

Modulated Transition Metal-Oxygen Covalency in Octahedral Sites of
CoFe Layered Double Hydroxides with Vanadium Doping Leading to
Highly Efficient Electrocatalyst

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Notes

The authors declare no competing financial interest.

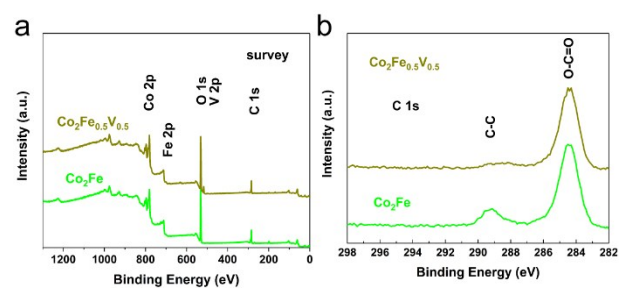


Figure S1 a) XPS survey of Co_2Fe and $\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}$; b) High-resolution XPS $\text{C } 1s$

spectrum of Co_2Fe and $\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}$.

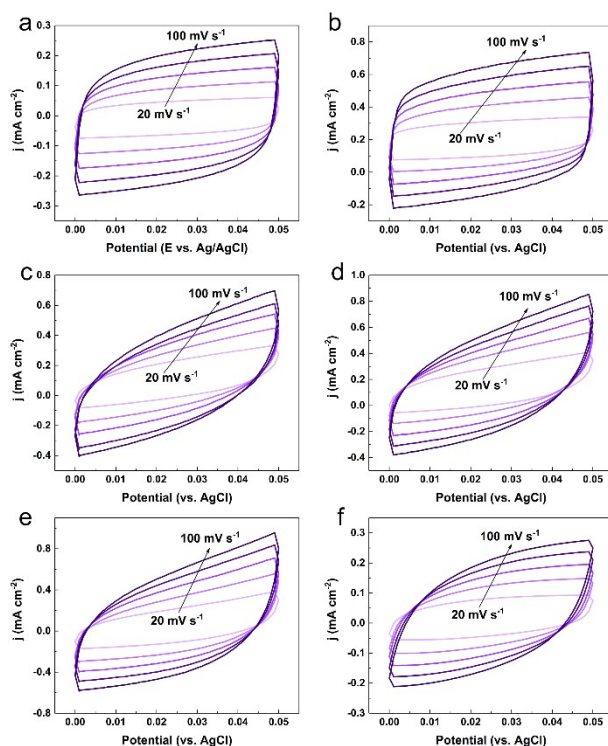


Figure S2 a-e) CV curves at various scan rate of $\text{Co}_2\text{Fe}_{0.5}\text{@CP}$, $\text{Co}_2\text{Fe@CP}$, $\text{Co}_2\text{Fe}_{0.67}\text{V}_{0.33}\text{@CP}$, $\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}\text{@CP}$ and, $\text{Co}_2\text{Fe}_{0.33}\text{V}_{0.67}\text{@CP}$ and $\text{Co}_2\text{V@CP}$, respectively.

Table S1 The fitting of electrochemical parameter

Samples	Tafel slope	C_{dl}	EIS		
	R^2	R^2	CPE-T	CPE-P	Chi-Squared
$\text{Co}_2\text{Fe}_{0.5}$	0.99	0.98	0.036	0.705	0.0039
Co_2Fe	0.99	0.99	0.105	0.723	0.0011
$\text{Co}_2\text{Fe}_{0.67}\text{V}_{0.33}$	0.99	0.98	0.099	0.814	0.0004

$\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}$	0.97	0.99	0.143	0.556	0.0003
$\text{Co}_2\text{Fe}_{0.33}\text{V}_{0.67}$	0.95	0.99	0.04	0.833	0.0006
Co_2V	0.96	0.99	0.013	0.885	0.003

Table S2 The fitting of EIS parameter

	$R_s (\Omega)$	$R_{ct} (\Omega)$
$\text{Co}_2\text{Fe}_{0.5}$	2.49	7.83
Co_2Fe	1.62	3.30
$\text{Co}_2\text{Fe}_{0.67}\text{V}_{0.33}$	1.48	1.95
$\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}$	1.43	0.58

$\text{Co}_2\text{Fe}_{0.33}\text{V}_{0.67}$	1.71	0.94
Co_2V	1.69	6.56

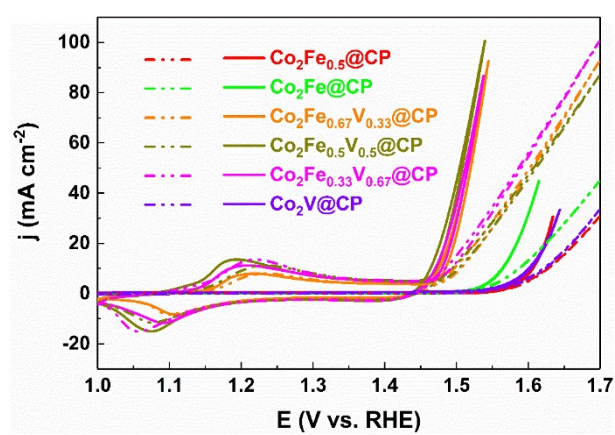


Figure S3 Original and IR-corrected CV polarization curves.

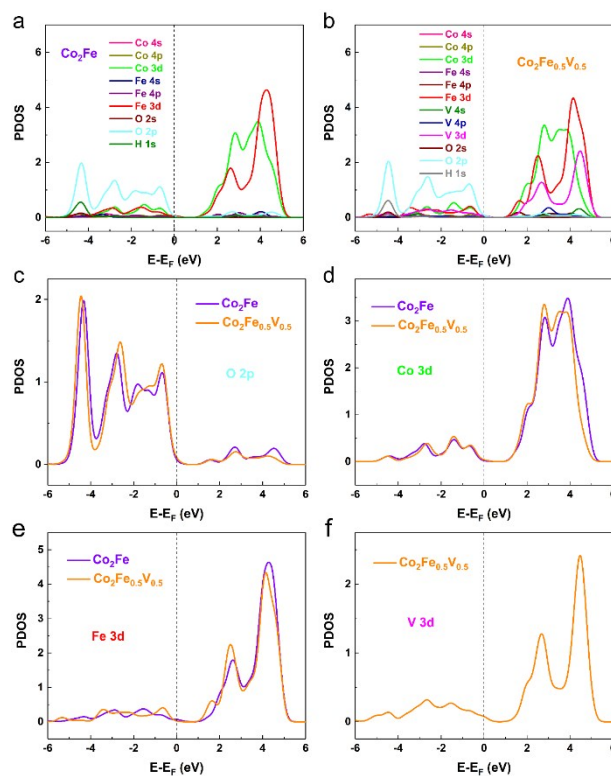


Figure S4 a) and b) TDOS of Co_2Fe and $\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}$, respectively. c)-e) PDOS of O 2p, Co 3d and Fe 3d in Co_2Fe and $\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}$, respectively. f) PDOS of V 3d in $\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}$.

Table S3 Comparison of catalytic performance of $\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}$ LDH to recently reported high performance metal oxide/hydroxide OER catalysts.

Electrocatalysts	electrolyte	j (mA cm^{-2})	η (mV)	Tafel slope (mV dec^{-1})	Ref.
$\text{Co}_2\text{Fe}_{0.5}\text{V}_{0.5}$ LDH@CP	1.0 M KOH	10	242	40	This work

CoFeMo (oxy)hydroxides/GC	1.0 M KOH	10	277	28	1
Fe-doped Co₃V₂O₈/GC	1.0 M KOH	10	307	36	2
Ni_xCo_{3-x}O₄ nanowires/NF	1.0 M KOH	10	337	75	3
Co₃Fe_{1.5}-LDH/NF	1.0 M KOH	10	284	45	4
CoFe-Bi@CoFe-LDH NA/TM	0.1 M KOH	10	418	108	5
CoFe-LDH/rGO	0.1 M KOH	10	325	-	6
Fe_{0.33}Co_{0.67}OOH PNSAs/CFC	0.1 M KOH	10	266	30	7
CuCo₂O₄/NrGO	1.0 M KOH	10	360	64	8
PA-CoS_x(OH)_y/NF	1.0 M KOH	10	261	-	9
Co/CoP-NC	1.0 KOH	10	300	44	10
LiCoO_x/CP	0.1 M KOH	10	290	50	11
NiCo oxides/NF	0.1 M KOH	10	370	-	12
FeCo_{1-x}ONS/GC	0.1 M KOH	10	308	36.8	13
Co₃S₄/NCNTs	0.1 M KOH	10	430	70	14

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