

Cu₃N Nanoparticles with Both (100) and (111) Facets for Enhancing the Selectivity and Activity of CO₂ Electroreduction to Ethylene

Hongzhi Wang, Xinze Bi, Yuezhu Zhao, Zhongxue Yang, Zhaoliang Wang,* Mingbo Wu*

Table. S1 Comparison of the activities of Cu₃N NPs with the reported catalysts for CO₂RR.

Catalyst	Electrolyte	Potential (vs. RHE)	Total j [mA cm ⁻²]	FE of ethylene	Reference
44 nm Cu nanocubes	KHCO ₃ (0.1M)	-1.1 V	≈3	41%	[1]
250 nm Cu cubes on Cu foils	KHCO ₃ (0.1M)	≈-1.03 V	n/a	48%	[2]
240 nm Cu cubes pre-treated with O ₂ plasma	KHCO ₃ (0.1M)	-1.0 V	≈34.8	45%	[3]
Star decahedron Cu	KHCO ₃ (0.1M)	-0.993 V	≈19	52.43%	[4]
Nanodeficient Cu nanosheets	K ₂ SO ₄ (0.1 M)	-1.18 V	58.8	83.20%	[5]
Graphite/carbon NPs/Cu/PTFE electrode	KOH (7 M)	-0.55 V	100	70%	[6]
Truncated-octahedral Cu ₂ O	KHCO ₃ (0.5M)	-1.1 V	≈37	59%	[7]
Branched CuO nanoparticles	KHCO ₃ (0.1M)	-1.05 V	≈25.3	68%	[8]
Electrochemical fragmented Cu ₂ O nanoparticles	KHCO ₃ (0.1M)	-1.1 V	≈17.5	27% to 57.3%	[9]
Cu ₃ N-derived Cu nanowires	KHCO ₃ (0.1M)	-1.0 V	≈56.8	66%	[10]
CuCl-derived Cu	KHCO ₃ (0.05M)	-2.6 V vs. Ag/AgCl	17	56%	[11]
HKUST-1-derived Cu cluster	KOH (0.1 M)	-1.07 V	262	45%	[12]
Phase-separated CuPd	KOH (0.1 M)	-0.74 V	360.5	≈48%	[13]
CuAg wire (Ag 6%)	KOH (1 M)	-0.68 V	≈300	55.20%	[14]
Dealloyed Cu–Al	KOH (1 M)	-1.5 V	400	80%	[15]
B-doped Cu	KHCO ₃ (0.1M)	-1.1 V	70	53%	[16]
F-modified Cu	KOH (0.75 M)	-0.89 V	1600	65%	[17]
Cu–PANI nanocatalyst	KHCO ₃ (0.1M)	-1.13 V	34.7	48.80%	[18]
EDTA-modified porous hollow Cu microspheres	KHCO ₃ (0.1M)	-0.82 V	≈7.5	50.10%	[19]
N-Aryl-dihydropyridine-based oligomer modified Cu	KHCO ₃ (1M)	-0.83 V	319	72%	[20]
Cu ₃ N NPs with both (100) and (111) facets	KHCO ₃ (0.1M)	-0.8 V	60	61.1%	This work

[1] A. Loiudice, P. Lobaccaro, E. A. Kamali, T. Thao, B. H. Huang, J. W. Ager and R. Buonsanti, *Angew. Chem., Int. Ed.*, 2016, **55**, 5789.

[2] P. Grosse, D. Gao, F. Scholten, I. Sinev, H. Mistry and B. R. Cuenya, *Angew. Chem., Int. Ed.*, 2018, **57**, 6192.

[3] D. Gao, I. Zegkinoglou, N. J. Divins, F. Scholten, I. Sinev, P. Grosse and B. R. Cuenya, *ACS Nano*, 2017, **11**, 4825.

[4] C. Choi, T. Cheng, M. F. Espinosa, H. Fei, X. Duan, W. A. Goddard and Y. Huang, *Adv. Mater.*, 2019, **31**, 1805405.

- [5] B. Zhang, J. Zhang, M. Hua, Q. Wan, Z. Su, X. Tan, L. Liu, F. Zhang, G. Chen, D. Tan, X. Cheng, B. Han, L. Zheng and G. Mo, *J. Am. Chem. Soc.*, 2020, **142**, 13606.
- [6] C. T. Dinh, T. Burdyny, M. G. Kibria, A. Seifitokaldani, C. M. Gabardo, F. P. García de Arquer, A. Kiani, J. P. Edwards, P. De Luna, O. S. Bushuyev, C. Zou, R. Quintero-Bermudez, Y. Pang, D. Sinton and E. H. Sargent, *Science*, 2018, **360**, 783.
- [7] Y. Gao, Q. Wu, X. Liang, Z. Wang, Z. Zheng, P. Wang, Y. Liu, Y. Dai, M. H. Whangbo and B. Huang, *Adv. Sci.*, 2020, **7**, 1902820.
- [8] J. Kim, W. Choi, J. W. Park, C. Kim, M. Kim and H. Song, *J. Am. Chem. Soc.*, 2019, **141**, 6986.
- [9] H. Jung, S. Y. Lee, C. W. Lee, M. K. Cho, D. H. Won, C. Kim, H. S. Oh, B. K. Min and Y. J. Hwang, *J. Am. Chem. Soc.*, 2019, **141**, 4624.
- [10] Y. Mi, S. Shen, X. Peng, H. Bao, X. Liu, J. Luo, *ChemElectroChem*, 2019, **6**, 2393.
- [11] M. G. Kibria, C. T. Dinh, A. Seifitokaldani, P. D. Luna, T. Burdyny, R. Q. Bermudez, M. B. Ross, O. S. Bushuyev, F. P. García de Arquer, P. Yang, D. Sinton and E. H. Sargent, *Adv. Mater.*, 2018, **30**, 1804867.
- [12] D. H. Nam, O. S. Bushuyev, J. Li, P. De Luna, A. Seifitokaldani, C. T. Dinh, F. P. García de Arquer, Y. Wang, Z. Liang, A. H. Proppe, C. S. Tan, P. Todorović, O. Shekhah, C. M. Gabardo, J. W. Jo, J. Choi, M.-J. Choi, S.-W. Baek, J. Kim, D. Sinton, S. O. Kelley, M. Eddaoudi and E. H. Sargent, *J. Am. Chem. Soc.*, 2018, **140**, 11378.
- [13] S. Ma, M. Sadakiyo, M. Heima, R. Luo, R. T. Haasch, J. I. Gold, M. Yamauchi and P. J. A. Kenis, *J. Am. Chem. Soc.*, 2017, **139**, 47.
- [14] T. T. H. Hoang, S. Verma, S. Ma, T. T. Fister, J. Timoshenko, A. I. Frenkel, P. J. A. Kenis and A. A. Gewirth, *J. Am. Chem. Soc.*, 2018, **140**, 5791.
- [15] M. Zhong, K. Tran, Y. Min, C. Wang, Z. Wang, C.-T. Dinh, P. De Luna, Z. Yu, A. S. Rasouli, P. Brodersen, S. Sun, O. Voznyy, C. S. Tan, M. Askerka, F. Che, M. Liu, A. Seifitokaldani, Y. Pang, S. C. Lo, A. Ip, Z. Ulissi and E. H. Sargent, *Nature*, 2020, **581**, 178.
- [16] Y. Zhou, F. Che, M. Liu, C. Zou, Z. Liang, P. De Luna, H. Yuan, J. Li, Z. Wang, H. Xie, H. Li, P. Chen, E. Bladt, R. Q. Bermudez, T. K. Shan, S. Bals, J. Hofkens, D. Sinton, G. Chen and E. H. Sargent, *Nat. Chem.*, 2018, **10**, 974.
- [17] W. Ma, S. Xie, T. Liu, Q. Fan, J. Ye, F. Sun, Z. Jiang, Q. Zhang, J. Cheng and Y. Wang, *Nat. Catal.*, 2020, **3**, 478.
- [18] X. Wei, Z. Yin, K. Lyu, Z. Li, J. Gong, G. Wang, L. Xiao, J. Lu, L. Zhuang, *ACS Catal.*, 2020, **10**, 4103.
- [19] J. Liu, J. Fu, Y. Zhou, W. Zhu, L. P. Jiang, Y. Lin, *Nano Lett.*, 2020, **20**, 4823.
- [20] F. Li, A. Thevenon, A. Rosas-Hernández, Z. Wang, Y. Li, C. M. Gabardo, A. Ozden, C. T. Dinh, J. Li, Y. Wang, J. P. Edwards, Y. Xu, C. McCallum, L. Tao, Z. Q. Liang, M. Luo, X. Wang, H. Li, C. P. O'Brien, C. S. Tan, D. H. Nam, R. Q. Bermudez, T. T. Zhuang, Y. C. Li, Z. Han, R. D. Britt, D. Sinton, T. Agapie, J. C. Peters and E. H. Sargent, *Nature*, 2020, **577**, 509.