Nanoparticles incorporated in N-doped Carbon as Bifunctional Oxygen Electrocatalyst for Rechargeable Zn-Air Battery**

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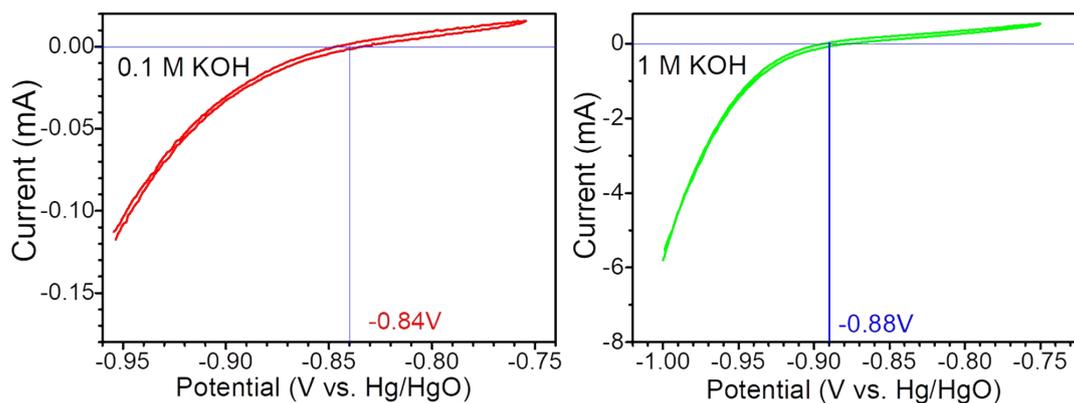


Fig. S1. Calibration of Hg/HgO reference electrode with respect to reversible hydrogen electrode (RHE).

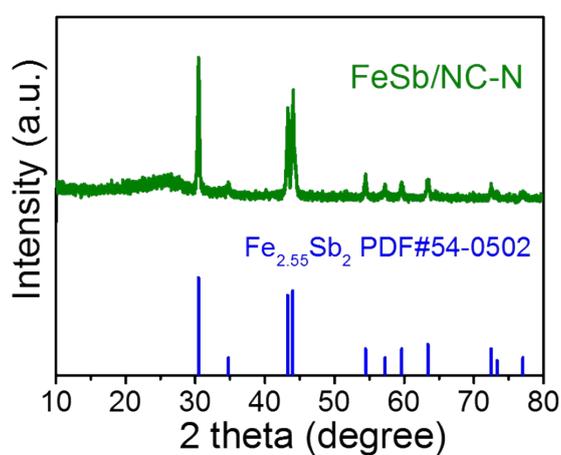


Fig. S2. XRD pattern of FeSb/NC-N catalyst.

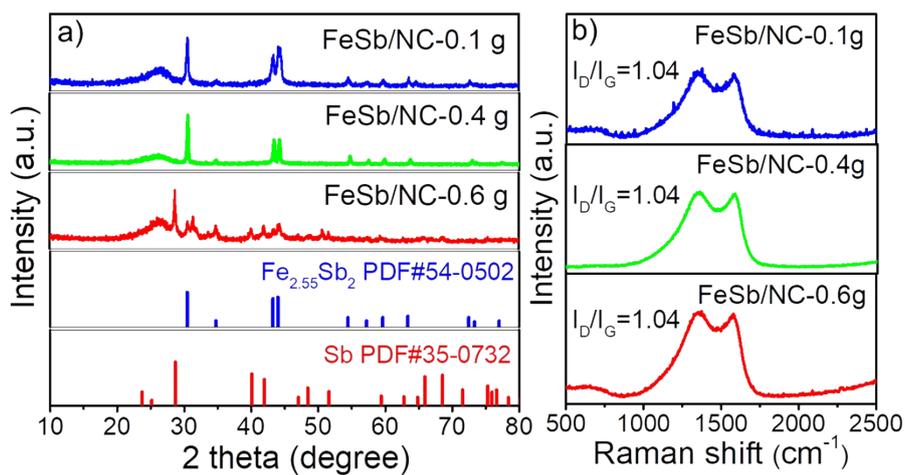


Fig. S3. a) XRD patterns and b) Raman spectra of FeSb/NC with different feeding amount of  $\text{SbCl}_3$ .

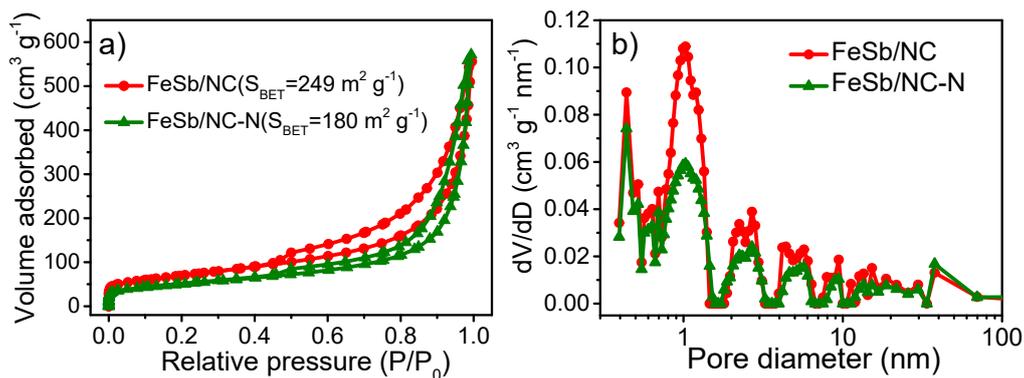


Fig. S4. a) N<sub>2</sub> adsorption-desorption isotherms and b) the corresponding pore size distribution curves of FeSb/NC and FeSb/NC-N catalysts.

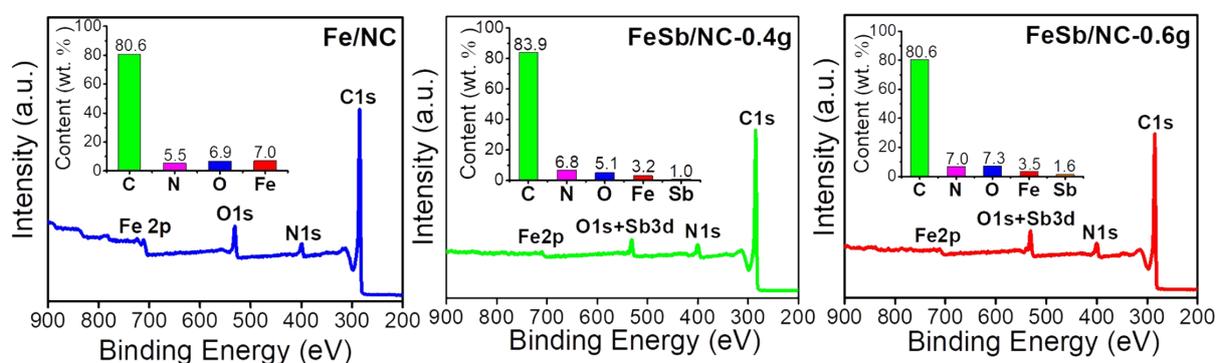


Fig. S5. The XPS survey spectra and the corresponding elemental contents of Fe/NC, FeSb/NC-0.4g and FeSb/NC-0.6g.

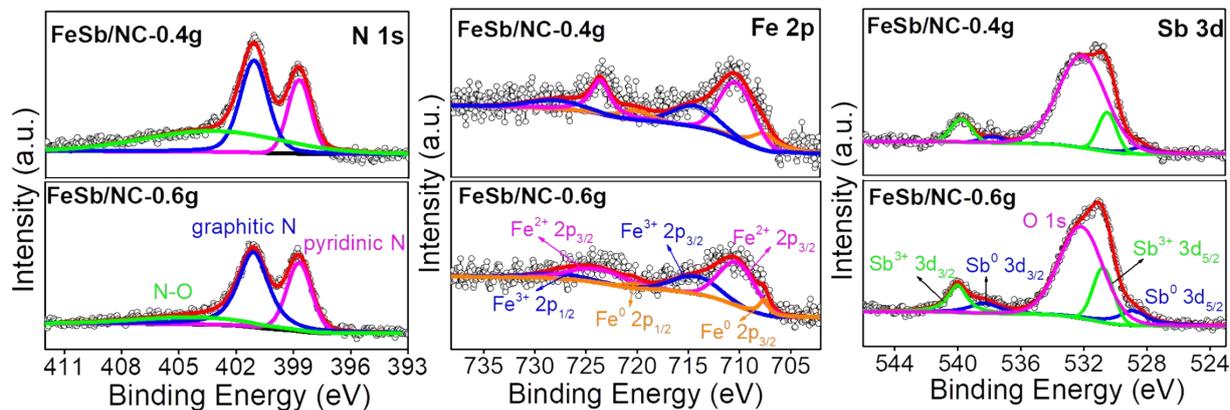


Fig. S6. High-resolution N 1s, Fe 2p and Sb 3d spectra of FeSb/NC-0.4g and FeSb/NC-0.6g.

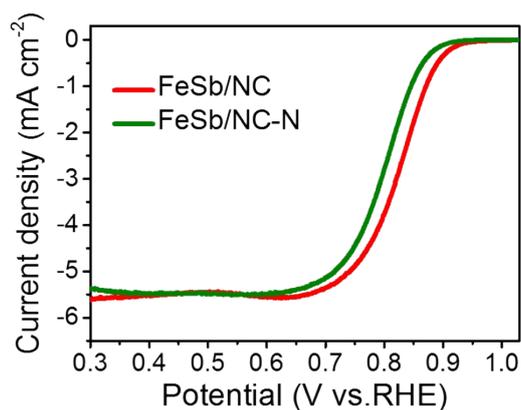


Fig. S7. LSV curves for ORR of FeSb/NC and FeSb/NC-N catalysts.

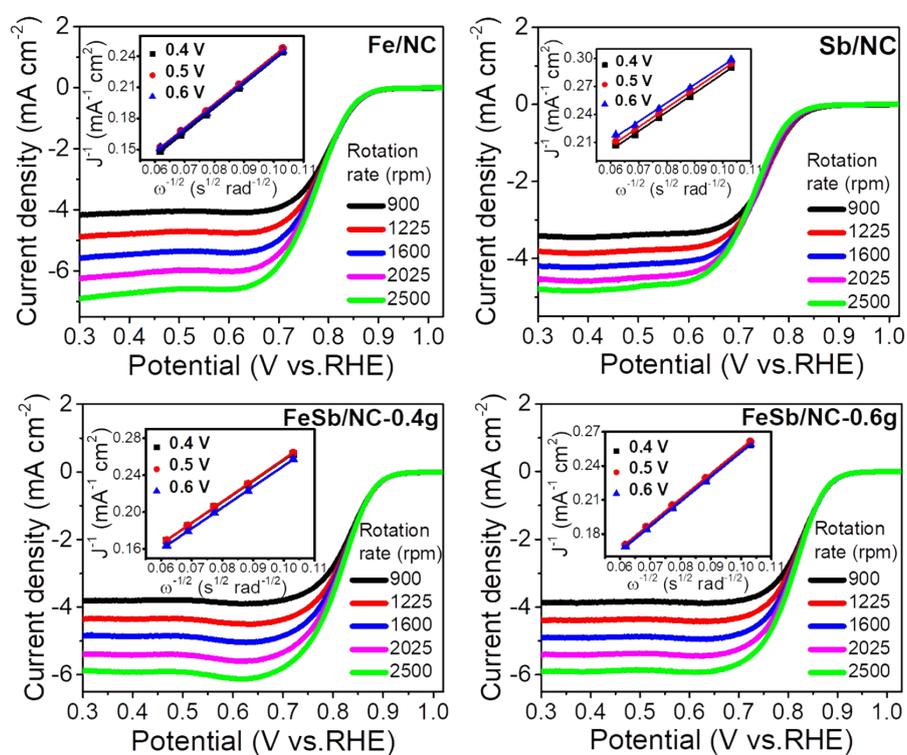


Fig. S8. LSV curves of Fe/NC, Sb/NC, FeSb/NC-0.4g and FeSb/NC-0.6g catalysts measured at different rotation rates and the corresponding K-L plots.

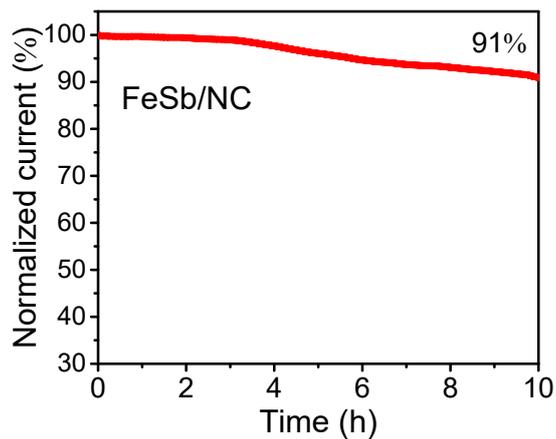


Fig. S9. ORR durability test of FeSb/NC performed on carbon paper.

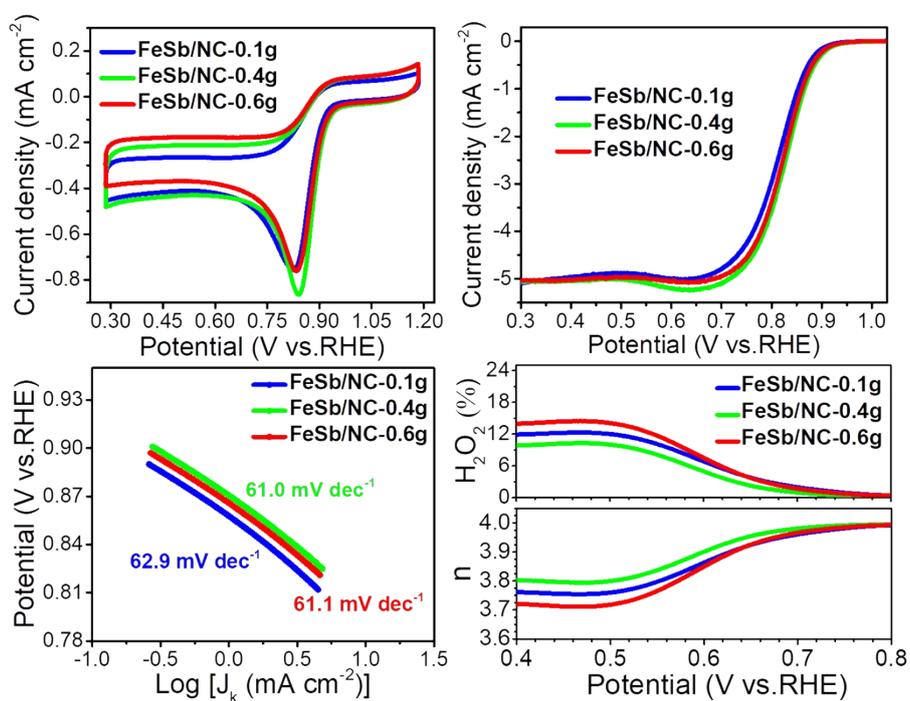


Fig. S10. ORR performance of FeSb/NC with different feeding amount of  $\text{SbCl}_3$ .

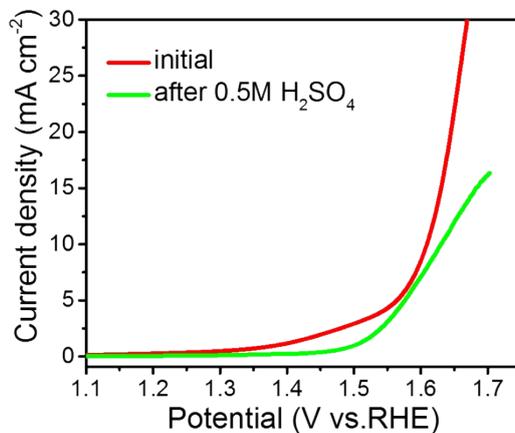


Fig. S11. OER LSV curves of FeSb/NC before and after acid leaching.

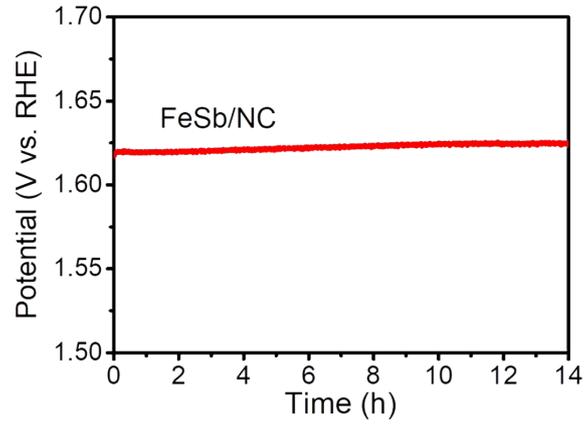


Fig. S12. Chronopotentiometric curve at a constant current density of  $10 \text{ mA cm}^{-2}$  for on FeSb/NC.

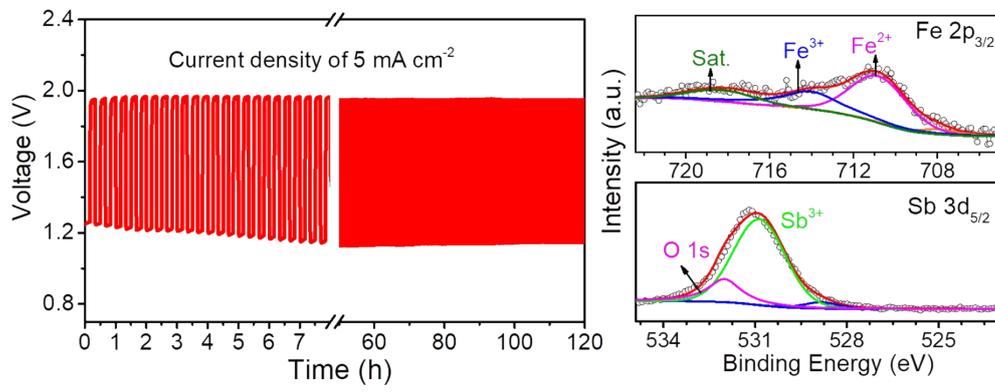


Fig. S13. High-resolution  $\text{Fe } 2p_{3/2}$  and  $\text{Sb } 3d_{5/2}$  spectra of FeSb/NC after 120 h of charge-discharge cycling test at  $5 \text{ mA cm}^{-2}$  for 120 h.

Table S1 ORR parameters for for FeSb/NC-0.1g, FeSb/NC-0.4g, FeSb/NC-0.6g.

Samples	Peak potential (V vs. RHE)	$E_{\text{onset}}$ (V vs. RHE)	$E_{1/2}$ (V vs. RHE)	$J_L$ (mA cm <sup>-2</sup> )	Tafel slope (mV dec <sup>-1</sup> )
FeSb/NC-0.1g	0.82	0.89	0.81	5.00	62.9
FeSb/NC-0.4g	0.84	0.90	0.82	5.24	61.0
FeSb/NC-0.6g	0.83	0.90	0.82	5.07	61.1

Table S2 Comparison of Zn-air battery performance of the FeSb/NC catalyst with recently reported electrocatalysts.

Catalysts	OCV (V)	Peak power density (mW cm <sup>-2</sup> )	Specific capacity (mA h g <sup>-1</sup> Zn)	Cycling durability @J(mA cm <sup>-2</sup> )	Ref.
FeSb/NC	1.46	175	751	887 h @5 616 h @10	This work
N-CoS <sub>2</sub> YSSs	1.41	81	744	165 h @10	[1]
FeNi <sub>3</sub> @NC	1.39	139	756	30 h @5	[2]
Co@hNCTs-800	1.45	149	746	500 h @5	[3]
Zn-Ni <sub>3</sub> FeN/NG	1.60	158	650	180 h @10	[4]
Fe-enriched-FeNi <sub>3</sub> /NC	1.43	89	734	14 h @10	[5]
CoSe <sub>2</sub> @NC	1.48	137	751	83 h @10	[6]
CoFe@NC/NC HNSs-700	1.49	184	774	50 h @5	[7]
Mn-RuO <sub>2</sub>	1.55	181	812	2500 h @10	[8]
Co <sub>6</sub> Mo <sub>6</sub> C <sub>2</sub> -Co@NC	1.38	45	760	300 h @10	[9]
CoFe/S-N-C	1.48	130	814	100 h @10	[10]
NiCo/NHCS-TUC-3	1.59	256	757	70 h @5	[11]
CS350-10Ar	1.36	135		120 h @5	[12]
Co/NGC-3		134	716	120 h @5	[13]
FeCo/Co <sub>2</sub> P@NPCF	1.44	154		107 h @10	[14]
MnSAC		258	675	100 h @5	[15]
Co <sub>9</sub> S <sub>8</sub> @Co/Mn-S,N-PC	1.49	80		210 h @10	[16]
CoFe-NCNFs	1.52	116		110 h @5	[17]
Fe-NC SAC		180	786	160 cycles @20	[18]
FeCo/Se-CNT	1.54	173		70 h @5	[19]
FeCu <sub>0.3</sub> -N/C	1.50	111	682	75 h @5	[20]
NiFe <sub>3</sub> @NGHS-NCNT <sub>s</sub>	1.51	127		166 h @10	[21]
f-FeCo-CNT	1.48	196	754	180 h @20	[22]
Catalysts	OCV (V)	Peak power density (mW cm <sup>-2</sup> )	Specific capacity (mA h g <sup>-1</sup> Zn)	Cycling durability @J(mA cm <sup>-2</sup> )	Ref.

<b>CoSb/NC-0.8</b>	1.42	180		160 h @10	[23]
<b>CoSb<sub>3</sub>/NCL-30</b>		211		60 h @10	[24]
<b>S-LaCoO<sub>3</sub></b>	1.47	92	747	100 h @2	[32]
<b>LSCP-3</b>	1.50	52	740	60 h @10	[33]
<b>Pb<sub>2</sub>Ru<sub>2</sub>O<sub>6.5</sub></b>		195		33 h @10	[34]
<b>YRO</b>	1.17	145		34 h @10	[35]

Table S3 Comparison of BI and SBI values of FeSb/NC catalyst with recently reported electrocatalysts.

<b>Catalysts</b>	<b>ORR (V) @-3 mA/cm<sup>2</sup><sub>geo</sub></b>	<b>OER (V) @10 mA/cm<sup>2</sup><sub>geo</sub></b>	<b>BI (V)</b>	<b>SBI (uA/cm<sup>2</sup><sub>BET</sub>)</b>	<b>Ref.</b>
<b>FeSb/NC</b>	<b>0.82</b>	<b>1.72</b>	<b>0.90</b>	<b>4.9</b>	<b>This work</b>
<b>Co<sub>9</sub>S<sub>8</sub>/(N,S-doped carbon)</b>	0.84	1.64	0.80	1.3	[25]
<b>N-doped CNT framework</b>	0.83	1.60	0.77	6.8	[26]
<b>N,P-doped C foam</b>	0.80	1.90	1.10	0.8	[27]
<b>Ba<sub>0.5</sub>Sr<sub>0.5</sub>Co<sub>0.8</sub>F<sub>e<sub>0.2</sub>O<sub>3-δ</sub></sub></b>	0.74	1.58	0.84	2.7	[28]
<b>α-MnO<sub>2</sub></b>	0.76	1.72	0.96	14.7	[29]
<b>Co<sub>x</sub>Mn<sub>3-x</sub>O<sub>4</sub>/C</b>	0.82	1.80	0.98	92.6	[30]
<b>Pb<sub>2</sub>Ru<sub>2</sub>O<sub>7-x</sub></b>	0.74	1.43	0.69	274.0	[31]

## References

- [1] X. F. Lu, S. L. Zhang, E. B. Shangguan, P. Zhang, S. Y. Gao, X. W. Lou, *Adv. Sci.* 7 (2020) 2001178.
- [2] D. Chen, J. W. Zhu, X. Q. Mu, R. L. Cheng, W. Q. Li, S. L. Liu, Z. H. Pu, C. Lin, S. C. Mu, *Appl. Catal. B Environ.* 268 (2020), 118729.
- [3] Q. Y. Zhou, Z. Zhang, J. J. Cai, B. Liu, Y. L. Zhang, X. F. Gong, X. L. Sui, A. P. Yu, L. Zhao, Z. B. Wang, Z. W. Chen, *Nano Energy* 71 (2020), 104592.
- [4] X. Y. He, Y. H. Tian, Z. L. Huang, L. Xu, J. C. Wu, J. C. Qian, J. M. Zhang, H. N. Li, *J. Mater. Chem. A* 9 (2021) 2301.
- [5] K. Chen, S. Kim, R. Rajendiran, K. Prabakar, G. Z. Li, Z. C. Shi, C. Jeong, J. Kang, O. L. Li, *J. Colloid Interface Sci.* 582 (2021) 977-990.
- [6] K. X. Ding, J. G. Hu, J. Luo, W. Jin, L. M. Zhao, L. R. Zheng, W. S. Yan, B. C. Weng, H. S. Hou, X. B. Ji, *Nano Energy* 91 (2022), 106675.
- [7] S. J. Wang, H. Y. Wang, C. Q. Huang, P. C. Ye, X. T. Luo, J. Q. Ning, Y. J. Zhong, Y. Hu, *Appl. Catal. B Environ.* 298 (2021), 120512.
- [8] C. H. Zhou, X. Chen, S. Liu, Y. Han, H. B. Meng, Q. Y. Jiang, S. M. Zhao, F. Wei, J. Sun, T. Tan, R. F. Zhang, *J. Am. Chem. Soc.* 144 (2022) 2694-2704.
- [9] Y. Q. Li, Z. H. Yin, M. Cui, S. R. Chen, T. L. Ma, *Mater. Today Energy* 18 (2020), 100565.
- [10] G. J. Li, Y. B. Tang, T. T. Fu, Y. Xiang, Z. P. Xiong, Y. J. Si, C. Z. Guo, Z. Q. Jiang, *Chem. Eng. J.* 429 (2022), 132174.
- [11] K. Sheng, Q. F. Yi, A-L. Chen, Y. B. Wang, Y. H. Yan, H. D. Nie, X. L. Zhou, *ACS Appl. Mater. Interfaces* 13 (2021) 45394-45405.
- [12] B. Li, H. G. Xue, H. Pang, Q. Xu, *Sci. China Chem.* 63 (2020) 475-482.
- [13] J. M. Li, Y. M. Kang, D. Liu, Z. Q. Lei, P. Liu, *ACS Appl. Mater. Interfaces* 12 (2020) 5717-5729.
- [14] Q. Shi, Q. Liu, Y. Ma, Z. Fang, Z. Liang, G. Shao, B. Tang, W. Y. Yang, L. Qin, X. S. Fang, *Adv. Energy Mater.* 10 (2020) 1903854.
- [15] H. S. Shang, W. M. Sun, R. Sui, J. J. Pei, L. R. Zheng, J. C. Dong, Z. L. Jiang, D. N. Zhou, Z. B. Zhuang, W. X. Chen, J. T. Zhang, D. S. Wang, Y. D. Li, *Nano Lett.* 20 (2020) 5443-5450.
- [16] R.-M. Sun, L. Zhang, J.-J. Feng, K.-M. Fang, A.-J. Wang, *J. Colloid Interface Sci.* 608 (2022) 2100-2110.
- [17] S.-Y. Lin, Y.-P. Chen, Y. Cao, L. Zhang, J.-J. Feng, A.-J. Wang, *J. Power Sources* 521 (2022), 230926.
- [18] C. Du, Y. J. Gao, J. G. Wang, W. Chen, *J. Mater. Chem. A* 8 (2020) 9981.
- [19] H. W. Zhang, M. Q. Zhao, H. R. Liu, S. R. Shi, Z. H. Wang, B. Zhang, L. Song, J. Z. Shang, Y. Yang, C. Ma, L. R. Zheng, Y. H. Han, W. Huang, *Nano Lett.* 21 (2021) 2255-2264.

- [20] B. Wang, L. Xu, G. P. Liu, Y. Z. Ye, Y. Quan, C. T. Wang, W. X. Wei, W. S. Zhu, C. X. Xu, H. M. Li, J. X. Xia, *J. Alloys Compd.* 826 (2020), 154152.
- [21] Y. F. Ma, W. H. Chen, Z. Q. Jiang, X. N. Tian, X. Y. WangGuo, G. L. Chen, Z.-J. Jiang, *J. Mater. Chem. A* (2022), Accepted Manuscript.
- [22] Y. Y. Wang, A. Kumar, M. Ma, Y. Jia, Y. Wang, Y. Zhang, G. X. Zhang, X. M. Sun, Z. F. Yan, *Nano Res.* 13 (2020) 1090-1099.
- [23] T. Gong, P. P. Sun, X. Xie, D. Zhang, Y. A. Wei, B. Li, N. Huang, L. Fang, X. W. Lv, X. H. Sun, *Appl. Surf. Sci.* 562 (2021), 150112.
- [24] T.-B. Yang, K.-Y. Zhou, G.-Y. Chen, W.-X. Zhang, J.-C. Liang, *RSC Adv.* 7 (2017), 33012.
- [25] Z.-Q. Cao, M.-Z. Wu, H.-B. Hu, G.-J. Liang, C.-Y. Zhi, *NPG Asia Mater.* 10 (2018) 670-684.
- [26] B. Y. Xia, Y. Yan, N. Li, H. B. Wu, X. W. Lou, X. Wang, *Nat. Energy* 1 (2016), 15006.
- [27] J. T. Zhang, Z. H. Zhao, Z. H. Xia, L. M. Dai, *Nat. Nanotechnol.* 10 (2015), 444.
- [28] J. Wang, H. Zhao, Y. Gao, D. J. Chen, C. Chen, M. Saccoccio, F. Ciucci, *Int. J. Hydrogen Energy* 41 (2016) 10744-10754.
- [29] Y. T. Meng, W. Q. Song, H. Huang, Z. Ren, S.-Y. Chen, S. L. Suib, *J. Am. Chem. Soc.* 136 (2014) 11452-11464.
- [30] C. Li, X. P. Han, F. Y. Cheng, Y. X. Hu, C. C. Chen, J. Chen, *Nat. Commun.* 6 (2015), 7345.
- [31] P. Gayen, S. Saha, K. Bhattacharyya, V. K. Ramani, *ACS Catal.* 10 (2020) 7734-7746.
- [32] J. Q. Ran, T. T. Wang, J. Y. Zhang, C. L. Xu, Y. G. Liu, S. B. Xi, D. Q. Gao, *Chem. Mater.* 32 (2020) 3439-3446.
- [33] R. Majee, T. Das, S. Chakraborty, S. Bhattacharyya, *ACS Appl. Mater. Interfaces* 12 (2020) 40355-40363.
- [34] J. Park, M. Risch, G. Nam, M. Park, T. J. Shin, S. Park, M. G. Kim, Y. Shao-Horn, J. Cho, *Energy Environ. Sci.* 10 (2017) 129-136.
- [35] J. Park, M. Park, G. Nam, M.-G. Kim, J. Cho, *Nano Lett.* 17 (2017) 3974-3981.