

Electronic Supplementary Information

NiCoP-CeO₂ Composites for Efficient Electrochemical Oxygen Evolution

Jiyu Li,^a Zeyan Wang,^{*a} Peng Wang,^a Zhaoke Zheng,^a Yuanyuan Liu,^a Hefeng Cheng,^a and Baibiao Huang^{*a}

a State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, China.

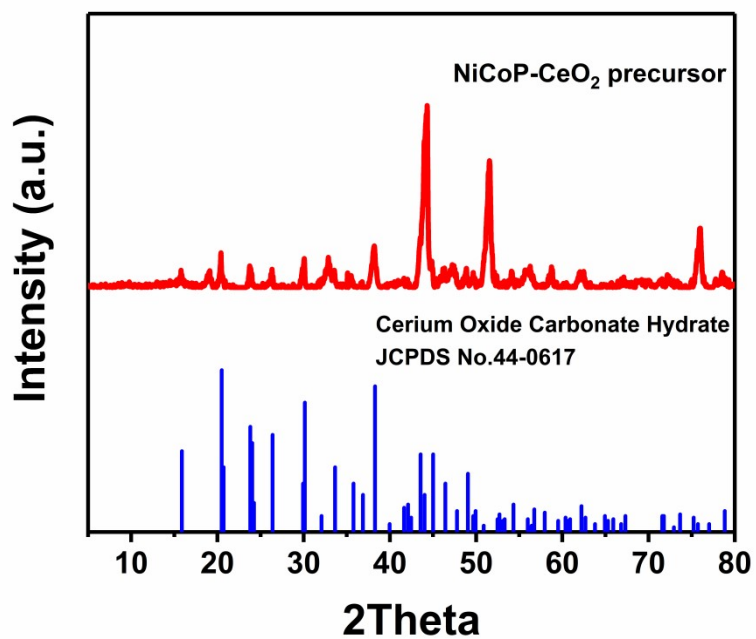


Fig. S1 XRD patterns of NiCoP-CeO₂ precursors.

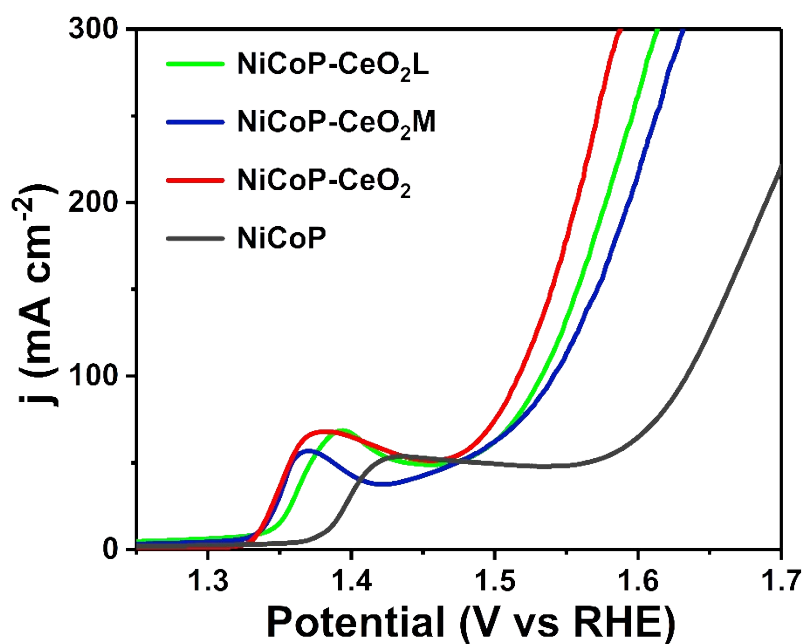


Fig. S2 LSV curves of NiCoP-CeO₂ electrodes with different amount loading on NiCoP in 1M KOH solution.

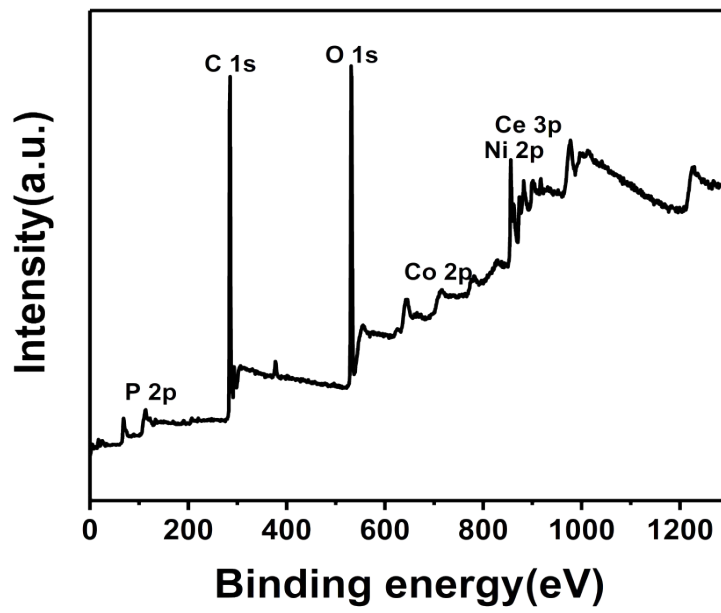


Fig. S3 XPS survey spectra of NiCoP-CeO₂.

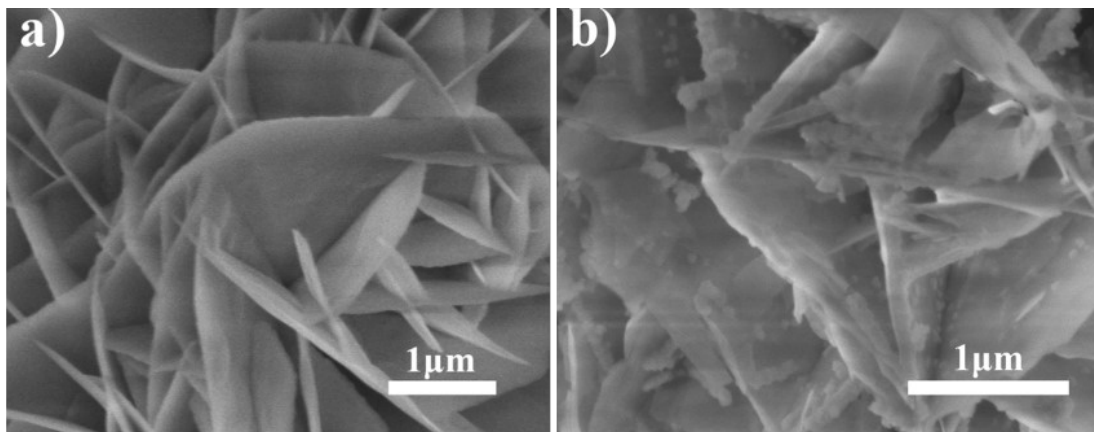


Fig. S4 SEM images of NiCo-LDHs (a) and NiCoP-CeO₂ precursors (b).

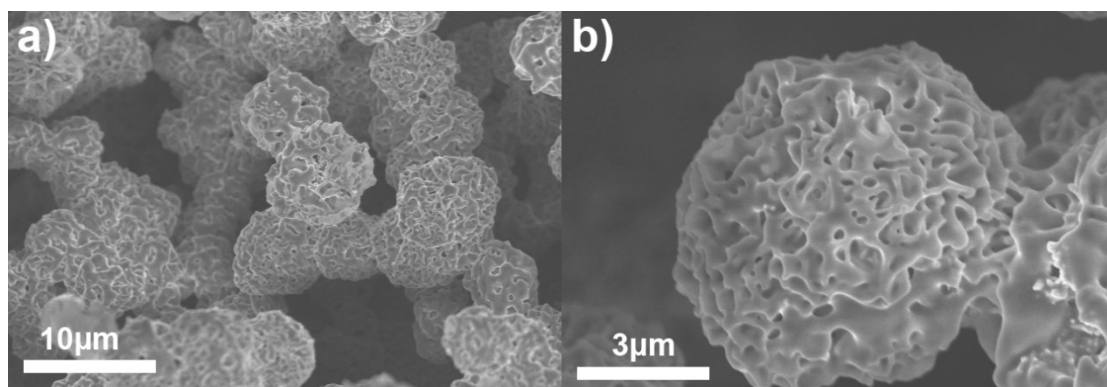


Fig. S5 SEM images of low (a) and high (b) magnification of NiCoP.

Table S1 Summary of electrocatalytic OER activities of LDHs-CeO₂ composites electrocatalysts^a

Catalyst	Overpotential (mV)	Tafel slope (mV dec ⁻¹)	References
NiFe-LDH/CeO ₂ @CeNC	235	128.8	1
CeO ₂ /NiFe-LDH	243	65	2
CeO _{2-x} @CoFe LDH	204 ^b	23.7	3
CeO ₂ -FeCo LDH	260	40	4
ceria/Ni-TMO	350	38	5
NF@NiFe LDH/CeO _x	280 ^c	--	6
Ni ₈₀ Fe ₂₀ /50wt%CeO ₂	289	40	7
NiCoP-CeO₂	217	45	this work

[a] except for special instructions, the value of catalyst overpotential in the table is at 10 mA cm⁻² of current density; [b]: the overpotential at 100mA cm⁻² of current density; [c] the overpotential of overall water splitting.

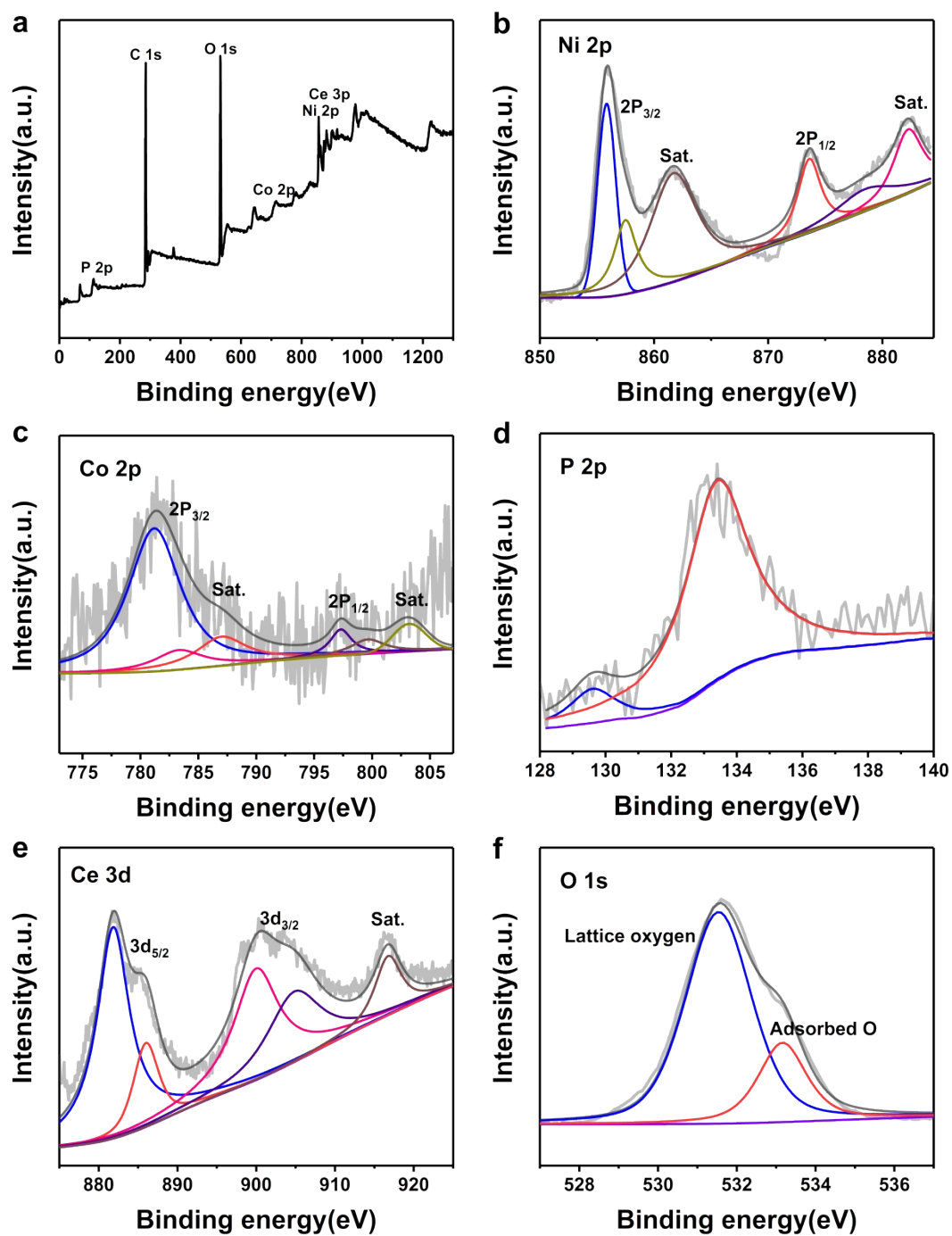


Fig. S6 XPS survey(a), Ni 2p(b), Co 2p(c), P 2p(d), Ce 3d(e) and O 1s(f) spectra of NiCoP-CeO₂ after stability test.

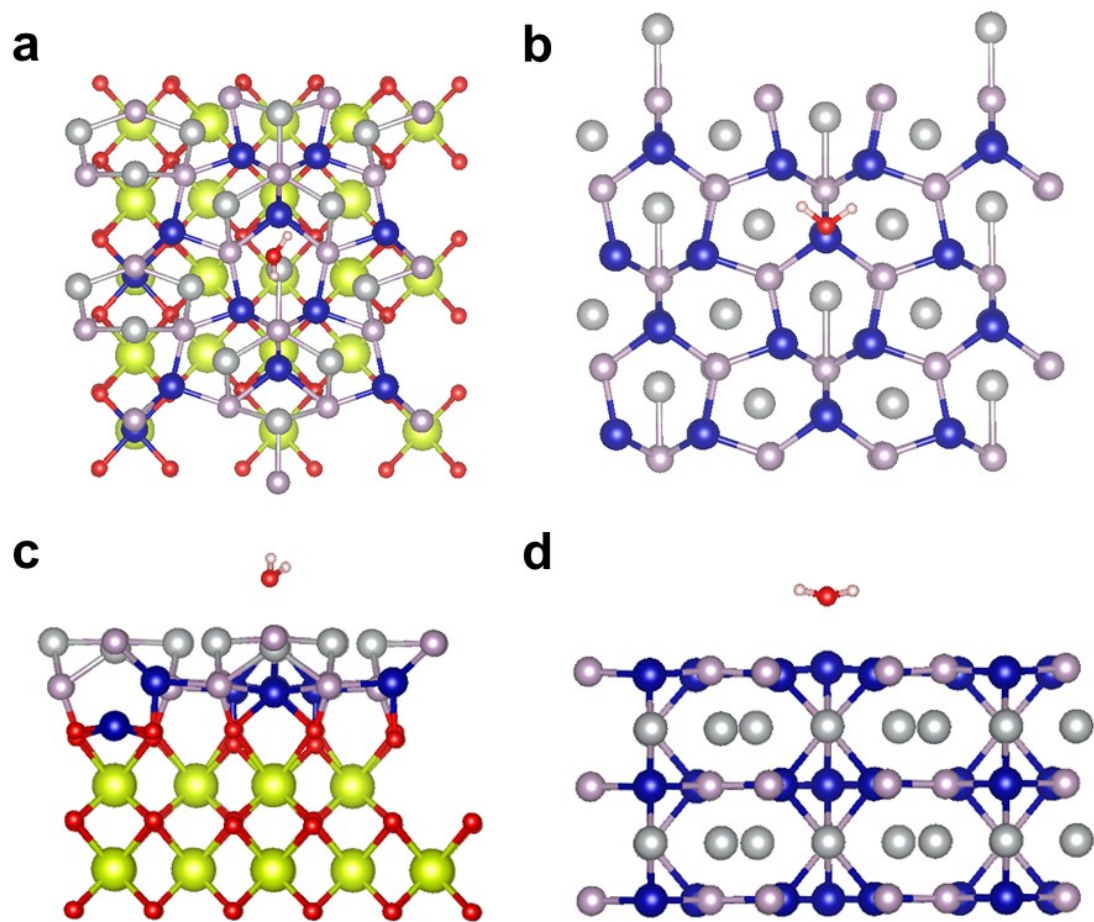


Fig. S7 Optimized adsorption structures of NiCoP-CeO₂ (a) and NiCoP (b).

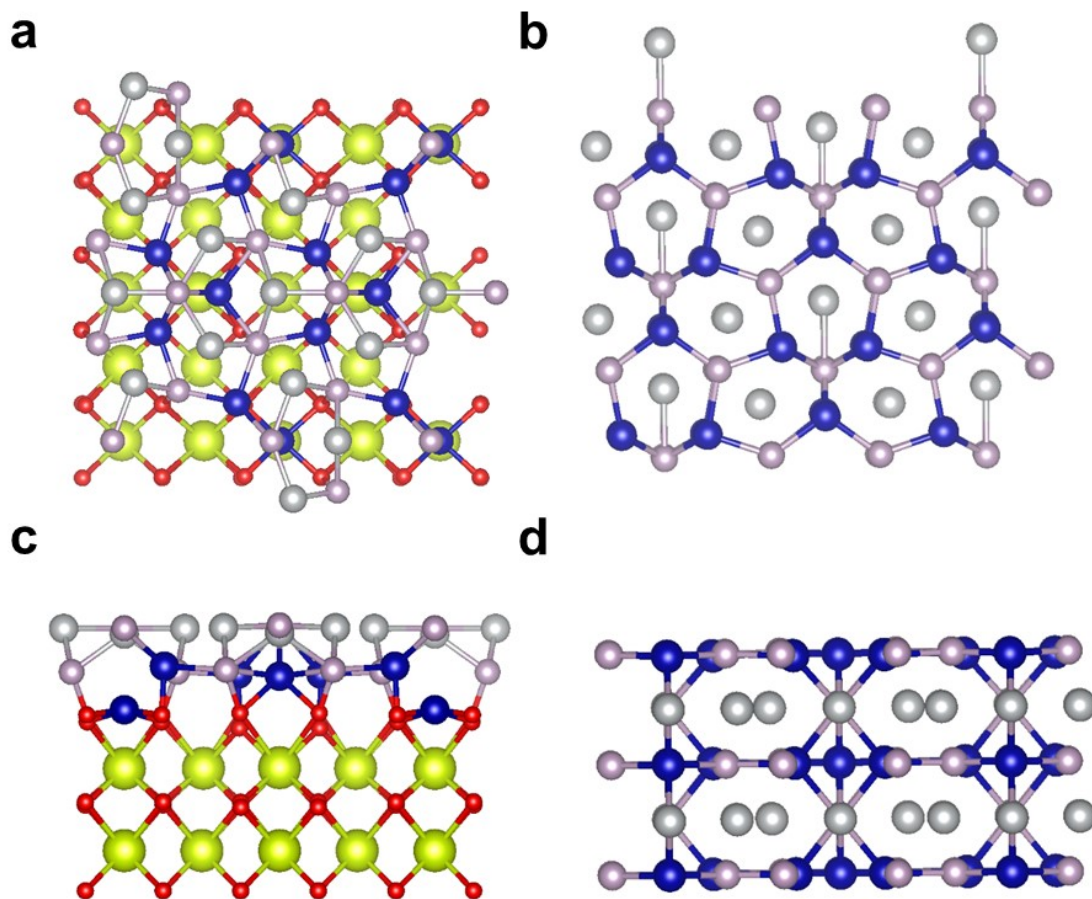


Fig. S8 The original structures of NiCoP-CeO₂ (a) and NiCoP (b).

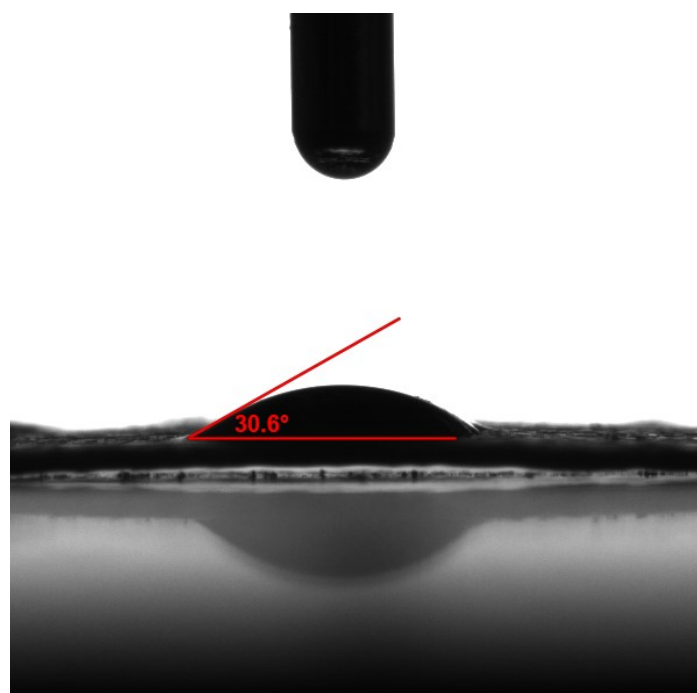


Fig. S9 Wetting-ability testing of CeO₂.

Table S2. The optimized cartesian coordinates of NiCoP-CeO₂ and NiCoP

NiCoP-CeO ₂			NiCoP		
0	0	1.35277	0.49529	5.07893	1.67548
0.02303	2.66743	4.10991	3.30659	10.31073	1.67548
2.88952	0.00396	4.11684	0.47161	5.07885	5.08629
2.8113	2.6159	1.35277	3.31533	10.28331	5.03904
0	5.2318	1.35277	3.84608	3.00033	1.67548
0.0229	7.80346	4.10779	1.03478	8.23213	1.67548
2.70454	5.23515	4.1506	3.83469	2.96915	5.06936
2.8113	7.8477	1.35277	1.0232	8.21316	5.03776
5.6226	0	1.35277	1.03478	1.92572	1.67548
5.64656	2.66787	4.13337	3.84608	7.15752	1.67548
8.50666	0.00342	4.11198	1.0181	1.93826	5.04106
8.4339	2.6159	1.35277	3.84654	7.1773	5.07086
5.6226	5.2318	1.35277	4.18934	5.07893	0
5.64689	7.80236	4.12983	1.37804	10.31073	0
8.32137	5.23387	4.13564	4.19638	5.07621	3.36693
8.4339	7.8477	1.35277	1.39179	10.31077	3.35792
1.43936	1.30994	2.97536	4.24351	5.07085	6.82256
4.19188	3.92649	2.99711	1.44424	10.3079	6.63614
4.21695	1.30795	0	4.81036	1.20583	0
4.32257	1.26128	5.70197	1.99906	6.43762	0
1.40565	3.92385	0	4.7809	1.22486	3.36791
1.37954	3.8927	5.46921	1.97409	6.45061	3.38077
1.40565	1.30795	0	4.77331	1.21183	6.63074
1.39606	1.28222	5.89543	1.94581	6.47496	6.60677
4.21695	3.92385	0	1.99906	3.72023	0
4.16594	3.91233	6.04234	4.81036	8.95203	0
4.23963	1.31061	2.88846	1.96904	3.7029	3.38286
1.38719	3.93027	2.80884	4.78893	8.92288	3.35985
1.38494	6.53675	2.80691	1.93216	3.67373	6.61286
4.23884	9.15753	2.88691	4.78379	8.92613	6.6404
4.21695	6.53975	0	5.54045	3.33506	0
4.17373	6.55994	6.03274	2.72915	8.56686	0
1.40565	9.15565	0	5.47971	3.3314	3.3706
1.39705	9.20253	5.89234	2.67424	8.55772	3.3613
1.40565	6.53975	0	5.48084	3.25982	6.69606
1.3934	6.59375	5.46542	2.67939	8.51565	6.75704
4.21695	9.15565	0	2.72915	1.5911	0
4.32511	9.21423	5.69747	5.54045	6.8229	0
4.19111	6.54119	2.99495	2.67108	1.59653	3.36251
1.4394	9.15852	2.97404	5.4839	6.81753	3.36675
7.05788	1.31191	2.98255	2.67286	1.63479	6.75106
9.81354	3.9277	2.971	5.48962	6.87733	6.69424
9.83955	1.30795	0	2.72915	5.07893	1.67548

9.95195	1.25816	5.6714	5.54045	10.31073	1.67548
7.02825	3.92385	0	2.77637	5.07218	5.09418
6.99383	3.89925	5.49056	5.56405	10.30184	5.05215
7.02825	1.30795	0	3.85531	5.06169	8.91448
7.01515	1.28136	5.89371	3.25541	4.30172	9.07331
9.83955	3.92385	0	3.31944	5.86151	9.10425
9.78452	3.90493	5.95578			
9.85916	1.30944	2.87771			
7.00423	3.927	2.8137			
7.00246	6.53882	2.81158			
9.85845	9.1581	2.87721			
9.83955	6.53975	0			
9.79058	6.5757	5.95274			
7.02825	9.15565	0			
7.015	9.19806	5.89494			
7.02825	6.53975	0			
7.00755	6.58306	5.48463			
9.83955	9.15565	0			
9.95457	9.2201	5.67129			
9.81292	6.53999	2.9704			
7.05851	9.15553	2.98083			
4.89192	5.06049	10.9447			
1.92742	0.00981	8.61797			
10.92348	5.25766	8.67953			
3.01019	3.31994	8.83502			
0.38039	8.41719	8.80759			
0.3809	2.07036	8.80809			
3.03003	7.16858	8.83196			
7.5936	0.00852	8.60129			
5.36187	5.274	8.86023			
8.72577	3.34305	8.82861			
6.02457	8.42635	8.80319			
6.0294	2.04678	8.79841			
8.72866	7.13126	8.82957			
11.21949	0.0087	6.05078			
3.37733	5.23954	7.276			
4.01392	1.35168	7.56515			
1.2307	6.62314	7.26885			
1.22699	3.8687	7.27464			
4.0168	9.12598	7.5596			
5.58773	0.00623	6.07427			
8.97638	5.24346	7.17657			
9.64897	1.35377	7.5303			
6.86323	6.61179	7.2981			

6.8567	3.87215	7.30716
9.64621	9.13019	7.52972
10.36712	3.44862	7.41042
1.94795	8.69486	7.34877
1.94645	1.79325	7.35101
10.36906	7.04267	7.40529
10.87765	0.01125	8.83688
1.89288	5.25345	8.97673
4.74549	3.46005	7.50141
7.58383	8.67942	7.34024
7.58401	1.80128	7.33733
4.75034	7.02393	7.48714
5.28314	0.0064	8.83368
7.60187	5.23894	8.95171
4.14623	5.57168	11.31531
5.61206	5.10058	11.60368

Table S3. The original cartesian coordinates of NiCoP-CeO₂ and NiCoP

NiCoP-CeO ₂			NiCoP		
0	0	1.35277	0.49529	5.07893	1.67548
0.03431	2.66848	4.12059	3.30659	10.31073	1.67548
2.90239	2.93E-04	4.1163	0.51711	5.07893	5.07034
2.8113	2.6159	1.35277	3.32841	10.31073	5.07034
0	5.2318	1.35277	3.84608	3.00033	1.67548
0.03607	7.79476	4.12049	1.03478	8.23213	1.67548
2.71648	5.23215	4.14039	3.85081	2.9635	5.0495
2.8113	7.8477	1.35277	1.03951	8.1953	5.0495
5.6226	0	1.35277	1.03478	1.92572	1.67548
5.65684	2.66835	4.1204	3.84608	7.15752	1.67548
8.52526	4.19E-04	4.11556	1.03951	1.96255	5.0495
8.4339	2.6159	1.35277	3.85081	7.19435	5.0495
5.6226	5.2318	1.35277	4.18934	5.07893	0
5.65813	7.7947	4.11969	1.37804	10.31073	0
8.33865	5.23224	4.14052	4.21375	5.07893	3.36596
8.4339	7.8477	1.35277	1.40245	10.31073	3.36596
1.44418	1.30832	2.99617	4.24186	5.07893	6.65575
4.20013	3.92466	2.98001	1.43056	10.31073	6.65575
4.21695	1.30795	0	4.81036	1.20583	0
4.34271	1.24827	5.6815	1.99906	6.43762	0
1.40565	3.92385	0	4.79816	1.22414	3.36686
1.41549	3.88011	5.47558	1.98686	6.45583	3.36686
1.40565	1.30795	0	4.80198	1.24067	6.63827

1.41296	1.26502	5.91852	1.99068	6.47247	6.63827
4.21695	3.92385	0	1.99906	3.72023	0
4.19986	3.89717	5.98113	4.81036	8.95203	0
4.24584	1.31021	2.88857	1.98686	3.70192	3.36686
1.38916	3.92882	2.80896	4.79816	8.93372	3.36686
1.39029	6.53486	2.81443	1.99068	3.68538	6.63827
4.24668	9.15426	2.88184	4.80198	8.91718	6.63827
4.21695	6.53975	0	5.54045	3.33506	0
4.2003	6.56623	5.9817	2.72915	8.56686	0
1.40565	9.15565	0	5.49564	3.33255	3.3579
1.41295	9.19826	5.91724	2.68434	8.56435	3.3579
1.40565	6.53975	0	5.50245	3.30597	6.71691
1.41607	6.58348	5.47734	2.69115	8.53777	6.71691
4.21695	9.15565	0	2.72915	1.5911	0
4.34306	9.21506	5.67932	5.54045	6.8229	0
4.20136	6.5388	2.98603	2.68434	1.59361	3.3579
1.44546	9.15492	2.98794	5.49564	6.82541	3.3579
7.06692	1.30849	2.99519	2.69115	1.62018	6.71691
9.82236	3.92471	2.98071	5.50245	6.85198	6.71691
9.83955	1.30795	0	2.72915	5.07893	1.67548
9.96534	1.24843	5.68037	5.54045	10.31073	1.67548
7.02825	3.92385	0	2.76452	5.07893	5.06071
7.03797	3.8802	5.47508	5.57582	10.31073	5.06071
7.02825	1.30795	0			
7.03554	1.26512	5.91814			
9.83955	3.92385	0			
9.82272	3.89711	5.98155			
9.86871	1.30997	2.88783			
7.01122	3.92901	2.8093			
7.01303	6.53524	2.81412			
9.86961	9.15393	2.8818			
9.83955	6.53975	0			
9.82303	6.56632	5.9823			
7.02825	9.15565	0			
7.03551	9.19846	5.9172			
7.02825	6.53975	0			
7.03819	6.58364	5.4769			
9.83955	9.15565	0			
9.96549	9.21533	5.67942			
9.82402	6.53868	2.98781			
7.06761	9.1551	2.98798			
2.0062	10.46274	8.63497			
10.99854	5.2313	8.68815			
3.12567	3.34735	8.8416			

0.42986	8.42027	8.81849
0.43058	2.04307	8.81939
3.1253	7.11605	8.84164
7.62889	2.72E-04	8.63513
5.37644	5.23167	8.68815
8.74802	3.34723	8.84135
6.05258	8.42031	8.81886
6.05325	2.04364	8.81899
8.74763	7.11613	8.84149
11.22993	5.23E-05	6.08561
3.41231	5.23165	7.21577
4.06001	1.34773	7.55126
1.27942	6.62797	7.28344
1.27965	3.83575	7.28188
4.06026	9.11575	7.54904
5.60762	10.46344	6.08615
9.03405	5.23174	7.21542
9.68297	1.34809	7.55015
6.90201	6.62829	7.283
6.90253	3.836	7.28178
9.68235	9.1161	7.54933
10.4118	3.43171	7.4306
1.99293	8.68828	7.35986
1.99301	1.77462	7.36093
10.41139	7.03201	7.4311
10.92284	10.4635	8.82934
1.97174	5.2314	8.92816
4.78921	3.43166	7.43049
7.61537	8.6889	7.35994
7.61568	1.77515	7.36038
4.78897	7.03186	7.43108
5.30021	2.09E-05	8.82978
7.59451	5.2314	8.92818

References

1. B. Wang, P. Xi, C. Shan, H. Chen, H. Xu, K. Iqbal, W. Liu and Y. Tang, *Advanced Materials Interfaces*, 2017, **4**, 1700272.
2. Q. Dong, C. Shuai, Z. Mo, N. Liu, G. Liu, J. Wang, H. Pei, Q. Jia, W. Liu and X. Guo, *Journal of Solid State Chemistry*, 2021, **296**, 121967.
3. Y. Hu, W. Liu, K. Jiang, L. Xu, M. Guan, J. Bao, H. Ji and H. Li, *Inorganic Chemistry Frontiers*, 2020, **7**, 4461-4468.
4. Y. Li, W. Luo, D. Wu, Q. Wang, J. Yin, P. Xi, Y. Qu, M. Gu, X. Zhang, Z. Lu and Z. Zheng, *Nano Research*, 2021.
5. X. Long, H. Lin, D. Zhou, Y. An and S. Yang, *ACS Energy Letters*, 2018, **3**, 290-296.
6. X. Wang, Y. Yang, L. Diao, Y. Tang, F. He, E. Liu, C. He, C. Shi, J. Li, J. Sha, S. Ji, P. Zhang, L. Ma and N. Zhao, *ACS Applied Material Interfaces*, 2018, **10**, 35145-35153.
7. E. Cossar, K. Agarwal, V. B. Nguyen, R. Safari, G. A. Botton and E. A. Baranova, *Electrocatalysis*, 2021, **12**, 605–618.