Supplementary Information (SI) for Journal of Materials Chemistry A.

Synergistic Modulation of CoOOH by Dual-defects to Enhance the Catalytic Performance of Oxygen Evolution Reaction

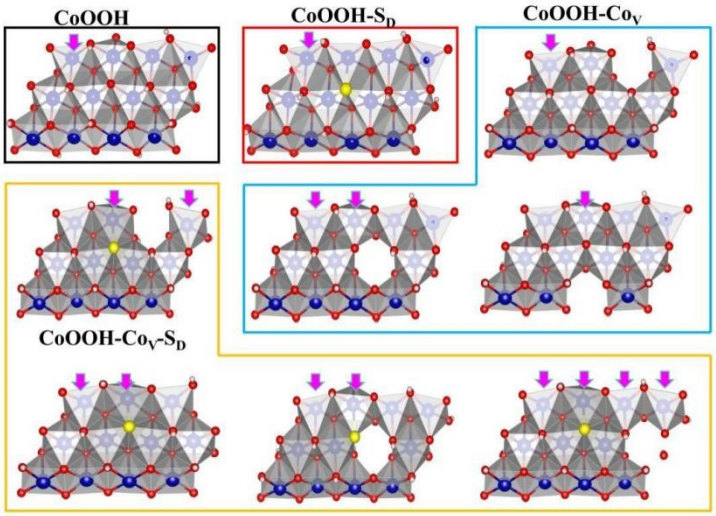

Figure S1. Considered active sites on (01-12) facets of different structure models for DFT+U calculations. CoOOH, CoOOH-S_D, CoOOH-Co_V and CoOOH-Co_V-S_D are framedin black, red, blue and yellow, respectively.

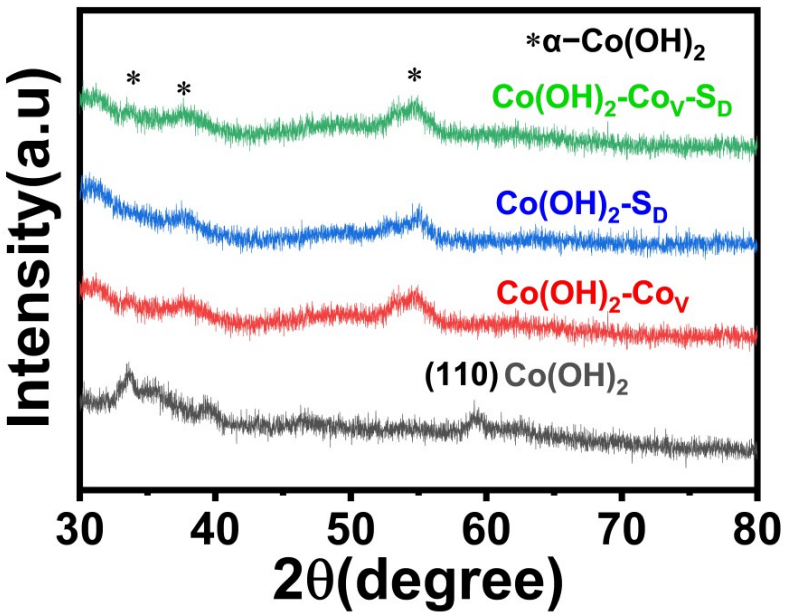

Figure S2. XRD images of CoOOH、CoOOH-Co_V、CoOOH-S_D and CoOOH-Co_V-S_D

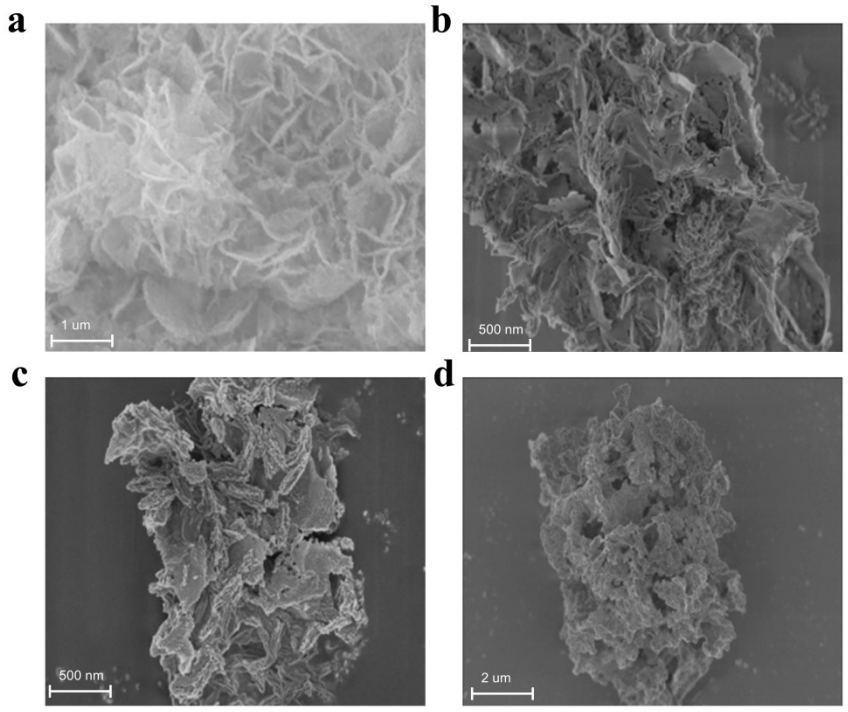

Figure S3. SEM images of CoOOH、CoOOH-Co_V、CoOOH-S_D and CoOOH-Co_V-S_D

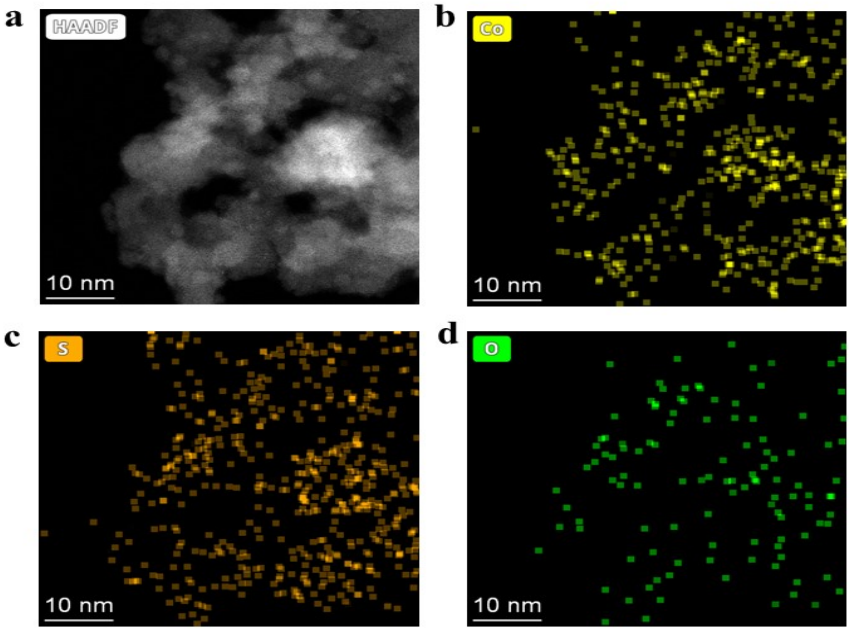

Figure S4. Elemental maps and HAADF-STEM images of Co, S, and O before catalysis.

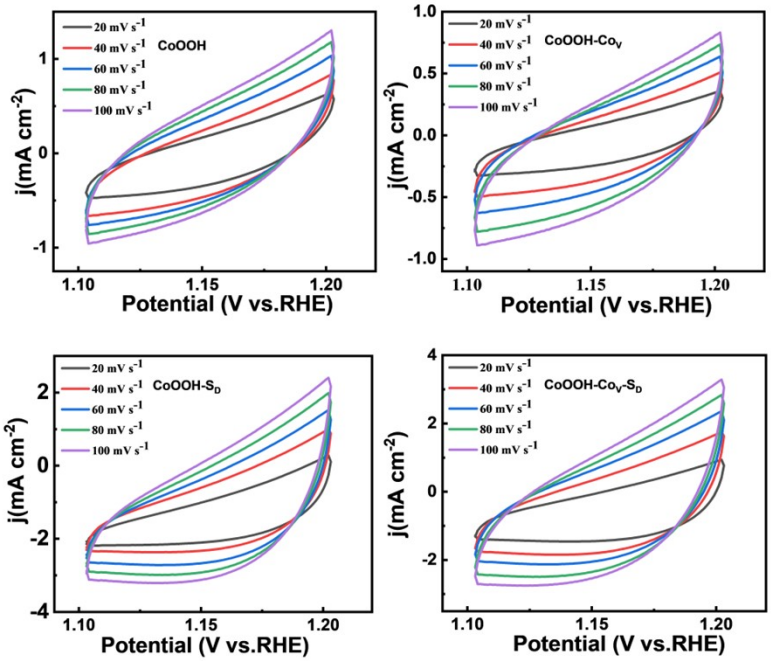

Figure S5. Cdl image of CoOOH, CoOOH-Co_V, CoOOH-S_D and CoOOH-Co_V-S_D at a sweep speed of 20~100mV/s

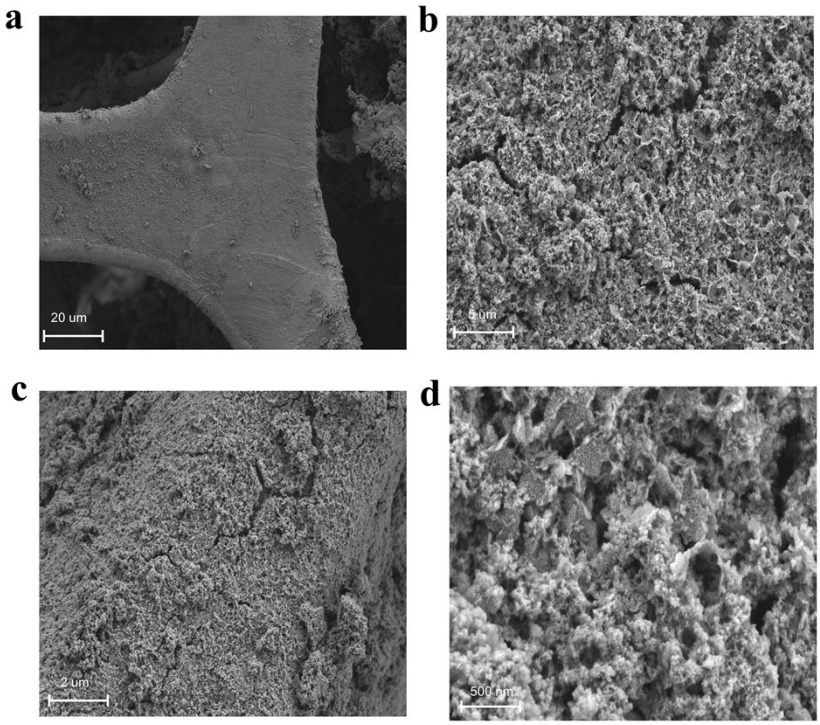

Figure S6. SEM images of CoOOH-Co_V-S_D after stability testing at differentmagnifications (a)20 um（b）5 um（c）2 um　(d) 500 nm

	Gibbs free energies (eV)			Gibbs free energy changes (eV)				η^{OER} (
	ΔG_{O*}	ΔG_{OH*}	ΔG_{OOH*}	ΔG_1	ΔG_2	ΔG_3	ΔG_4	mV)
CoOOH-Co	2.36	0.62	3.92	0.62	1.74	1.56	1	510
CoOOH-S_D-1	2.84	1.06	3.96	1.06	1.78	1.12	0.96	550
CoOOH-Co_V-1-Co1	2.62	1.09	4.02	1.09	1.53	1.4	0.9	300
CoOOH-Co_V-2-Co1	2.62	1.02	4.08	1.02	1.6	1.46	0.84	370
CoOOH-Co_V-2-Co2	3.5	1.78	4.63	1.78	1.72	1.13	0.29	550
CoOOH-Co_V-3-Co1	2.88	1.16	3.97	1.16	1.72	1.09	0.95	490
CoOOH-Co_V-S_D-1-Co1	3.03	1.29	3.7	1.29	1.74	0.67	1.22	510
CoOOH-Co_V-S_D-1-Co2	3.09	1.28	4.3	1.28	1.81	1.21	0.62	580
CoOOH-Co_V-S_D-2-Co1	2.69	1.29	4.32	1.29	1.4	1.63	0.6	400
CoOOH-Co_V-S_D-2-Co2	2.83	1.16	4.08	1.16	1.67	1.25	0.84	440
CoOOH-Co_V-S_D-3-Co1	2.52	1.06	3.99	1.06	1.46	1.47	0.93	240
CoOOH-Co_V-S_D-3-Co2	3.58	1.9	4.7	1.9	1.68	1.12	0.22	670
CoOOH-Co_V-S_D-4-Co1	2.27	1.12	4.07	1.12	1.15	1.8	0.85	570
CoOOH-Co_V-S_D-4-Co2	2.83	1.17	4.05	1.17	1.66	1.22	0.87	430
CoOOH-Co_V-S_D-4-Co3	3.03	1.32	4.09	1.32	1.71	1.06	0.83	480
CoOOH-Co_V-S_D-4-Co4	3.44	1.3	4.21	1.3	2.14	0.77	0.71	910

Table S1. Calculated energetics and overpotentials of different metal sites.

Sample number	Sample size (g)	Constant volume V0 (mL)	Test elements	concentration C0 (mg/L)	Dilution factor f	Digestion solution/ concentration of the original sample C1 (mg/L)	Elemental content Cx (mg/kg)	Elemental content W (%)
	0.033	25	S	4.133	100	413.30	313106.06	31.3
$Co(OH)_2$-Co_V-S_D	0.033	25	S	4.086	100	408.60	309545.45	31.0

	0.033	25	S	4.141	100	414.10	313712.12	31.4
	0.0329	25	S	13.82	1	13.82	10501.52	1.05
CoOOH-Co_V-S_D	0.0329	25	S	13.837	1	13.84	10514.44	1.05
	0.0329	25	S	13.814	1	13.81	10496.96	1.05

Table S2. Detail Inductive Coupled Plasma (ICP) data of S in $Co(OH)_2$-Co_V-S_D and CoOOH-Co_V-S_D

catalyst	Activation technique	Electrolyte	η (mV) at 10 mA cm-2	Tafel slope	Ref
Co_3S_4-Cu	Cu doping	1 M KOH	279	113	1
LaZn-Co_3O_4	La doping & Zn doping	1 M KOH	273	18.08	2
$Co(OH)_2$@NCDs	N doping	1 M KOH	296	70.5	3
Cu-$Co(OH)_2$	Cu doping	1 M KOH	300	47	4
Mo/$Co(OH)_2$-20	Mo doping	1 M KOH	288	69.72	5
Ag-CoOOH	Ag doping	1 M KOH	256	64.6	6
MoCo$(OH)_2$/CoP/NF	Mo doping & P doping	1 M KOH	287	143	7
Mo-$Co(OH)_2$	Mo doping	1 M KOH	218	90	8

EP(black)/V–CoO_2-xH_2	**O vacancies & V doping**	**1 M KOH**	**269**	**31**	**9**
Ir–$Co(OH)_x$	**Ir doping**	**1 M KOH**	**251**	**75.4**	**10**
CoOOH-Co_V-S_D	**Co vacancies & S doping**	**1 M KOH**	**251**	**51.85**	**Our work**

Table S3. Comparison of the catalytic performance between CoOOH-Co_V-S_D and previously reported CoOOH-based catalysts.

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