

Supporting Information

Integrating Single Atoms with Nanoparticles Catalysts for Efficient

Electrochemical Energy Conversion

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Table S1. Performance of SA/NPCs in different electrocatalytic reactions.

Catalysts	Single atoms	Nano particles	Performance	Type	Electrolyte (M)	Ref.
Fe/NC	FeN ₄	Fe	$E_{1/2} = 0.90$ V	ORR	KOH (1.0)	1
			$E_{1/2} = 0.71$ V		H ₂ SO ₄ (1.0)	
Fe-N-HMCTs	FeN _x	Fe ₃ C	$E_{1/2} = 0.872$ V	ORR	KOH (0.1)	2
			$E_{1/2} = 0.71$ V		H ₂ SO ₄ (0.5)	
Fe SAs/NPs@NC	Fe	Fe	$E_{1/2} = 0.898$ V	ORR	KOH (0.1)	3
Pt ₃ Co/FeN ₄ -C	FeN ₄	Pt ₃ Co	$E_{1/2} = 0.90$ V	ORR	HClO ₄ (0.1)	4
Pt-Fe-N-C	Pt/Fe	PtFe	$E_{1/2} = 0.909$ V	ORR	HClO ₄ (0.1)	5
Fe/Meso-NC-1000	Fe	Fe	$E_{1/2} = 0.885$ V	ORR	KOH (0.1)	6
FeN ₃ -Pd@NC NB	FeN ₃	Pd	$E_{1/2} = 0.926$ V	ORR	KOH (0.1)	7
FeSA-FeNC@NSC	Fe	Fe	$E_{1/2} = 0.90$ V	ORR	KOH (0.1)	8

Co-SAs/SNPs@NC	Co	Co	$E_{1/2} = 0.898$ V	ORR	KOH (0.1)	9
Cu ₁ Co _p -N-C	Cu	Co	$E_{1/2} = 0.87$ V	ORR	KOH (0.1)	10
Co ₃ Fe ₇ @Co/Fe-SAC	CoFe	Co ₃ Fe ₇	$E_{1/2} = 0.84$ V	ORR	KOH (0.1)	11
Fe _{NPs} /MnFe _{SAs} -NC	Mn/Fe	Fe	$E_{1/2} = 0.91$ V	ORR	KOH (0.1)	12
Fe ₃ O ₄ @FeNC	Fe	Fe ₃ O ₄	$E_{1/2} = 0.89$ V	ORR	KOH (0.1)	13
FeSA/FeAC-NC 900	Fe	Fe	$E_{1/2} = 0.90$ V	ORR	KOH (0.1)	14
			$E_{1/2} = 0.80$ V		HClO ₄ (0.1)	
nPtCo/NC	CoN ₄	Pt ₃ Co	$E_{1/2} = 0.89$ V	ORR	HClO ₄ (0.1)	15
Catalysts	Single atoms	Nano particles	Performance	Type	Electrolyte (M)	Ref.
Co-NCS-2	Co	Co	$E_{1/2} = 0.90$ V	ORR	KOH (0.1)	16
RuCo@NC	Co-N _x	RuCo	$E_{j=10} = 1.46$ V	OER	KOH (1.0)	17
Ni SAs/Fe-NiOOH	NiC ₄	Fe- NiOOH	$E_{j=10} = 1.499$ V	OER	KOH (1.0)	18
Co _n Ir ₁ /N-C	Ir	Co	$E_{j=10} = 1.492$ V	OER	KOH (1.0)	19
Cu/Rh(SAs)+ Cu ₂ Rh(NPs)/G	CuRu	Cu ₂ Rh	$\eta_{10} = 8$ mV	HER	H ₂ SO ₄ (0.5)	20
Ru/Co@OG	Co	Ru	$\eta_{10} = 13$ mV	HER	KOH (1.0)	21
Ru@Co-SAs/N-C	Co	Ru	$\eta_{10} = 7$ mV	HER	KOH (1.0)	22
			$\eta_{10} = 57$ mV		H ₂ SO ₄ (0.5)	
Ru/Fe-N-C	Ru-N ₄	Ru	$\eta_{10} = 9$ mV	HER	KOH (1.0)	23
	Fe-N-C					
Ni SA/NP-NCF-800	Ni-N ₄	Ni	$\eta_{10} = 137.3$ mV	HER	KOH (1.0)	24
Ru _{NP} -Ru _{SA} @CFN-	Ru	Ru	$\eta_{10} = 33$ mV	HER	KOH (1.0)	25

Ru _{NP} @RuN _x - OFC/NC	Ru	Ru	$\eta_{10} = 19 \text{ mV}$ $\eta_{10} = 10 \text{ mV}$ $\eta_{10} = 71 \text{ mV}$	HER	KOH (1.0) H ₂ SO ₄ (0.5) KOH (1.0)	26
CoSe/Co-N-C	Co	CoCe	$\eta_{10} = 63 \text{ mV}$ $\eta_{10} = 128 \text{ mV}$	HER	H ₂ SO ₄ (0.5) PBS (1.0)	27
Ni SAs-Pd@NC	Ni	Pd	$E_{1/2} = 0.84 \text{ V}$ $E_{j=10} = 1.61 \text{ V}$	ORR OER	KOH (0.1)	28
Catalysts	Single atoms	Nano particles	Performance	Type	Electrolyte (M)	Ref.
Co _{SA} &Co _{NP-10}	Co	Co	$E_{1/2} = 0.86 \text{ V}$ $E_{j=10} = 1.62 \text{ V}$	ORR OER	KOH (0.1)	29
Co@NCNT/Co- SA@NCMT	Co	Co	$E_{1/2} = 0.870 \text{ V}$ $E_{j=10} = 1.6 \text{ V}$	ORR OER	KOH (1.0)	30
Co@N-C/PCNF	Co	Co	$E_{1/2} = 0.85 \text{ V}$ $E_{j=10} = 1.519 \text{ V}$	ORR OER	KOH (0.1) KOH (1.0)	31
CNT@CoSA- Co/NCP	Co	Co	$E_{1/2} = 0.87 \text{ V}$ $E_{j=10} = 1.61 \text{ V}$	ORR OER	KOH (0.1) KOH (1.0)	32
CoNP- CoSA@DSCB	Co	Co	$E_{1/2} = 0.886 \text{ V}$ $E_{j=10} = 1.571 \text{ V}$	ORR OER	KOH (0.1) KOH (1.0)	33
Co-Co ₃ O ₄ @NAC	Co	Co ₃ O ₄	$E_{1/2} = 0.795 \text{ V}$ $E_{j=10} = 1.61 \text{ V}$	ORR OER	KOH (0.1)	34
RuCo@Co-N-C	Co	RuCo	$E_{1/2} = 0.90 \text{ V}$ $E_{j=10} = 1.55 \text{ V}$	ORR OER	KOH (0.1) KOH (1.0)	35

CoNi/Co-N@HNC	Co	CoNi	$E_{1/2} = 0.86 \text{ V}$	ORR	KOH (0.1)	36
			$E_{j=10} = 1.59 \text{ V}$	OER		
NiFe@C@Co CNFs	Co	NiFe	$E_{1/2} = 0.87 \text{ V}$	ORR	KOH (0.1)	37
			$E_{j=10} = 1.57 \text{ V}$	OER	KOH (1.0)	
SD-Fe-N/C	Fe	Fe	$E_{1/2} = 0.852 \text{ V}$	ORR	KOH (0.1)	38
			$E_{j=10} = 1.565 \text{ V}$	OER		
Fe-N-C/Fe ₃ C-op	Fe	Fe ₃ C	$E_{1/2} = 0.911 \text{ V}$	ORR	KOH (0.1)	39
			$E_{j=10} = 1.579 \text{ V}$	OER	KOH (1.0)	

Catalysts	Single atoms	Nano particles	Performance	Type	Electrolyte (M)	Ref.
FePc CNTs NiCo/CP	Fe	NiCo	$E_{1/2} = 0.89 \text{ V}$	ORR	KOH (0.1)	40
			$E_{j=10} = 1.58 \text{ V}$	OER		
H-CoFe@NCNF	Fe	Co _{5.47} N	$E_{1/2} = 0.77 \text{ V}$	ORR	KOH (0.1)	41
			$E_{j=10} = 1.68 \text{ V}$	OER		
FePc NiFe ₂ O ₄ /G	Fe	NiFe ₂ O ₄	$E_{1/2} = 0.85 \text{ V}$	ORR	KOH (0.1)	42
			$E_{j=10} = 1.57 \text{ V}$	OER		
FeCo NPs/NC	FeCo	FeCo	$E_{1/2} = 0.82 \text{ V}$	ORR	KOH (0.1)	43
			$E_{j=10} = 1.49 \text{ V}$	OER	KOH (1.0)	
SA&NP-FeCo-NTS	FeN ₄	FeCo	$E_{1/2} = 0.87 \text{ V}$	ORR	KOH (0.1)	44
	CoN ₄		$E_{j=10} = 1.58 \text{ V}$	OER	KOH (1.0)	
Fe/Ni-NC FeNi@G	FeNi	FeNi	$E_{1/2} = 0.885 \text{ V}$	ORR	KOH (0.1)	45
			$E_{j=10} = 1.503 \text{ V}$	OER	KOH (1.0)	
Ni, Fe-DSAs/NCs	NiFe	NiFe	$E_{1/2} = 0.895 \text{ V}$	ORR	KOH (0.1)	4
			$E_{j=10} = 1.612 \text{ V}$	OER		

metal/NG	AuPtIr	AuPtIr	$E_{1/2} = 0.855 \text{ V}$	ORR	KOH (0.1)	46
			$E_{j=10} = 1.493 \text{ V}$	OER	KOH (1.0)	
$\text{Ni}_{\text{SA}}\text{Fe}_{\text{SA}}\text{-Ni}_x\text{Fe/CNT}$	NiFe	NiFe	$E_{j=10} = 1.457 \text{ V}$	OER	KOH (1.0)	47
			$\eta_{10} = 64 \text{ mV}$	HER		
CoRu-MoS ₂	Co	Ru	$E_{j=10} = 1.538 \text{ V}$	OER	KOH (1.0)	48
			$\eta_{10} = 52 \text{ mV}$	HER		
CoNG/Ru	Co	Ru	$E_{j=10} = 1.58 \text{ V}$	OER	KOH (1.0)	49
			$\eta_{10} = 15 \text{ mV}$	HER		

Catalysts	Single atoms	Nano particles	Performance	Type	Electrolyte (M)	Ref.
Mo-CoP/Co-N-C	Co	Mo-CoP	$E_{j=10} = 1.431 \text{ V}$	OER	KOH (1.0)	50
			$\eta_{10} = 45 \text{ mV}$	HER		
$\text{Cu}_{1+n}/\text{BDNC}$	Cu	Cu	$E_{j=10} = 1.43 \text{ V}$	OER	KOH (1.0)	51
			$\eta_{10} = 216 \text{ mV}$	HER		
Au-Fe ₁ NC/NF	Fe	Au	$E_{j=10} = 1.476 \text{ V}$	OER	KOH (1.0)	52
			$\eta_{10} = 35.6 \text{ mV}$	HER		
FeCoSe@NCNSs	Fe	CoSe	$E_{j=10} = 1.55 \text{ V}$	OER	KOH (1.0)	53
			$\eta_{10} = 99 \text{ mV}$	HER		
Ir-SA@Fe@NCNT	Ir	Fe	$E_{j=10} = 1.48 \text{ V}$	OER	H ₂ SO ₄ (0.5)	54
			$\eta_{10} = 26 \text{ mV}$	HER		
CoNC	Co	Co	$E_{j=10} = 1.459 \text{ V}$	OER	KOH (1.0)	55
			$\eta_{10} = 36 \text{ mV}$	HER	KOH (1.0)	
			$E_{1/2} = 0.858 \text{ V}$	ORR	KOH (0.1)	

CoSA + Co ₉ S ₈ /HCNT	Co	Co ₉ S ₈	$E_{j=10} = 1.56 \text{ V}$	OER	KOH (0.1)	56
			$\eta_{10} = 250 \text{ mV}$	HER	KOH (1.0)	
			$E_{1/2} = 0.855 \text{ V}$	ORR	KOH (0.1)	

References

1. M. Liu, J. Lee, T. C. Yang, F. Zheng, J. Zhao, C. M. Yang and L. Y. S. Lee, *Small Methods*, 2021, **5**, 2001165.
2. X. Cui, L. Gao, S. Lei, S. Liang, J. Zhang, C. D. Sewell, W. Xue, Q. Liu, Z. Lin and Y. Yang, *Adv. Funct. Mater.*, 2021, **31**, 2170064.
3. W.-J. Niu, Y.-Y. Yan, R.-J. Li, W.-W. Zhao, J.-L. Chen, M.-J. Liu, B. Gu, W.-W. Liu and Y.-L. Chueh, *Chem. Eng. J.*, 2023, **456**, 140858.
4. Z. Wang, X. Jin, R. Xu, Z. Yang, S. Ma, T. Yan, C. Zhu, J. Fang, Y. Liu, S.-J. Hwang, Z. Pan and H. J. Fan, *ACS Nano*, 2023, **17**, 8622-8633.
5. Z. Qiao, C. Wang, C. Li, Y. Zeng, S. Hwang, B. Li, S. Karakalos, J. Park, A. J. Kropf and E. C. Wegener, *Energy Environ. Sci.*, 2021, **14**, 4948-4960.
6. S. N. Zhao, J. K. Li, R. Wang, J. Cai and S. Q. Zang, *Adv. Mater.*, 2022, **34**, 2107291.
7. Z. Lin, A. Yang, B. Zhang, B. Liu, J. Zhu, Y. Tang and X. Qiu, *Adv. Funct. Mater.*, 2022, **32**, 2107683.
8. W. Zhai, S. Huang, C. Lu, X. Tang, L. Li, B. Huang, T. Hu, K. Yuan, X. Zhuang and Y. Chen, *Small*, 2022, **18**, 2107225.
9. Z. Wang, C. Zhu, H. Tan, J. Liu, L. Xu, Y. Zhang, Y. Liu, X. Zou, Z. Liu and X. Lu, *Adv. Funct. Mater.*, 2021, **31**, 2104735.
10. C. Zhang, J. Liu, Y. Zhang, W. Yang and H. Lu, *Appl. Surf. Sci.*, 2023, **611**, 155779.
11. B. Liu, S. Wang, R. Feng, Y. Ni, F. Song and Q. Liu, *ACS Appl. Mater. Interfaces*, 2022, **14**, 38739-38749.
12. J. Bai, Y. Fu, P. Zhou, P. Xu, L. Wang, J. Zhang, X. Jiang, Q. Zhou and Y. Deng, *ACS Appl. Mater. Interfaces*, 2022, **14**, 29986-29992.
13. S. Hu, W. Ni, D. Yang, C. Ma, J. Zhang, J. Duan, Y. Gao and S. Zhang, *Carbon*, 2020, **162**, 245-255.
14. F.-Y. Zheng, R. Li, S. Xi, F. Ai and J. Wang, *J. Mater. Chem. A*, 2023, **11**, 8202-8212.
15. X. Li, Y. He, S. Cheng, B. Li, Y. Zeng, Z. Xie, Q. Meng, L. Ma, K. Kisslinger

- and X. Tong, *Adv. Mater.*, 2021, **33**, 2106371.
16. C. Shi, Y. Liu, R. Qi, J. Li, J. Zhu, R. Yu, S. Li, X. Hong, J. Wu and S. Xi, *Nano Energy*, 2021, **87**, 106153.
 17. B. Sarkar, D. Das and K. K. Nanda, *Green Chem.*, 2020, **22**, 7884-7895.
 18. H. Liu, X. Xu, H. Xu, S. Wang, Z. Niu, Q. Jia, L. Yang, R. Cao, L. Zheng and D. Cao, *Appl. Catal. B*, 2021, **297**, 120451.
 19. X. Ding, C. Jia, P. Ma, H. Chen, J. Xue, D. Wang, R. Wang, H. Cao, M. Zuo, S. Zhou, Z. Zhang, J. Zeng and J. Bao, *Nano Lett.*, 2023, **23**, 3309-3316.
 20. S. Sultan, M. H. Diorizky, M. Ha, J. N. Tiwari, H. Choi, N. K. Dang, P. Thangavel, J. H. Lee, H. Y. Jeong and H. S. Shin, *J. Mater. Chem. A*, 2021, **9**, 10326-10334.
 21. P. Su, W. Pei, X. Wang, Y. Ma, Q. Jiang, J. Liang, S. Zhou, J. Zhao, J. Liu and G. Q. Lu, *Angew. Chem. Int. Ed. Engl.*, 2021, **60**, 16044-16050.
 22. S. Yuan, Z. Pu, H. Zhou, J. Yu, I. S. Amiinu, J. Zhu, Q. Liang, J. Yang, D. He and Z. Hu, *Nano Energy*, 2019, **59**, 472-480.
 23. C. Hu, E. Song, M. Wang, W. Chen, F. Huang, Z. Feng, J. Liu and J. Wang, *Adv. Sci.*, 2021, **8**, 2001881.
 24. J. Yu, J. Li, C.-Y. Xu, Q. Liu, J. Liu, R. Chen, J. Zhu, R. Li and J. Wang, *Carbon*, 2021, **185**, 96-104.
 25. T. Luo, J. Huang, Y. Hu, C. Yuan, J. Chen, L. Cao, K. Kajiyoshi, Y. Liu, Y. Zhao and Z. Li, *Adv. Funct. Mater.*, 2023, **33**, 2213058.
 26. Y. Feng, W. Feng, J. Wan, J. Chen, H. Wang, S. Li, T. Luo, Y. Hu, C. Yuan and L. Cao, *Appl. Catal. B*, 2022, **307**, 121193.
 27. S. Che, N. Ta, F. Yang, X. Yan, H. Liu, N. Chen, S. Sun, C. Wang, B. Jiang and Y. Sun, *Mater. Chem. Front.*, 2022, **6**, 3577-3588.
 28. Q. Lu, H. Wu, X. Zheng, Y. Chen, A. Rogach, X. Han, D. Yida and W. Hu, *Adv. Sci.*, 2021, **8**, 2101438.
 29. J. Guo, W. Li, Y. Xu, Y. Mao, Z. Mei, H. Li, Y. He, X. San, K. Xu and X. Liang, *Small Methods*, 2023, **7**, 2201371.
 30. J. Sun, P. Leng, Y. Xie, X. Yu, K. Qu, L. Feng, H. Bao, F. Luo and Z. Yang, *Appl. Catal. B*, 2022, **319**, 121905.
 31. Q. Lu, H. Wu, X. Zheng, Y. Chen, A. L. Rogach, X. Han, Y. Deng and W. Hu, *Adv. Sci.*, 2021, **8**, 2101438.
 32. J.-C. Li, Y. Meng, L. Zhang, G. Li, Z. Shi, P.-X. Hou, C. Liu, H.-M. Cheng and M. Shao, *Adv. Funct. Mater.*, 2021, **31**, 2103360.
 33. J. Hong, M. Chen, L. Zhang, L. Qin, J. Hu, X. Huang, C. Zhou, Y. Zhou, T. Wågberg and G. Hu, *Chem. Eng. J.*, 2023, **455**, 140401.
 34. X. Zhong, W. Yi, Y. Qu, L. Zhang, H. Bai, Y. Zhu, J. Wan, S. Chen, M. Yang, L. Huang, M. Gu, H. Pan and B. Xu, *Appl. Catal. B*, 2020, **260**, 118188.
 35. X. Luo, S. Zhao, Z. Luo, S. Li, X. Zhao, Q. Fang, X. Wei, H. Wang, C. Wang and Z. Zhu, *Chem. Eng. J.*, 2023, **463**, 142184.
 36. Y. Tan, Z. Zhang, Z. Lei, L. Yu, W. Wu, Z. Wang and N. Cheng, *Appl. Catal. B*, 2021, **304**, 121006.
 37. X. Chen, J. Pu, X. Hu, Y. Yao, Y. Dou, J. Jiang and W. Zhang, *Small*, 2022, **18**, 2200578.
 38. J.-C. Li, Y. Meng, H. Zhong, L. Zhang, S. Ding, Z. Lyu Or Lv, S. Beckman, P.-X. Hou, Y. Mei, H.-M. Cheng and C. Liu, *Carbon*, 2023, **205**, 302-309.
 39. J. Chang, Q. Zhang, J. Yu, W. Jing, S. Wang, G. Yin, G. Waterhouse and S. Lu, *Adv. Sci.*, 2023, **10**, 2301656.
 40. S. Ding, L. He, L. Fang, Y. Zhu, T. Li, Z. Lyu Or Lv, D. Du, Y. Lin and J.-C. Li,

- Adv. Energy Mater.*, 2022, **12**, 2202984.
41. X. Zhang, P. Yu, G. Xing, Y. Xie, X. Zhang, G. Zhang, S. Fanfei and L. Wang, *Small*, 2022, **18**, 2205228.
 42. H. Hu, Y. Meng, Y. Mei, P. X. Hou, C. Liu, H. M. Cheng, M. Shao and J. C. Li, *Energy Stor. Mater.*, 2023, **54**, 517-523.
 43. D. Xie, D. Yu, Y. Hao, S. Han, G. Li, X. Wu, F. Hu, L. Li, H.-Y. Chen, Y.-F. Liao and S. Peng, *Small* 2021, **17**, 2007239.
 44. Q. Zhang, P. Liu, X. Fu, Y. Yuan, L. Wang, R. Gao, L. Zheng, L. Yang and Z. Bai, *Adv. Funct. Mater.*, 2022, **32**, 2112805.
 45. Z. Xu, G. Chen, F. Yang, J. Jang, G. Liu, F. Xiao, Y. Sun, X. Qiu, W. Chen, D. Su, M. Gu and M. Shao, *Electrochim. Acta*, 2023, **458**, 142549.
 46. X. Lin, H. Yixuan, K. Hu, X. Lin, G. Xie, X. Liu, K. Reddy and H.-J. Qiu, *ACS Mater. Lett.*, 2022, **4**, 978-986.
 47. W. Luo, Y. Wang, L. Luo, S. Gong, M. Wei, Y. Li, X. Gan, Y. Zhao, Z. Zhu and Z. Li, *ACS Catal.*, 2022, **12**, 1167-1179.
 48. I. S. Kwon, T. T. Debela, I. H. Kwak, Y. C. Park, J. Seo, J. Y. Shim, S. J. Yoo, J. G. Kim, J. Park and H. S. Kang, *Small*, 2020, **16**, 2000081.
 49. T. He, Y. Peng, Q. Li, J. Lu, Q. Liu, R. Mercado, Y. Chen, F. Nichols, Y. Zhang and S. Chen, *ACS Appl. Mater. Interfaces*, 2019, **11**, 46912–46919.
 50. G. Li, F. Yang, S. Che, H. Liu, N. Chen, J. Qian, C. Yu, B. Jiang, M. Liu and Y. Li, *J Mater Sci Technol*, 2023, **166**, 58-66.
 51. W. Zhang, R. Liu, Z. Fan, H. Wen, Y. Chen, R. Lin, Y. Zhu, X. Yang, Z. Chen and W. Zhang, *Inorg. Chem. Front.*, 2023, **10**, 443-453.
 52. Y. Q. Sun, J. Q. Luo, M. X. Zhang, J. Li, J. K. Yu, S. Y. Lu, W. Y. Song, Y. C. Wei, Z. X. Li and J. Liu, *ACS Appl. Mater. Interfaces*, 2023, **18**, 10696–10708.
 53. Y. Pan, M. Wang, M. Li, G. Sun, Y. Chen, Y. Liu, W. Zhu and B. Wang, *J. Energy Chem.*, 2022, **68**, 699-708.
 54. F. Luo, H. Hu, X. Zhao, Z. Yang, Q. Zhang, J. Xu, T. Kaneko, Y. Yoshida, C. Zhu and W. Cai, *Nano Lett.*, 2020, **20**, 2120-2128.
 55. H. J. Son, M. J. Kim and S. H. Ahn, *Chem. Eng. J.*, 2021, **414**, 128739.
 56. Y. Li, R. Cao, L. Li, X. Tang, T. Chu, B. Huang, K. Yuan and Y. Chen, *Small*, 2020, **16**, 1906735.