Unrevealing the multicomponent Metal ion incorporation and sulfide modification in cobalt oxide for efficient water Oxidation

Muzzayab Masood¹, Muhammad Aamir^{1*}, Muhammad Ejaz Khan², Muhammad Sher³, Khush Bakhat Akram,⁴ Hafiz Zahid Shafi,⁵ Hamad Almohamadi,⁶ Md. Akhtaruzzaman,^{*7} Md. Shahiduzzaman,⁸

¹ Department of Chemistry, Mirpur University of Science and Technology(MUST), Mirpur-10250 (AJK), Pakistan.

² Department of Computer Engineering, National University of Technology, Islamabad 44000, Pakistan

³Department of Chemistry, Allama Iqbal Open University, H-8, Islamabad, Pakistan.

⁴Applied Sciences and Humanities Department, National University of Technology, Islamabad 44000, Pakistan

⁵Materials Division, National Institute of Lasers & Optronics College (NILOP-C), Pakistan Insti-

tute of Engineering & Applied Science (PIEAS), P.O. Nilore 45650, Islamabad, Pakistan.

6Department of Chemical Engineering, Faculty of Engineering, Islamic University of Madinah, Madinah, Abo Bakr Al Siddiq, Al Jamiah, Madinah 42351, Saudi Arabia

⁷The Department of Chemistry, Faculty of Science, The Islamic University of Madinah, Madinah, Abo Bakr Al Siddiq, Al Jamiah, Madinah 42351, Saudi Arabia

⁸Nanomaterials Research Institute, Kanazawa University, Kakuma, Kanazawa 920-1192, Japan

*Corresponding Authors:

Muhammad Aamir Email: amir.chem@must.edu.pk

Table S1. Comparison of overpotential and Tefal slope values of the various reported cobalt based electrocatalysts for OER activity with the as-synthesized electrocatalysts.

Catalyst	Electrolyte	Overpotential (mV)	Tafel Slope	Ref.
	_	at 10 mAcm ⁻²	$(mV dec^{-1})$	
CdCoO	1 M KOH	208	81.98	Our Work
CdCoS	1 M KOH	199	63.45	Our Work
CdCoO@CuCoO	1 M KOH	215	83.05	Our Work
CdCoS@CuCoS	1 M KOH	208	69.91	Our Work
Co ₃ O ₄ -GC	1 M KOH	350	60.5	[1]
LaxSr1-xCoO3-δ-GC	1 M KOH	250	NA	[2]
Co ₂ FeO ₄ -GC	1 M KOH	359	43	[3]
CoOOH-CC	1 M KOH	426	60	[4]
Zn0.2Co0.8OOH-GC	1 M KOH	235	35.7	[5]
LiCoO1.8Cl0.2-GC	1 M KOH	276.8	55.4	[6]
NiCo ₂ O ₄ -CP	1 M KOH	270	39	[7]
SrCoO _{3-δ} -GC	1 M KOH	417	66	[8]
FeCoSe2-GC	1 M KOH	370	53.5	[9]
Fe ₃ Co(PO ₄) ₄ -GC	1 M KOH	237	57	[10]
CoAl ₂ O ₄ -GC	1 M KOH	290	70	[11]
Zn0.35Co0.65O-GC	1 M KOH	290	42.6	[12]
CoFe ₂ O ₄ -NF	1 M KOH	248	54.2	[13]
CaCoO ₃ -GC	1 M KOH	260	38	[14]
Co ₂ (OH) ₃ Cl-GC	1 M KOH	270	42	[15]
$Co_3Sn_2S_2$ -CW	1 M KOH	300	74	[16]
γ-CoOOH-CC	1 M KOH	300	38	[17]
CoS-Co(OH) ₂ -NF	1 M KOH	380	68	[18]
GC = Glassy Carbon, NF = Nickel Foam, CC = Carbon Cloth, CW = Copper Wire, CP = Carbon				
Paper				

- Zhang, R., et al., *Tracking the role of defect types in Co3O4 structural evolution and active motifs during oxygen evolution reaction*. Journal of the American Chemical Society, 2023. 145(4): p. 2271-2281.
- 2. Lu, M., et al., Artificially steering electrocatalytic oxygen evolution reaction mechanism by regulating oxygen defect contents in perovskites. Science advances, 2022. **8**(30): p. eabq3563.
- 3. Xiang, W., et al., 3D atomic-scale imaging of mixed Co-Fe spinel oxide nanoparticles during oxygen evolution reaction. Nature Communications, 2022. **13**(1): p. 179.
- 4. Wang, S., et al., *Identifying the geometric catalytic active sites of crystalline cobalt oxyhydroxides for oxygen evolution reaction*. Nature Communications, 2022. **13**(1): p. 6650.

- 5. Huang, Z.-F., et al., *Chemical and structural origin of lattice oxygen oxidation in Co–Zn oxyhydroxide oxygen evolution electrocatalysts*. Nature Energy, 2019. **4**(4): p. 329-338.
- 6. Wang, J., et al., *Redirecting dynamic surface restructuring of a layered transition metal oxide catalyst for superior water oxidation*. Nature Catalysis, 2021. **4**(3): p. 212-222.
- 7. Li, J., et al., *Boosted oxygen evolution reactivity by igniting double exchange interaction in spinel oxides.* Journal of the American Chemical Society, 2019. **142**(1): p. 50-54.
- 8. Pan, Y., et al., *Direct evidence of boosted oxygen evolution over perovskite by enhanced lattice oxygen participation*. Nature communications, 2020. **11**(1): p. 2002.
- 9. Dou, Y., et al., *Approaching the activity limit of CoSe2 for oxygen evolution via Fe doping and Co vacancy.* Nature Communications, 2020. **11**(1): p. 1664.
- 10. Sultan, S., et al., Superb water splitting activity of the electrocatalyst Fe3Co (PO4) 4 designed with computation aid. Nature Communications, 2019. **10**(1): p. 5195.
- 11. Wu, T., et al., *Iron-facilitated dynamic active-site generation on spinel CoAl2O4 with selftermination of surface reconstruction for water oxidation.* Nature Catalysis, 2019. **2**(9): p. 763-772.
- 12. Wahl, S., et al., Zn0. 35Co0. 65O–A stable and highly active oxygen evolution catalyst formed by zinc leaching and tetrahedral coordinated cobalt in wurtzite structure. Advanced Energy Materials, 2019. 9(20): p. 1900328.
- 13. Huang, L., et al., *Zirconium-regulation-induced bifunctionality in 3D cobalt–iron oxide nanosheets for overall water splitting*. Advanced Materials, 2019. **31**(28): p. 1901439.
- 14. Li, X., et al., *Exceptional oxygen evolution reactivities on CaCoO3 and SrCoO3*. Science advances, 2019. **5**(8): p. eaav6262.
- 15. Jiang, H., et al., *Tracking structural self-reconstruction and identifying true active sites toward cobalt oxychloride precatalyst of oxygen evolution reaction*. Advanced Materials, 2019. **31**(8): p. 1805127.
- 16. Li, G., et al., Surface states in bulk single crystal of topological semimetal Co3Sn2S2 toward water oxidation. Science Advances, 2019. **5**(8): p. eaaw9867.
- 17. Seh, Z.W., et al., *Combining theory and experiment in electrocatalysis: Insights into materials design.* Science, 2017. **355**(6321): p. eaad4998.
- Yoon, T. and K.S. Kim, One-Step Synthesis of CoS-Doped β-Co (OH) 2@ Amorphous MoS2+ x Hybrid Catalyst Grown on Nickel Foam for High-Performance Electrochemical Overall Water Splitting. Advanced Functional Materials, 2016. 26(41): p. 7386-7393.