Supporting Information

Facile Synthesis of Hierarchical Porous Ni_xCo_{1-x}SeO₃ Networks with Controllable Composition as a New and Efficient Water Oxidation Catalyst

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Figure S1. Digital image of NF and Ni_{0.5}Co_{0.5}SeO₃/NF.



Figure S2. XRD pattern of the $Ni_{0.5}Co_{0.5}SeO_3/NF$ networks catalyst.



Figure S3. SEM images of Ni_{0.5}Co_{0.5}SeO₃/NF.



Figure S4. SEM images of NiSeO₃/NF.



Figure S5. SEM images of CoSeO₃/NF.



Figure S6. TEM images of Ni_{0.5}Co_{0.5}SeO₃.



Figure S7. The electron image of the elemental mapping region and corresponding EDS spectrum for $Ni_{0.5}Co_{0.5}SeO_3$.



Figure S8. EPMA data for NiSeO₃/NF, CoSeO₃/NF, and Ni_{0.5}Co_{0.5}SeO₃/NF.



Figure S9. a) Nitrogen adsorption-desorption isotherms of $Ni_{0.5}Co_{0.5}SeO_3/NF$. b) The corresponding pore distribution curve obtained on the Barrett-Joyner-Halenda (BJH) model.



Figure S10. Cyclic voltammetry curves of (a) $Ni_{0.5}Co_{0.5}SeO_3/NF$, (b) $NiSeO_3/NF$, and (c) $CoSeO_3/NF$.



Figure S11. TOF curve of the Ni_{0.5}Co_{0.5}SeO₃ catalyst in 1 M KOH solution.



Figure S12. (a) LSV curves, (b) overpotentials at 100 mA cm⁻² and (c) current density at 1.73 V obtained on the NiCoSeO₃ integrated electrocatalysts with different Ni/Co ratios in NiCoSeO₃.



Figure S13. Crystal structure of NiSeO₃, Ni_{0.5}Co_{0.5}SeO₃, and CoSeO₃.



Figure S14. The density of states of a) NiSeO₃, b) Ni_{0.5}Co_{0.5}SeO₃, and c) CoSeO₃.



Figure S15. Estimation of C_{dl} for Ni_{0.5}Co_{0.5}SeO₃/NF and RuO₂.



Figure S16. Cyclic voltammetry curves of (a) NiCoSeO₃ and (b) RuO₂.



Figure S17. The SEM images of $Ni_{0.5}Co_{0.5}SeO_3$ after the stability test.

Table S1.	ICP	results	for	Ni	and	Co	in	Ni_0	₅ Co	0.5SeC	D3.
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Sample	m _{Ni} (mg)	m _{Co} (mg)	Atomic ratio of Ni/Co
Ni _{0.5} Co _{0.5} SeO ₃	0.736	0.829	0.47/0.53

Table	S2.	Comparison	of th	ne OER	activity	of	the	Ni _{0.5} Co _{0.5} SeO ₃ /NF	with	some	reported
nonpre	cious	s electrocataly	sts in	alkaline	condition	1.					

Catalysts	Overpotential at 100 mA cm ⁻² (mV)	Tafel slope (mV dec ⁻¹)	References
Ni _{0.5} Co _{0.5} SeO ₃	380	44	This work
Co-S/Ti mesh	430	64	Electrochem. Commun.,
			2015 , 60, 92.
Co-P film	413	47	Angew. Chem. Int. Ed.,
			2015 , 54, 6251.
$\mathrm{Co}_3\mathrm{V}_2\mathrm{O}_8$	497	65	J. Mater. Chem. A, 2014,
			2, 18435.
Mn_3N_2	390	101	Angew. Chem., 2018, 130,
			706.
NiV LDH	390	72	Adv. Energy Mater., 2018,
			1703341

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Time (min)	15	30	45	60	75	90
Calculated O2 (mL)	6.83959	13.63492	20.36705	27.02332	33.59109	40.05772
Measured O2 (mL)	6.731	13.221	19.821	26.301	32.651	39.231
Faradaic efficiency (%)	98.41	96.96	97.32	97.33	97.20	97.94
Average (%)			97	.53		

Table S3. The theoretical values, measured values and the Faradaic efficiencies of the amount of O_2 production at different periods.

Table S4. Lattice Constants (Å), Magnetic Coupling state (Ferromagnetic (FM) or Antiferromagnetic (AFM)) and band gaps.

	а	b	с	Magnetic Coupling	Band Gap (eV)
NiSeO ₃	6.037	7.013	5.230	FM	1.440
CoSeO ₃	4.972	5.887	7.208	AFM	2.497
Ni _{0.5} Co _{0.5} SeO ₃	5.886	7.244	5.027	AFM	1.362

Computational Methods:

The first-principles calculations within density-functional theory (DFT) were implemented by the Vienna Ab-initio Simulation Package (VASP)[1]. A generalized gradient approximation (GGA) in the form of Perdew-Burke-Ernzerhof (PBE) [2] is adopted to describe the electron-electron interactions. We also adopted a GGA + U strategy to describe the strong Coulomb interaction between the partially filled 3d-shells of the transition metals in all frameworks. The values of the Coulomb parameter U and exchange parameter J were set to 4.0 eV and 0.0 eV, respectively. The energy cut-off employed for plane-wave expansion of electron wavefunctions was set to 520 eV and the electron-ion interactions were treated using projector-augmented-wave (PAW) potentials[3]. The system is modeled by unit cells repeated periodically on the x-y plane, while a vacuum region of about 20 Å was applied along the z-direction to avoid mirror interaction between neighboring images. Structural optimization was carried out using a conjugate gradient (CG) method until the remaining force on each atom is less than 0.05 eV/ Å.

References

- (1) G. Kresse and J. Hafner, Journal of Physics: Condensed Matter, 1994, 6(40), 8245.
- (2) J.P. Perdew, K. Burke and M. Ernzerhof, Physical review letters, 1996, 77(18), 3865.
- (3) G. Kresse and D. Joubert, Physical Review B, 1999, 59(3), 1758.