

Supporting Information

Vanadium-doped cobalt selenide: an efficient bifunctional electrocatalyst for overall water splitting

Ankita Sahu, ^{a,b} Manisha Sadangi, ^{a,b} and J. N. Behera ^{a,b*}

a: School of Chemical Science, National Institute of Science Education and Research (NISER), an OCC of Homi Bhabha National Institute (HBNI), Khurda, Odisha, India, 752050

b: Centre for Interdisciplinary Sciences (CIS), NISER, Khurda, Odisha, India, 752050

Email: jnbehera@niser.ac.in

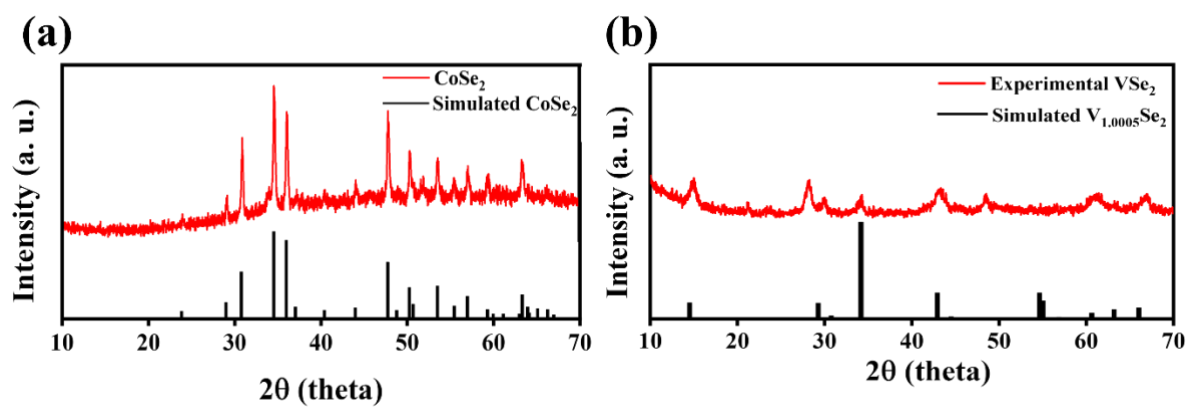


Fig. S1 (a) PXRd of CoSe₂, (b) PXRd of VSe₂.

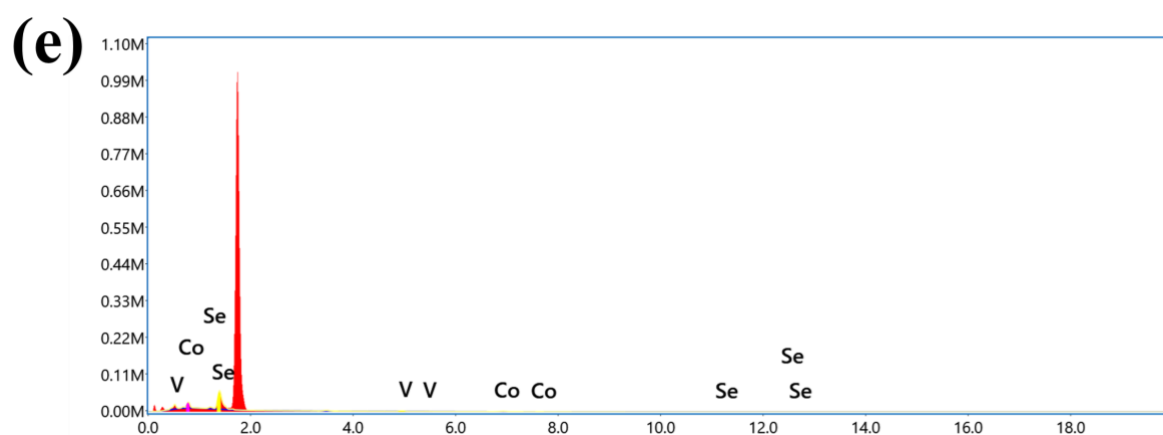
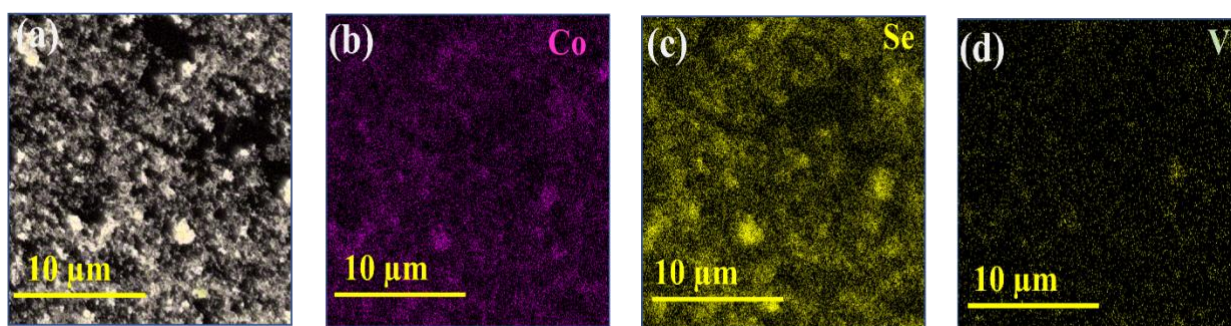


Fig. S2 (a-d) Elemental mapping, (e) EDAX spectrum of V@CoSe₂-1.

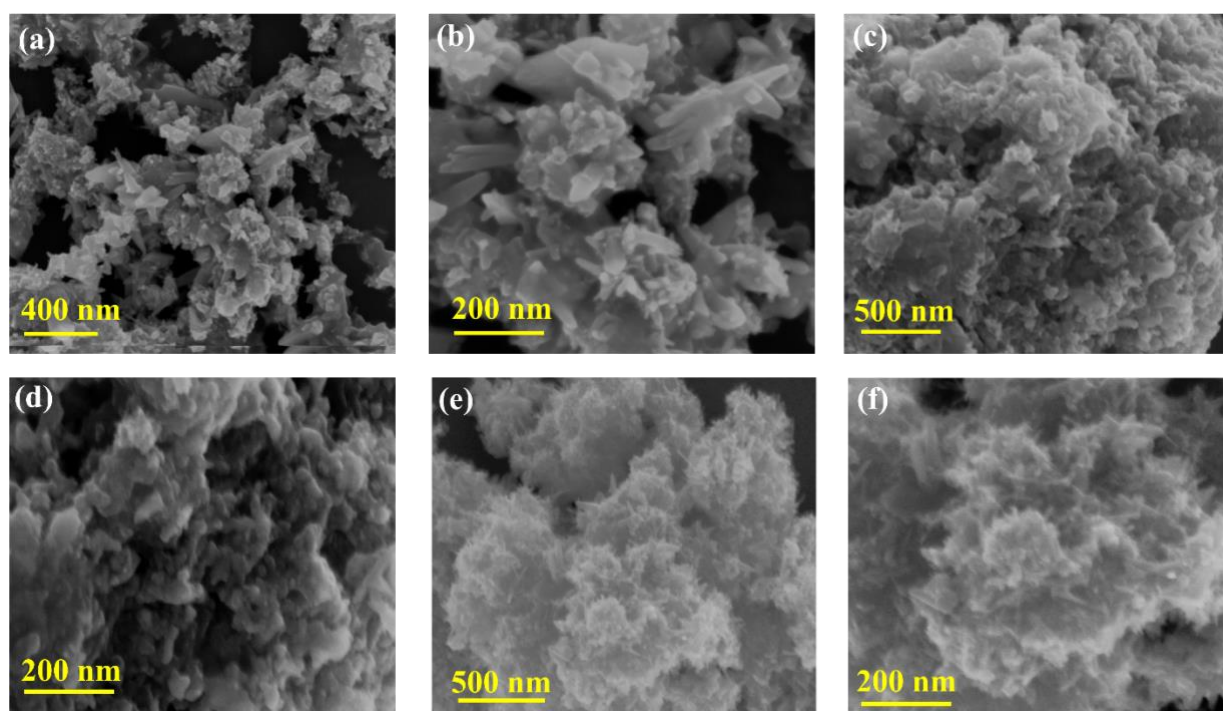


Fig. S3 (a, b) FESEM images of V@CoSe₂-2, (c, d) FESEM images of V@CoSe₂-3, (e, f) FESEM images of CoSe₂.

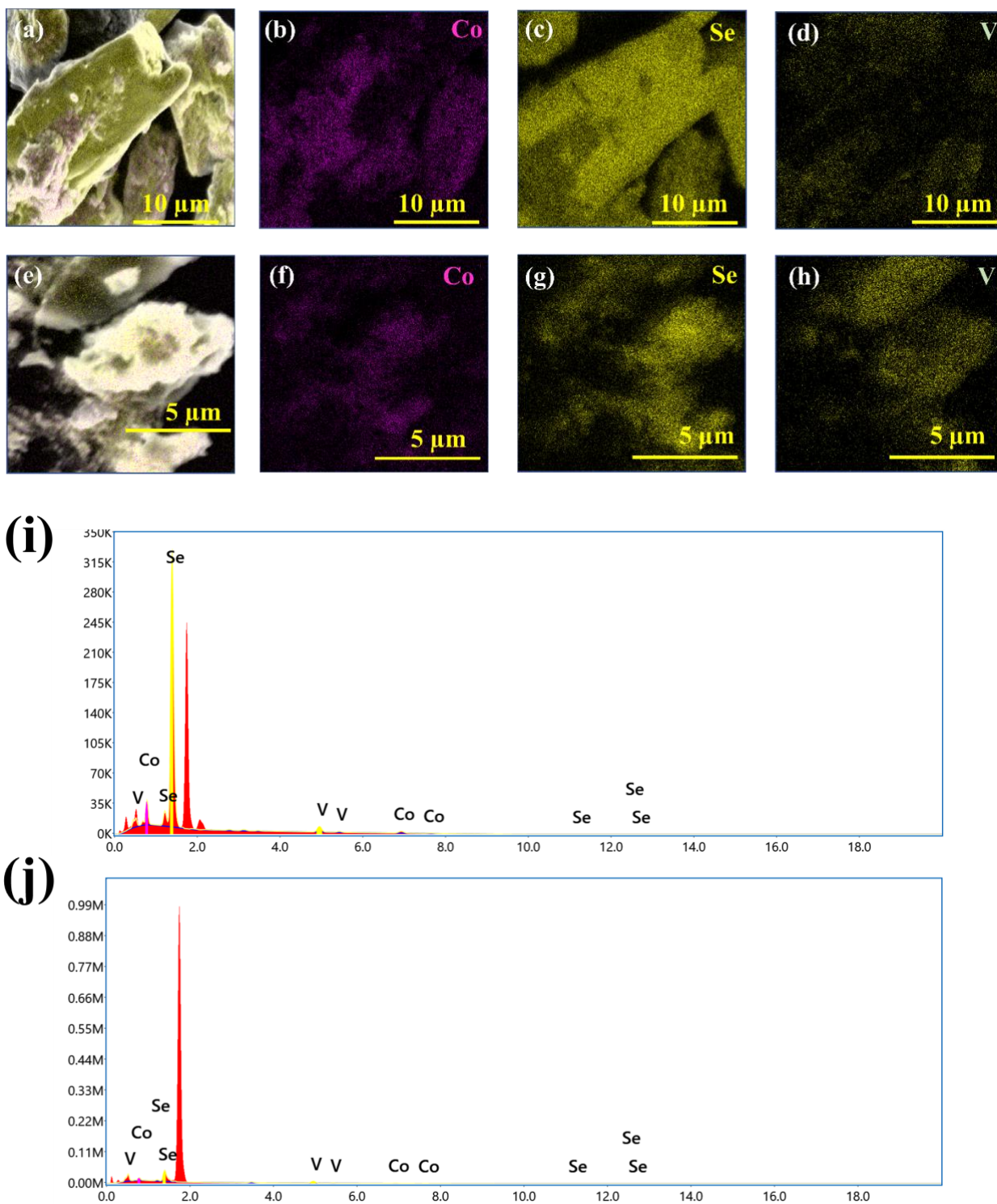


Fig. S4 (a-d) Elemental mapping of V@CoSe₂-2, (e-h) Elemental mapping of V@CoSe₂-3, (i) EDAX spectrum of V@CoSe₂-2, (j) EDAX spectrum of V@CoSe₂-3.

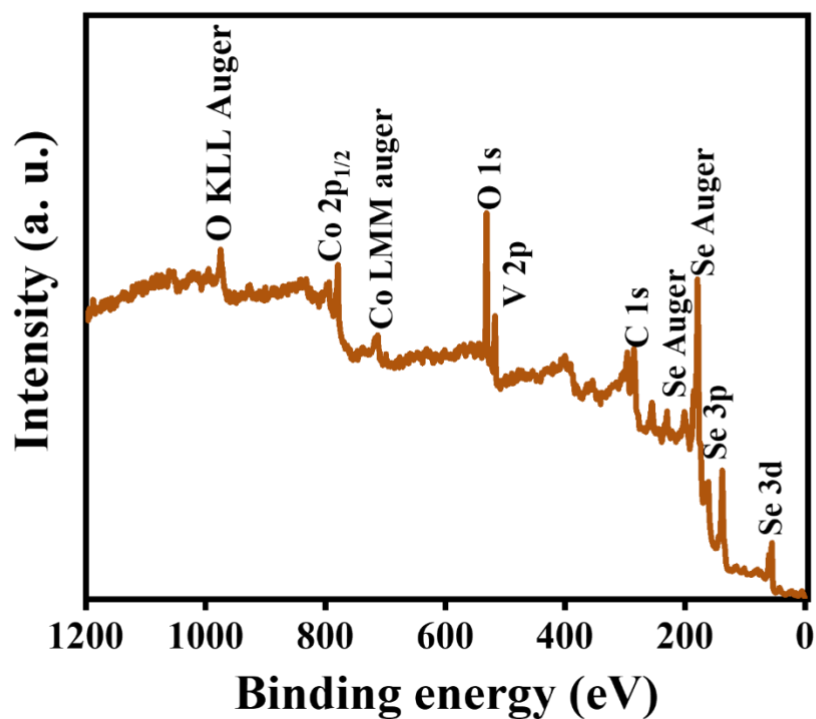


Fig. S5 Full survey spectrum of V@CoSe₂-1.

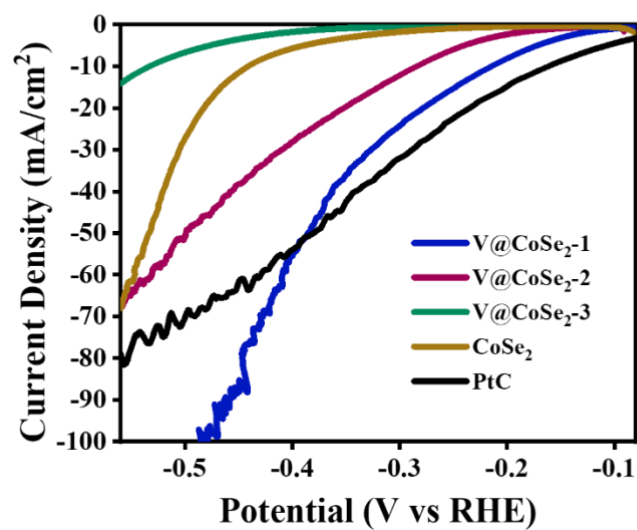


Fig. S6 Full range current density LSV of alkaline HER.

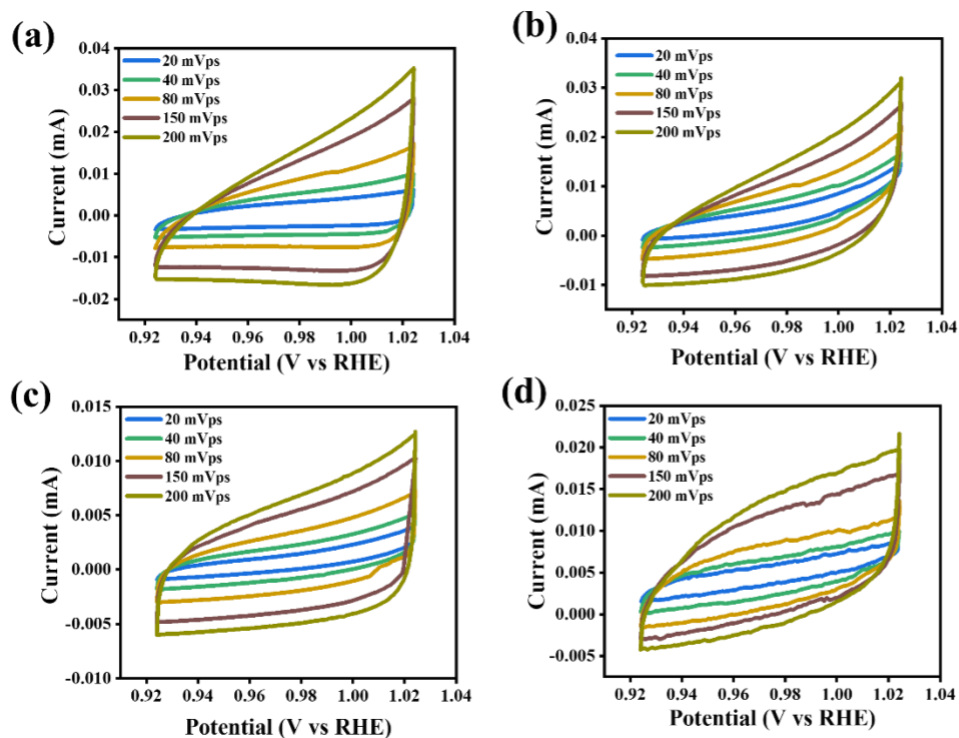


Fig. S7 CV curves of (a) V@CoSe₂-1, (b) V@CoSe₂-2, (c) V@CoSe₂-3, (d) CoSe₂ in the potential window of 0.92 V to 1.02 V for OER application.

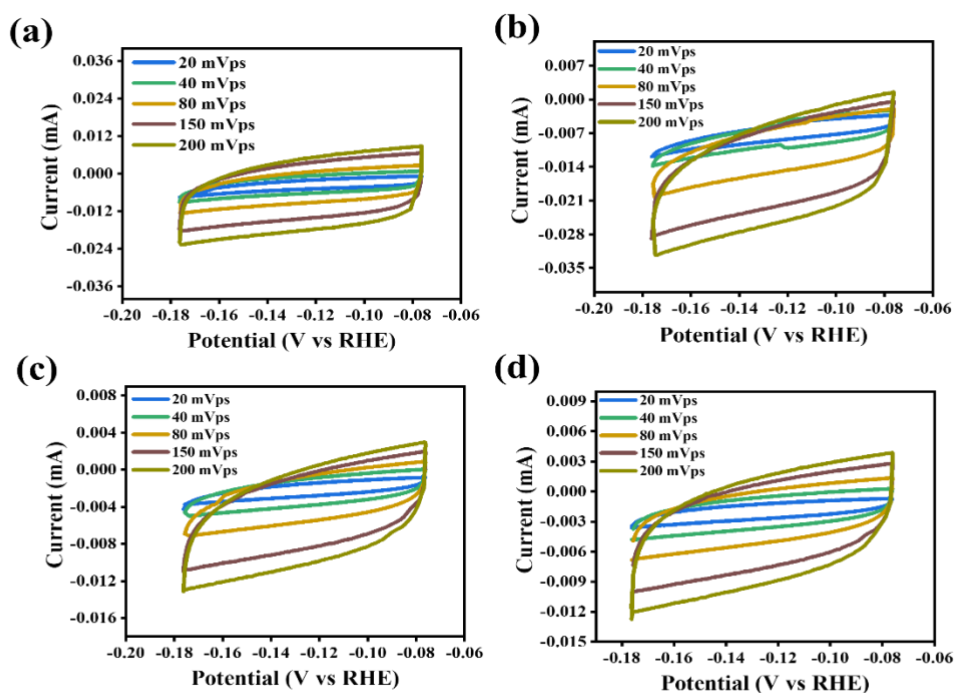


Fig. S8 CV curves of (a) V@CoSe₂-1, (b) V@CoSe₂-2, (c) V@CoSe₂-3, (d) CoSe₂ in the potential window of -0.08 V to -0.18 V for HER application.

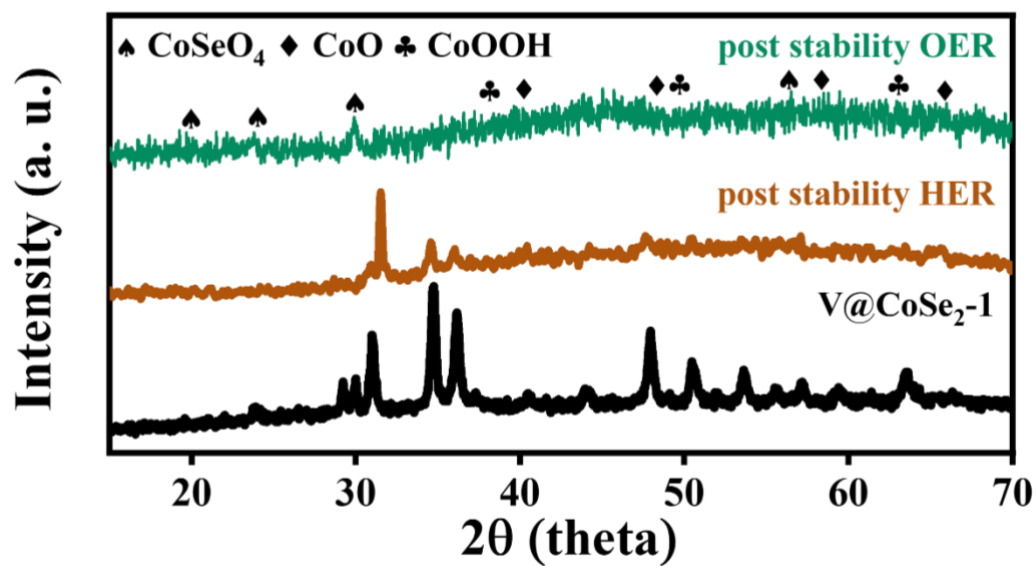


Fig. S9 PXR D of post-stability OER and HER of V@CoSe₂-1.

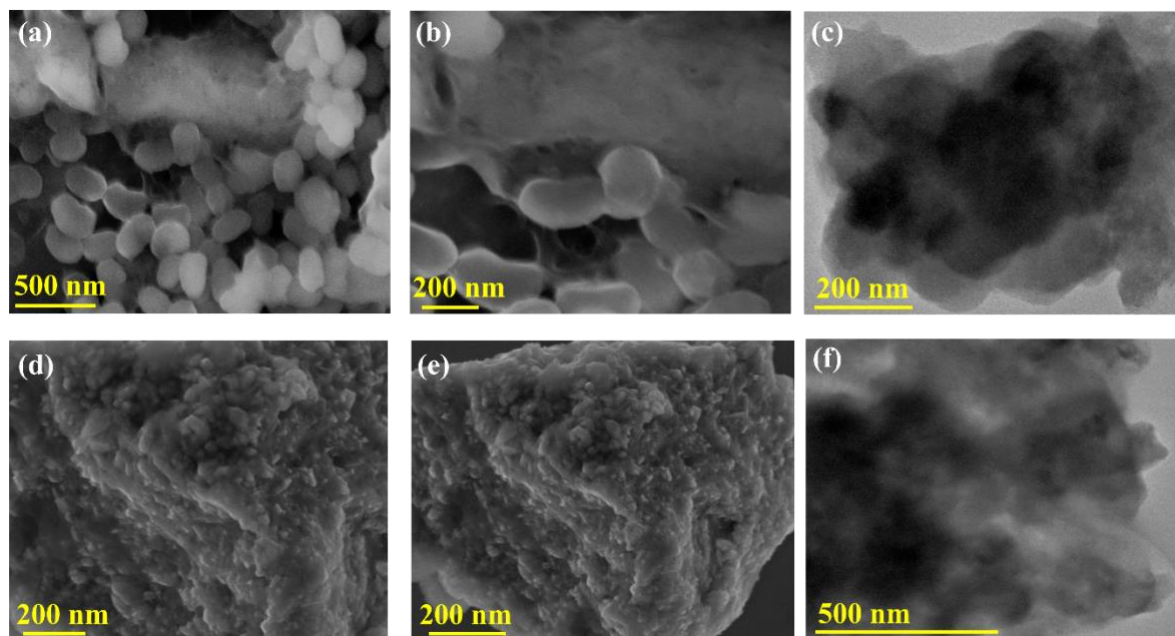


Fig. S10 (a, b) FESEM images of V@CoSe₂-1 post OER, (c) TEM image of V@CoSe₂ process -1 post OER, (d-e) FESEM images of V@CoSe₂-1 post HER, (f) TEM image of V@CoSe₂-1 post HER.

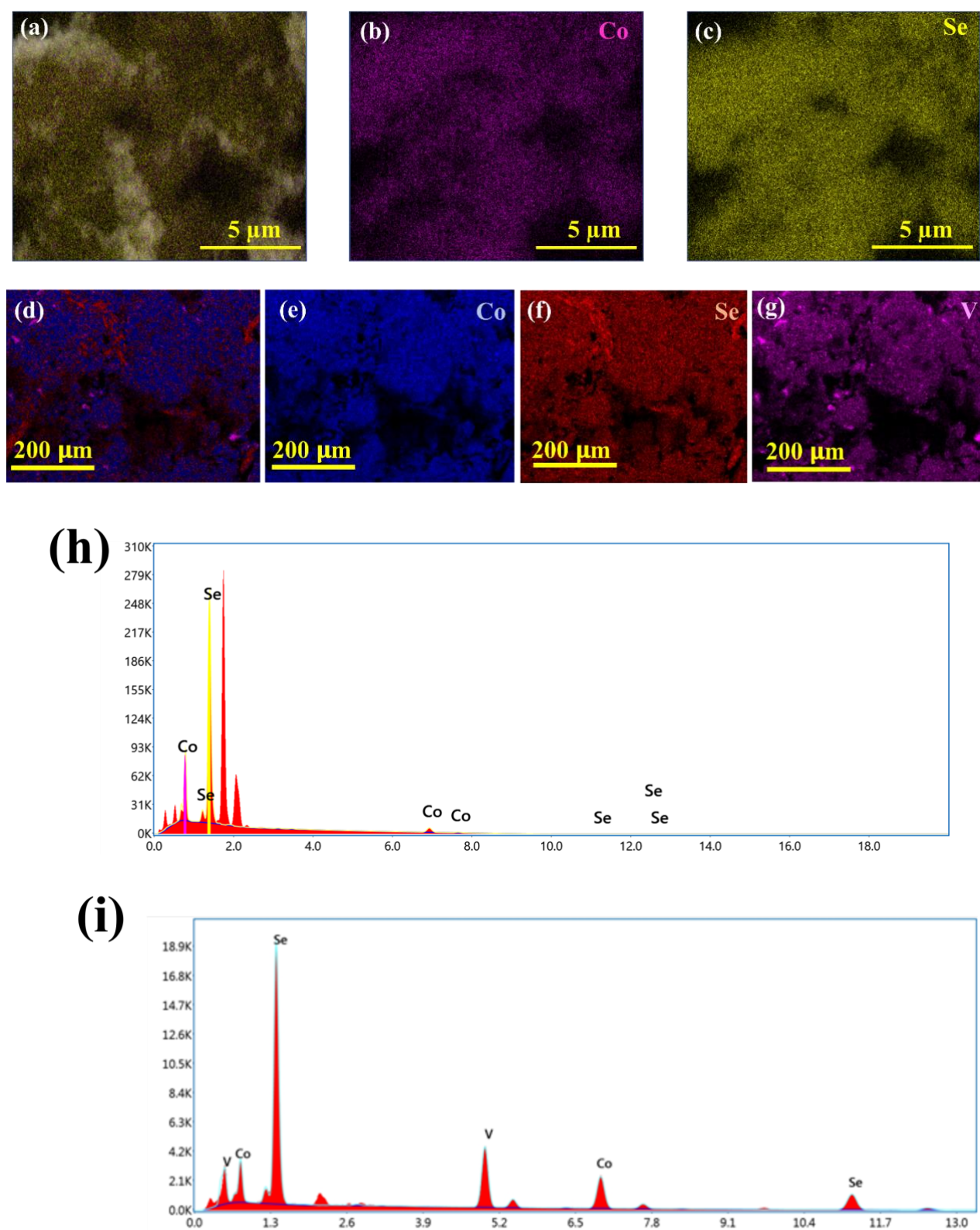


Fig.S11 (a-c) elemental mapping of post stability OER, (d-g) elemental mapping of post stability HER, (i) EDAX spectrum of post stability OER, (j) EDAX spectrum of post-stability HER of V@CoSe₂-1

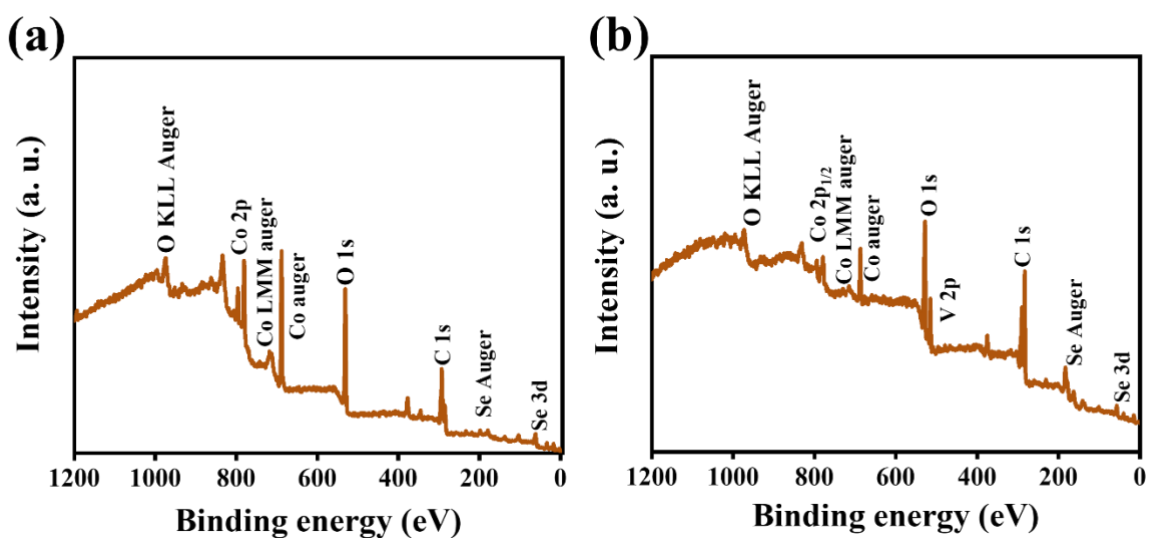


Fig. S12 (a) Full survey spectrum of post-OER, (b) full survey spectrum of post HER of V@CoSe₂-1.

Table S1: Comparison of weight % and atomic % of different electrocatalysts observed in EDAX spectra.

Electrocatalyst	Weight %			Atomic %		
	Co	Se	V	Co	Se	V
V@CoSe ₂ -1	20.40	67.60	12.10	24	59.50	16.50
V@CoSe ₂ -2	7.30	80.40	12.30	8.90	73.60	17.40
V@CoSe ₂ -3	11.90	40.90	47.20	12.30	31.50	56.30
V@CoSe ₂ -1 (post OER)	20.80	79.20	—	26	74	—
V@CoSe ₂ -1 (post HER)	18.90	70.71	10.40	22.58	63.05	14.37

Table S2: Molar ratios of elements of each electrocatalyst calculated from XPS spectra.

Electrocatalyst	Molar ratio
V@CoSe ₂ -1	Co:V:Se (1.5:1:3.5)
After OER V@CoSe ₂ -1	Co:Se (1:1.25)
After HER V@CoSe ₂ -1	Co:V:Se (1.7:1:1.6)

Table S3: R_s, R_{ct}, C_{dl}, ECSA of different electrocatalysts.

Electrocatalyst	R _s (Ω)		R _{ct} (Ω)		C _{dl} (μF)		ECSA (cm ²)	
	OER	HER	OER	HER	OER	HER	OER	HER
V@CoSe ₂ -1	11.89	14.9	13.16	36.9	62.7	56.1	1.56	1.40
V@CoSe ₂ -2	11.89	14.9	16.23	72.47	45.7	52	1.14	1.28
V@CoSe ₂ -3	11.89	14.9	38.91	106.7	27	22.4	0.67	0.56
CoSe ₂	—	—	—	—	29.4	25	0.73	0.63

Table S4: Comparison of different bifunctional electrocatalysts for alkaline water splitting at 10 mA/cm² current density.

Electrocatalyst	1 M KOH η HER/OER (mV)	1 M KOH Cell voltage (V)	Tafel (mV/dec) HER/OER	Substrate taken as electrode	Ref.
V@CoSe ₂ -1	270/315	1.96	124/63	Glassy carbon/ graphite sheet	This work
Ni-CoSe ₂	250/325	1.69	69.3/58.6	Glassy carbon	1
Co ₂ B/CoSe ₂	300/320	1.73	76/56	Carbon fibre cloth	2
RuSe ₂ CoSe ₂ /NC	31/248	1.57	20.8/58.1	Glassy carbon	3
CoSe ₂ @MoSe ₂	183/309	1.524	87.69/84.04	Glassy Carbon/Ni foam	4
Co-BTC	370/437	2.03	115.1/89.1	Carbon cloth	5
H-CoS _x @NiFe LDH/NF	95/250	1.98	90/49	Nikel foam	6
Cu ₂ Se/CoSe ₂	110/170	1.56	140/130	Cu foam	7
NiSe ₂ -CoSe ₂	66/220	1.56	57/99.57	Carbon cloth	8

References

- 1 G. Yang, Y. Zhang, J. Liu, M. Wang, C. Gu and J. Li, *Int. J. Hydrogen Energy*, 2022, **47**, 38920–38929.
- 2 Y. Guo, Z. Yao, C. Shang and E. Wang, *ACS Appl. Mater. Interfaces*, 2017, **9**, 39312–39317.
- 3 L. Li, J. Qu, L. Zhang, L. Wei, J. Su and L. Guo, *ACS Appl. Mater. Interfaces*, 2024, **16**, 24660–24670.
- 4 Z. Chen, W. Wang, S. Huang, P. Ning, Y. Wu, C. Gao, T. T. Le, J. Zai, Y. Jiang, Z. Hu and X. Qian, *Nanoscale*, 2020, **12**, 326–335.
- 5 S. Naik Shreyanka, J. Theerthagiri, S. J. Lee, Y. Yu and M. Y. Choi, *Chem. Eng. J.*, 2022, **446**, 137045.
- 6 Y. J. Lee and S. K. Park, *Small*, 2022, **18**, 2200586.
- 7 M. Das, G. Kumar and R. S. Dey, *ACS Appl. Energy Mater.*, 2022, **5**, 3915–3925.
- 8 H. Liu, F. Yang, F. Chen, S. Che, N. Chen, C. Xu, N. Wu, W. Wei and Y. Li, *Mater. Chem. Front.*, 2023, **7**, 1365–1373.