

Supporting information

Regulation of intrinsic physicochemical properties of metal oxide nanomaterials for energy conversion and environmental detection applications

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Table S1 Detailed comparison of OER activity for metal oxide nanomaterials with different size

Metal oxide nanomaterials	Size(nm)	BET SA (m ² / g)	Potential (mV) at 10 mA/cm ²	Tafel slope (mV dec ⁻¹)	Electrolyte	Ref.
Co ₃ O ₄	5.9	111.2	534	-47±7	1M KOH	S1
	21.1	27.93	569			
	46.9	7.80	588			
Co ₃ O _{4-δ} quantum dots	2	-	270	38.8	1M KOH	S2
NiO	3.3	210	300 (7.5 mA/cm ²)	40	0.5M KOH	S3

Table S2 The intrinsic physicochemical properties of metal oxide nanomaterials and their corresponding performance for electrocatalytic water splitting

Electrocatalysts	Size [nm]	Reactions	Electrolyte	overpotential [mV] at 10 mA cm ⁻²	η Tafel slope [mV dec ⁻¹]	Ref.
Co ₃ O ₄	5.9	OER	1.0 M KOH	534	-47±7	S1
	21.1			569		
	46.9			588		
Co ₃ O _{4-δ} quantum dots	2	OER	1.0 M KOH	270	38.8	S2
NiO	3.3	OER	0.1 M KOH	300 (7.5 mA/cm ²)	40.0	S3
Electrocatalysts	Shape	Reactions	Electrolyte	overpotential [mV] at 10 mA cm ⁻²	η Tafel slope (mV dec ⁻¹)	Ref.
MoO ₂	nanosheets	HER	1.0 M KOH	27	41.0	S4
		OER		200	54.0	
NiCo ₂ O ₄	microcuboids	HER	1.0 M NaOH	50	49.7	S5
		OER		230	53.0	
NiFe-Oxide	nanocubes	HER	1.0 M KOH	271	48.0	S6
		OER		197	58.0	
Co ₃ O ₄	hollow microspheres	OER	0.1 M KOH	~400	-	S7
Co ₃ O ₄	nanoparticle	OER	1.0 M KOH	497	-	S8
Co ₃ O ₄	nanoparticle	OER	1.0 M KOH	314(0.5 mA/cm ²)	-	S9
Co ₃ O ₄	microtube	OER	1.0 M KOH	290	84	S10
Co ₃ O ₄	nano-islands	OER	1.0 M KOH	376	59	S11
Co ₃ O ₄	nanorods	OER	1.0 M KOH	275	-	S12
Co ₃ O ₄	nanowire	OER	0.1 M KOH	290	70	S13
Electrocatalysts	Defect type	Reactions	Electrolyte	overpotential [mV] at 10 mA cm ⁻²	η Tafel slope (mV dec ⁻¹)	Ref.
MoO _{3-x}	OVs	HER	0.1 M KOH	170	56	S14
NiO	OVs	HER	1 M KOH	110	100	S15
NiCo ₂ O ₄	OVs	OER	0.1 M KOH	320	30	S16

Co ₃ O ₄	OVs	OER	0.1 M KOH	220	68	S17
Fe _x Co _y -oxide	OVs	OER	0.1 M KOH	350	36.8	S18
Ca ₂ Mn ₂ O ₅	OVs	OER	0.1 M KOH	100	149	S19
Electrocatalysts	Defect type	Reactions	Electrolyte	overpotential [mV] at 10 mA cm ⁻²	η Tafel slope (mV dec ⁻¹)	Ref.
Co _{3-x} O ₄	MVs	OER	1.0 M KOH	268	38.2	S20
δ -FeOOH	MVs	HER	1.0 M KOH	108	68	S21
		OER		265	53	

Table S3 The intrinsic physicochemical properties of metal oxide nanomaterials and their corresponding performance for photocatalytic water splitting

Catalyst	Size [nm]	Reactor/Parameter	Product (H ₂)	Ref.
Cu ₂ O	50	200 W Hg-Xe lamp, $\lambda > 420$ nm	0.007 $\mu\text{mol g}^{-1} \text{h}^{-1}$	S22
	100		0.009 $\mu\text{mol g}^{-1} \text{h}^{-1}$	
	300		0.012 $\mu\text{mol g}^{-1} \text{h}^{-1}$	
	500		0.013 $\mu\text{mol g}^{-1} \text{h}^{-1}$	
Catalyst	Shape	Reactor/Parameter	Product (H ₂)	Ref.
Conventional Cu ₂ O	nanocubes	200 W Hg-Xe light source	$\sim 1.2 \mu\text{mol g}^{-1} \text{h}^{-1}$	S23
Hierarchical Cu ₂ O			15 $\mu\text{mol g}^{-1} \text{h}^{-1}$	
Cu ₂ O	cubes	300 W Hg lamp, $\lambda > 420$ nm	24.7 $\mu\text{mol h}^{-1}$	S24
	concave cubes		70.5 $\mu\text{mol h}^{-1}$	
	octapods		145.1 $\mu\text{mol h}^{-1}$	
TiO ₂	nanotube	250 W Xe lamp, 1.15 $\times$ 10 ⁵ lx	4.6 mmol h ⁻¹ g ⁻¹	S25
	nanorods		2.9 mmol h ⁻¹ g ⁻¹	
	nanosquares		2.1 mmol h ⁻¹ g ⁻¹	
Catalyst	Defect type	Reactor/Parameter	Product (H ₂)	Ref.
SrTiO ₃	OVs	300 W Xe lamp	2.2 mmol h ⁻¹ g ⁻¹	S26
In ₂ O ₃	OVs	300 W Xe lamp, $\lambda > 420$ nm	-	S27
Catalyst	Defect type	Reactor/Parameter	Product (H ₂)	Ref.
TiO ₂	MVs	300 W Xe lamp, $\lambda > 420$ nm	29.86 mmol h ⁻¹ g ⁻¹	S28
Catalyst	Crystal facets	Reactor/Parameter	Product (H ₂)	Ref.
TiO ₂ Nanobelts	{001} and {101}	300 W Xe lamp, 400 < λ < 800 nm	670 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S29
Solid TiO ₂	{111}	300 W Xe lamp	$\sim 80 \mu\text{mol h}^{-1} \text{g}^{-1}$	S30
mesoporous TiO ₂			$\sim 3.2 \mu\text{mol h}^{-1} \text{g}^{-1}$	
SrTiO ₃	{023} and {001}	300 W Xe lamp	71.1 $\mu\text{mol h}^{-1}$ 30.0 $\mu\text{mol /h}^{-1} (\text{O}_2)$	S31
Cu ₂ O	{100}	300 W Hg lamp, $\lambda > 420$ nm	0.88 $\mu\text{mol h}^{-1}$	S32
	{111}		1.23 $\mu\text{mol h}^{-1}$	
	{544}		1.55 $\mu\text{mol h}^{-1}$	
	{104}		1.88 $\mu\text{mol h}^{-1}$	

WO ₃	{002}	300W Xe lamp, $\lambda > 420$ nm	3 $\mu\text{mol h}^{-1} \text{cm}^{-2}$	S33
α -Fe ₂ O ₃	{012} and {104}	300W Xe lamp, $\lambda > 420$ nm	309.4 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S34
	{101} and {111}		(O ₂) 3.68 $\mu\text{mol h}^{-1} \text{g}^{-1}$ (O ₂)	
BiVO ₄	{040}	300 W Xe lamp, $\lambda \geq 420$ nm	310 mmol h^{-1}	S35

Table S4 The intrinsic physicochemical properties of metal oxide nanomaterials and their corresponding performance for photocatalytic reduction of CO₂

Photocatalyst	Size [nm]	Major Products	Yields	Ref.
TiO ₂	4.5	CH ₄	0.15 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S36
	6		0.29 $\mu\text{mol h}^{-1} \text{g}^{-1}$	
	8		0.31 $\mu\text{mol h}^{-1} \text{g}^{-1}$	
	14		0.37 $\mu\text{mol h}^{-1} \text{g}^{-1}$	
	29		0.27 $\mu\text{mol h}^{-1} \text{g}^{-1}$	
Photocatalyst	Shape	Major Products	Yields	Ref.
W ₁₈ O ₄₉	nanowires	CH ₄	2.2 $\text{mmol L}^{-1} \text{g}^{-1} \text{h}^{-1}$	S37
Bi ₂ WO ₆	nanoplates	CH ₄	1.1 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S38
WO ₃	nanosheets	CH ₄	~1.2 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S39
ZnO-Cu ₂ O	sphere	CH ₄	1080 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S40
Photocatalyst	Crystal facets	Major Products	Yields	Ref.
TiO ₂	{001} and {101}	CH ₄	1.35 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S41
Co ₃ O ₄	{112} and {111}	CO	1672 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S42
	{111}		1238 $\mu\text{mol h}^{-1} \text{g}^{-1}$	
CeO ₂	{100} and {111}	CH ₄	0.86 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S43
BiOI	{001}	CO	0.259 $\mu\text{mol h}^{-1}$	S44
		CH ₄	0.089 $\mu\text{mol h}^{-1}$	
	{100}	CO	0.076 $\mu\text{mol h}^{-1}$	
		CH ₄	0.075 $\mu\text{mol h}^{-1}$	
BiOI/O ₃	{010} and {100}	CO	5.42 $\mu\text{mol h}^{-1} \text{g}^{-1}$	S45

References:

- S1. J. Esswein, M. J. McMurdo, P. N. Ross, A. T. Bell and T. D. Tilley, *J. Phys. Chem. C*, 2009, **113**, 15068-15072.
- S2. G. X. Zhang, J. Yang, H. Wang, H. B. Chen, J. L. Yang and F. Pan, *ACS Appl. Mater. Interfaces*, 2017, **9**, 16159-16167.
- S3. Fominykh, J. M. Feckl, J. Sicklinger, M. Döblinger, S. Böcklein, J. Ziegler, L. Peter, J. Rathousky, E. W. Scheidt, T. Bein and D. Fattakhova-Rohlfing, *Adv. Funct. Mater.*, 2014, **24**, 3123-3129.
- S4. Y. S. Jin, H. T. Wang, J. J. Li, X. Yue, Y. J. Han, P. K. Shen and Y. Cui, *Adv. Mater.*, 2016, **28**, 3785-3790.
- S5. X. H. Gao, H. X. Zhang, Q. G. Li, X. G. Yu, Z. L. Hong, X. W. Zhang, C. D. Liang and Z. Lin, *Angew. Chem. Int. Edit.*, 2016, **55**, 6290-6294.
- S6. A. Kumar and S. Bhattacharyya, *ACS Appl. Mater. Interfaces*, 2017, **9**, 41906-41915.
- S7. J. Zhao, Y. C. Zou, X. X. Zou, T. Y. Bai, Y. P. Liu, R. Q. Gao, D. J. Wang and G. D. Li, *Nanoscale*, 2014, **6**, 7255-7262.
- S8. N. H. Chou, P. N. Ross, A. T. Bell and T. D. Tilley, *ChemSusChem*, 2011, **4**, 1566-1569.

- S9. J. D. Blakemore, H. B. Gray, J. R. Winkler and A. M. Müller, *ACS Catal.*, 2013, **3**, 2497-2500.
- S10. Y. P. Zhu, T. Y. Ma, M. Jaroniec and S. Z. Qiao, *Angew. Chem. Int. Edit.*, 2017, **56**, 1324-1328.
- S11. G. Y. Liu, S. K. Karuturi, A. N. Simonov, M. Fekete, H. J. Chen, N. Nasiri, N. H. Le, P. R. Narangari, M. Lysevych, T. R. Gengenbach, A. Lowe, H. H. Tan, C. Jagadish, L. Spiccia and A. Tricoli, *Adv. Energy Mater.*, 2016, 1600697.
- S12. G. H. Cheng, T. Y. Kou, J. Zhang, C. H. Si, H. Gao and Z. H. Zhang, *Nano Energy*, 2017, **38**, 155-166.
- S13. Y. Ma, S. Dai, M. Jaroniec and S. Z. Qiao, *J. Am. Chem. Soc.*, 2014, **136**, 13925-13931.
- S14. Zhu, F. Shi, X. F. Zhu and W. S. Yang, *Nano Energy*, 2020, **73**, 104761.
- S15. Luo, R. Miao, T. D. Huan, I. M. Mosa, A. S. Poyraz, W. Zhong, J. E. Cloud, D. A. Kriz, S. Thanneeru, J. K. He, Y. S. Zhang, R. Ramprasad and S. L. Suib, *Adv. Energy Mater.*, 2016, 1600528.
- S16. X. D. Zhang and Y. Xie, *Chem. Soc. Rev.*, 2013, **42**, 8187-8199.
- S17. J. Bao, X. D. Zhang, B. Fan, J. J. Zhang, M. Zhou, W. L. Yang, X. Hu, H. Wang, B. C. Pan and Y. Xie, *Angew. Chem. Int. Edit.*, 2015, **54**, 7399-7404.
- S18. L. Z. Zhuang, L. Ge, Y. S. Yang, M. R. Li, Y. Jia, X. D. Yao and Z. H. Zhu, *Adv. Mater.*, 2017, **29**, 1606793.
- S19. J. Kim, X. Yin, K. C. Tsao, S. H. Fang and H. Yang, *J. Am. Chem. Soc.*, 2014, **136**, 14646-14649.
- S20. R. R. Zhang, Y. C. Zhang, L. Pan, G. Q. Shen, N. Mahmood, Y. H. Ma, Y. Shi, W. Y. Jia, L. Wang, X. W. Zhang, W. Xu and J. J. Zou, *ACS Catal.*, 2018, **8**, 3803-3811.
- S21. B. Liu, Y. Wang, H. Q. Peng, R. Yang, Z. Jiang, X. T. Zhou, C. S. Lee, H. J. Zhao and W. J. Zhang, *Adv. Mater.*, 2018, **30**, 1803144.
- S22. S. Karthikeyan, S. Kumar, L. J. Durndell, M. A. Isaacs, C. M. A. Parlett, B. Coulson, R. E. Douthwaite, Z. Jiang, K. Wilson and A. F. Lee, *ChemCatChem*, 2018, **10**, 3554-3563.
- S23. S. Kumar, C. M. A. Parlett, M. A. Isaacs, D. V. Jowett, R. E. Douthwaite, M. C.R. Cockett, A. F. Lee, *Appl. Catal. B-Environ.*, 2016, **189**, 226-232.
- S24. Y. H. Zhang, B. B. Jiu, F. L. Gong, J. L. Chen and H. L. Zhang, *J. Alloy. Compd.*, 2017, **729**, 563-570.
- S25. D. P. Kumar, V. D. Kumari, M. Karthik, M. Sathish and M. V. Shankar, *Sol. Energy Mat. Sol. C.*, 2017, **163**, 113-119.
- S26. H. Q. Tan, Z. Zhao, W. B. Zhu, E. N. Coker, B. S. Li, M. Zheng, W. X. Yu, H. Y. Fan and Z. C. Sun, *ACS Appl. Mater. Interfaces*, 2014, **6**, 19184-19190.
- S27. F. C. Lei, Y. F. Sun, K. T. Liu, S. Gao, L. Liang, B. C. Pan and Y. Xie, *J. Am. Chem. Soc.*, 2014, **136**, 6826-6829.
- S28. S. B. Wang, L. Pan, J. J. Song, W. B. Mi, J. J. Zou, L. Wang and X. W. Zhang, *J. Am. Chem. Soc.*, 2015, **137**, 2975-2983.
- S29. S. C. Sun, P. Gao, Y. R. Yang, P. P. Yang, Y. J. Chen and Y. B. Wang, *ACS Appl. Mater. Interfaces*, 2016, **8**, 18126-18131.
- S30. T. T. Wu, X. D. Kang, M. W. Kadi, I. Ismail, G. Liu and H. M. Cheng, *Chinese J. Catal.*, 2015, **36**, 2103-2108.
- S31. B. Wang, S. H. Shen and L. J. Guo, *Appl. Catal. B-Environ.*, 2015, **166-167**, 320-326.
- S32. L. Z. Zhang, J. W. Shi, M. C. Liu, D. W. Jing and L. J. Guo, *Chem. Commun.*, 2014, **50**, 192-194.
- S33. J. J. Zhang, P. Zhang, T. Wang and J. L. Gong, *Nano Energy*, 2015, **11**, 189-195.
- S34. Y. L. Wang, Y. H. Li, X. L. Wang, Y. Hou, A. P. Chen and H. G. Yang, *Appl. Catal. B-Environ.*, 2017, **206**, 216-220.
- S35. D. G. Wang, H. F. Jiang, X. Zong, Q. Xu, Y. Ma, G. L. Li and C. Li, *Chem. Eur. J.*, 2011, **17**, 1275-1282.
- S36. K. Kočí, L. Obalová, L. Matějová, D. Plachá, Z. Lacný, J. Jirkovský and O. Šolcová, *Appl. Catal. B-Environ.*, 2009, **89**, 494-502.

- S37. G. C. Xi, S. X. Ouyang, P. Li, J. H. Ye, Q. Ma, N. Su, H. Bai and C. Wang, *Angew. Chem. Int. Edit.*, 2012, **51**, 2395-2399.
- S38. Y. Zhou, Z. P. Tian, Z. Y. Zhao, Q. Liu, J. H. Kou, X. Y. Chen, J. Gao, S. C. Yan and Z. Q. Zou, *ACS Appl. Mater. Interfaces*, 2011, **3**, 3594-3601.
- S39. X. Y. Chen, Y. Zhou, Q. Liu, Z. D. Li, J. G. Liu and Z. G. Zou, *ACS Appl. Mater. Interfaces*, 2012, **4**, 3372-3377.
- S40. K. L. Bae, J. Kim, C. K. Lim, K. M. Nam and H. Song, *Nat. Commun.*, 2017, **8**, 1156.
- S41. J. G. Yu, J. X. Low, W. Xiao, P. Zhou and M. Jaroniec, *J. Am. Chem. Soc.*, 2014, **136**, 8839-8842.
- S42. C. Gao, Q. Q. Meng, K. Zhao, H. J. Yin, D. W. Wang, J. Guo, S. L. Zhao, L. Chang, M. He, Q. X. Li, H. J. Zhao, X. J. Huang, Y. Gao and Z. Y. Tang, *Adv. Mater.*, 2016, **28**, 6485-6490.
- S43. P. Li, Y. Zhou, Z. Y. Zhao, Q. F. Xu, X. Y. Wang, M. Xiao and Z. G. Zou, *J. Am. Chem. Soc.*, 2015, **137**, 9547-9550.
- S44. L. Q. Ye, X. L. Jin, X. X. Ji, C. Liu, Y. R. Su, H. Q. Xie and C. Liu, *Chem. Eng. J.*, 2016, **291**, 39-46.
- S45. F. Chen, H. W. Huang, L. Q. Ye, T. R. Zhang, Y. H. Zhang, X. P. Han and T. Y. Ma, *Adv. Funct. Mater.*, 2018, **28**, 1804284.