Supporting Information

Title: Itinerant ferromagnetic half metallic Iro-Cobalt couple: promising bifunctional electrocatalysts for ORR and OER

Yuling Sun, Jing Wang, Qian Liu, Meirong Xia, Yongfu Tang, Faming Gao, Yanglong Hou, John Tse*, Yufeng Zhao**

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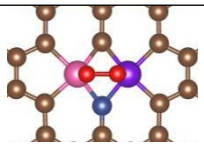
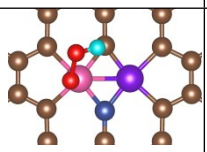
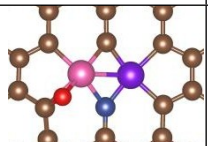
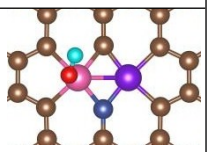
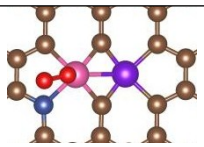
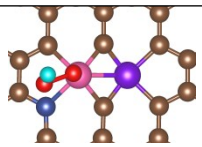
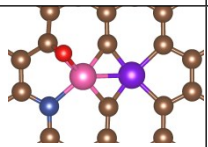
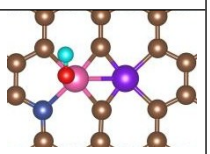
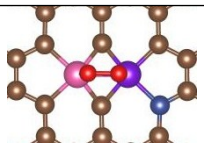
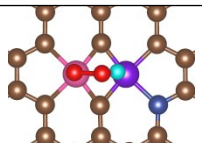
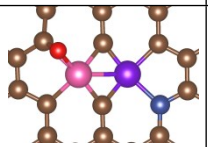
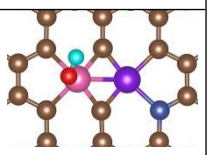
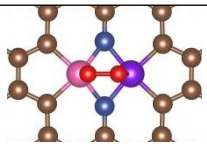
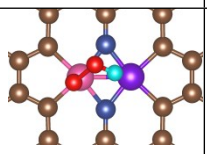
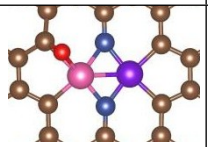
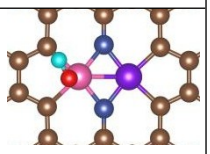
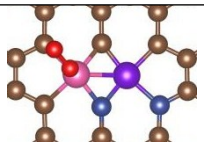
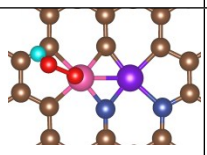
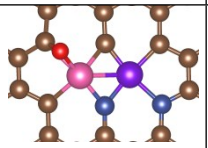
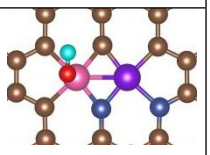
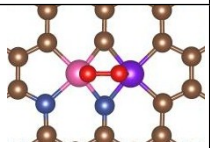
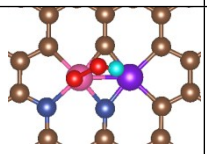
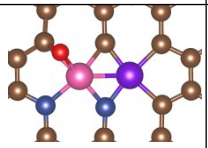
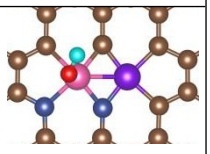
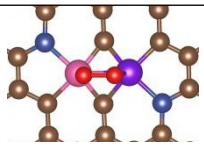
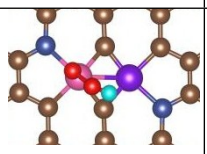
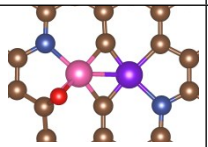
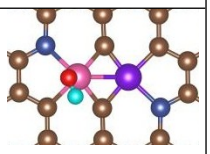
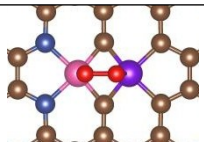
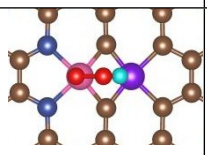
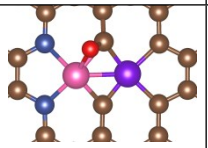
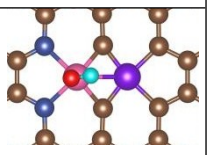
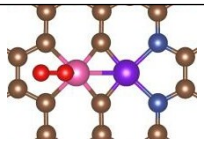
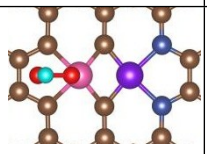
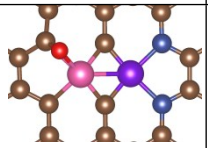
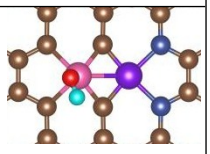
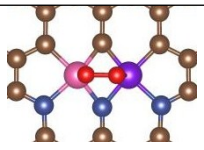
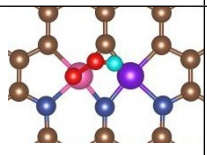
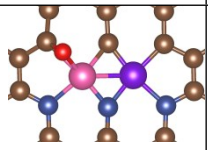
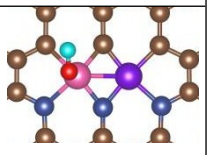
$FeCoN_1$-gra(Ⅰ)				
$FeCoN_1$-gra(Ⅱ)				
$FeCoN_1$-gra(Ⅲ)				
$FeCoN_2$-gra(Ⅰ)				
$FeCoN_2$-gra(Ⅱ)				
$FeCoN_2$-gra(Ⅲ)				
$FeCoN_2$-gra(Ⅳ)				
$FeCoN_2$-gra(Ⅴ)				
$FeCoN_2$-gra(Ⅵ)				
$FeCoN_3$-gra(Ⅰ)				

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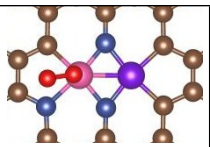
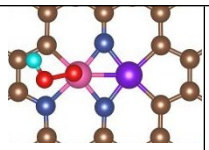
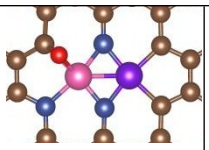
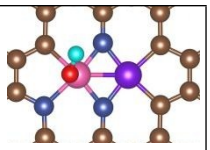
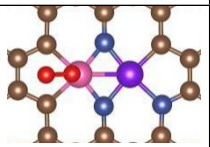
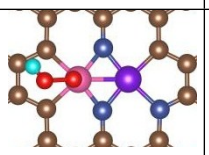
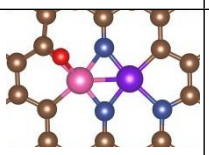
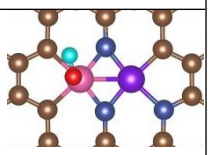
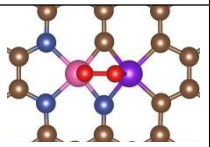
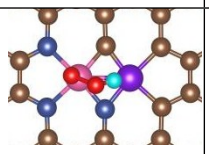
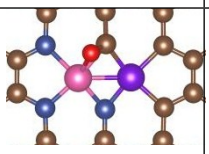
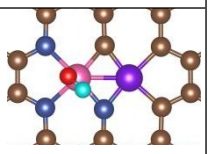
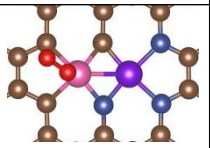
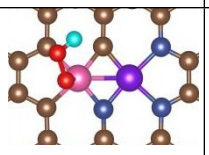
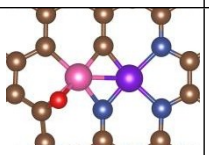
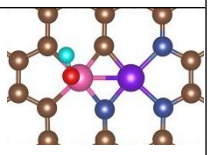
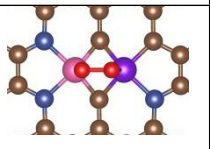
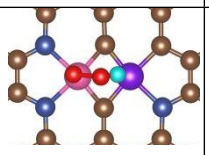
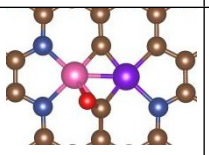
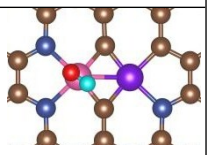
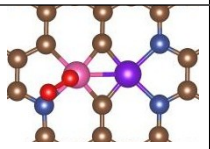
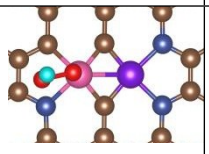
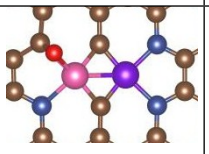
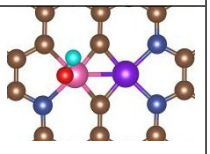
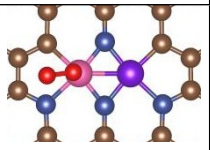
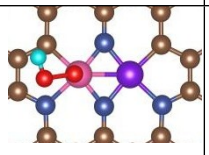
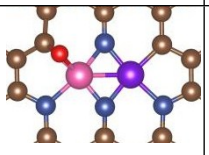
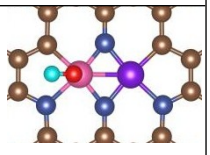
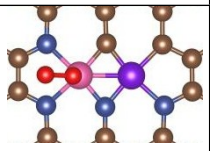
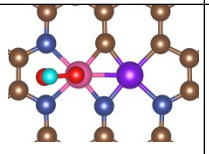
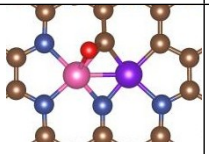
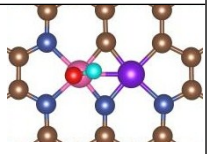
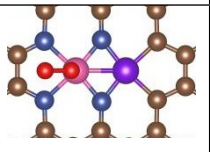
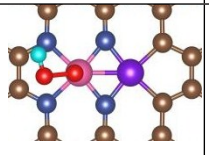
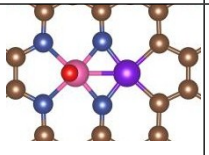
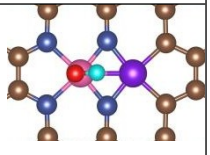
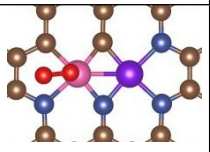
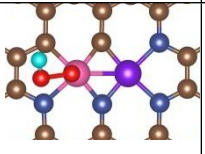
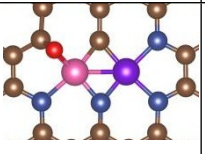
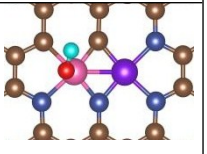
$FeCoN_3$-gra(Ⅱ)				
$FeCoN_3$-gra(Ⅲ)				
$FeCoN_3$-gra(Ⅳ)				
$FeCoN_3$-gra(Ⅴ)				
$FeCoN_3$-gra(Ⅵ)				
$FeCoN_3$-gra(Ⅶ)				
$FeCoN_4$-gra(Ⅰ)				
$FeCoN_4$-gra(Ⅱ)				
$FeCoN_4$-gra(Ⅲ)				
$FeCoN_4$-gra(Ⅳ)				
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To be continued

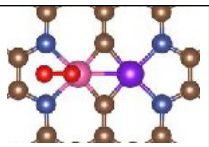
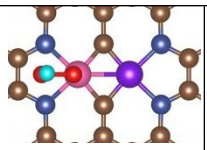
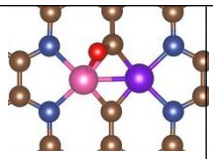
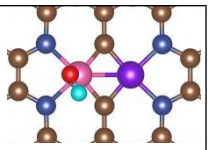
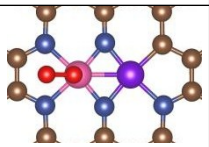
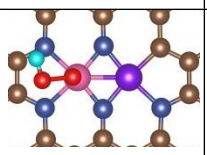
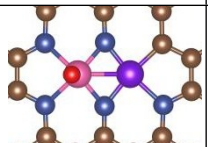
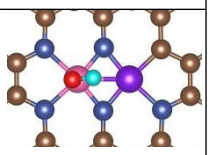
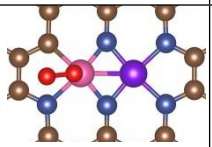
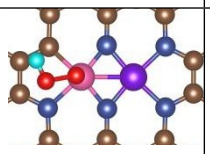
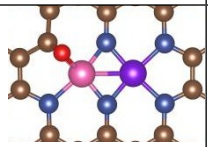
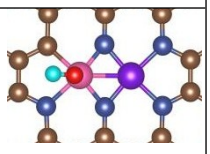
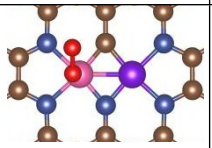
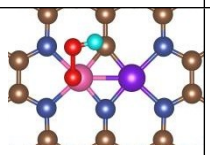
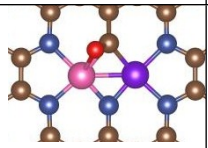
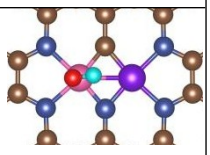
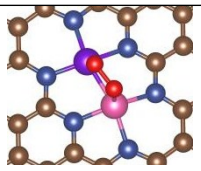
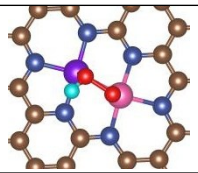
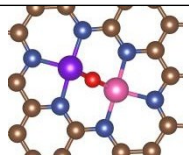
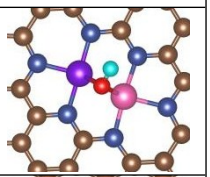
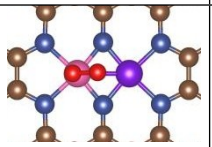
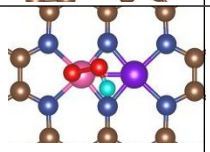
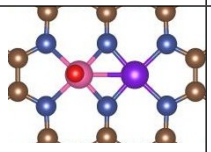
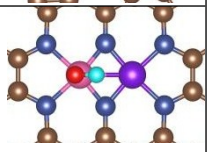
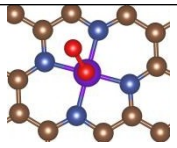
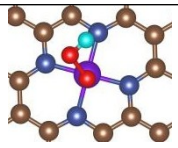
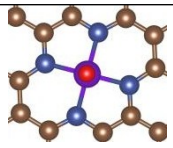
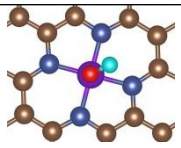
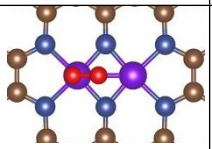
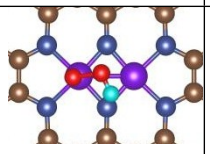
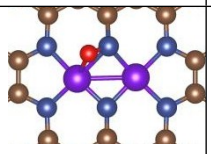
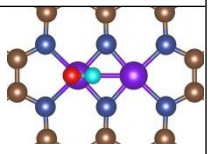
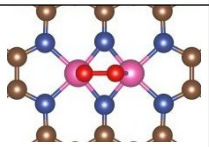
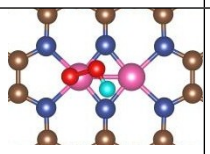
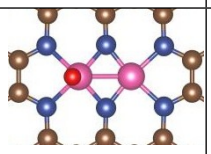
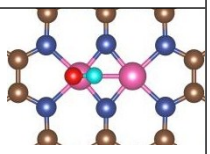
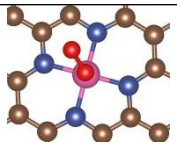
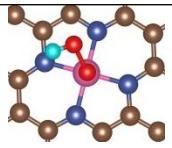
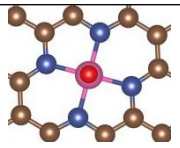
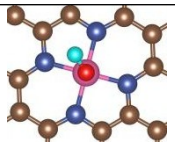
$FeCoN_4$-gra(Ⅵ)				
$FeCoN_5$-gra(Ⅰ)				
$FeCoN_5$-gra(Ⅱ)				
$FeCoN_5$-gra(Ⅲ)				
$FeCoN_6$-gra(Ⅰ)				
$FeCoN_6$-gra(Ⅱ)				
CoN_4-gra				
$CoCoN_6$-gra				
$FeFeN_6$-gra				
FeN_4-gra				

Figure S1.

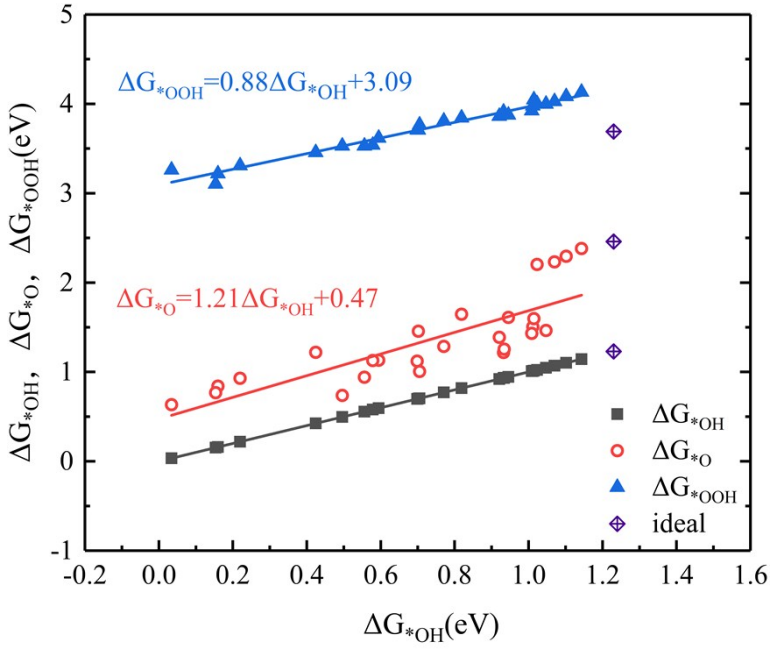

ΔG*OOH=0.88ΔG*OH+3.09
ΔG*O=1.21ΔG*OH+0.47
ΔG*OH
ΔG*O
ΔG*OOH
ideal
ΔG*OH, ΔG*O, ΔG*OOH(eV)
ΔG*OH(eV)
5
4
3
2
1
0
-1
-0.2
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6

Figure S2.

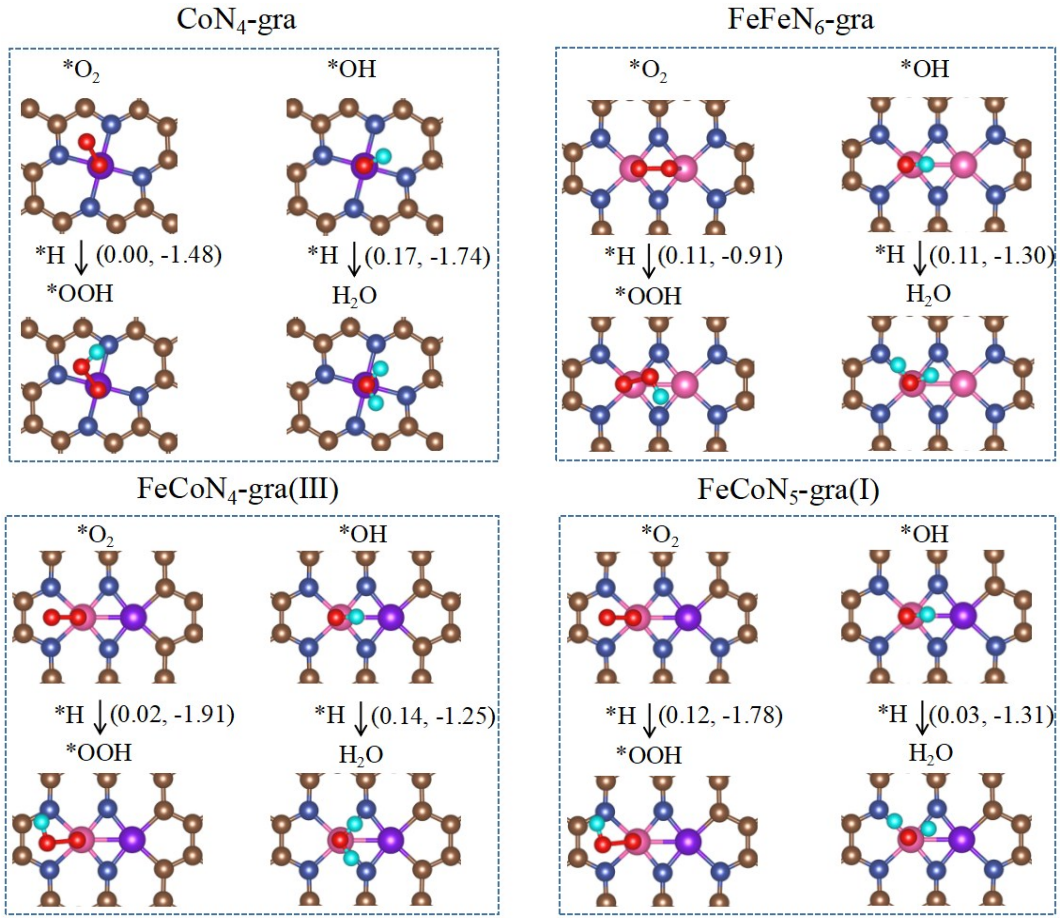
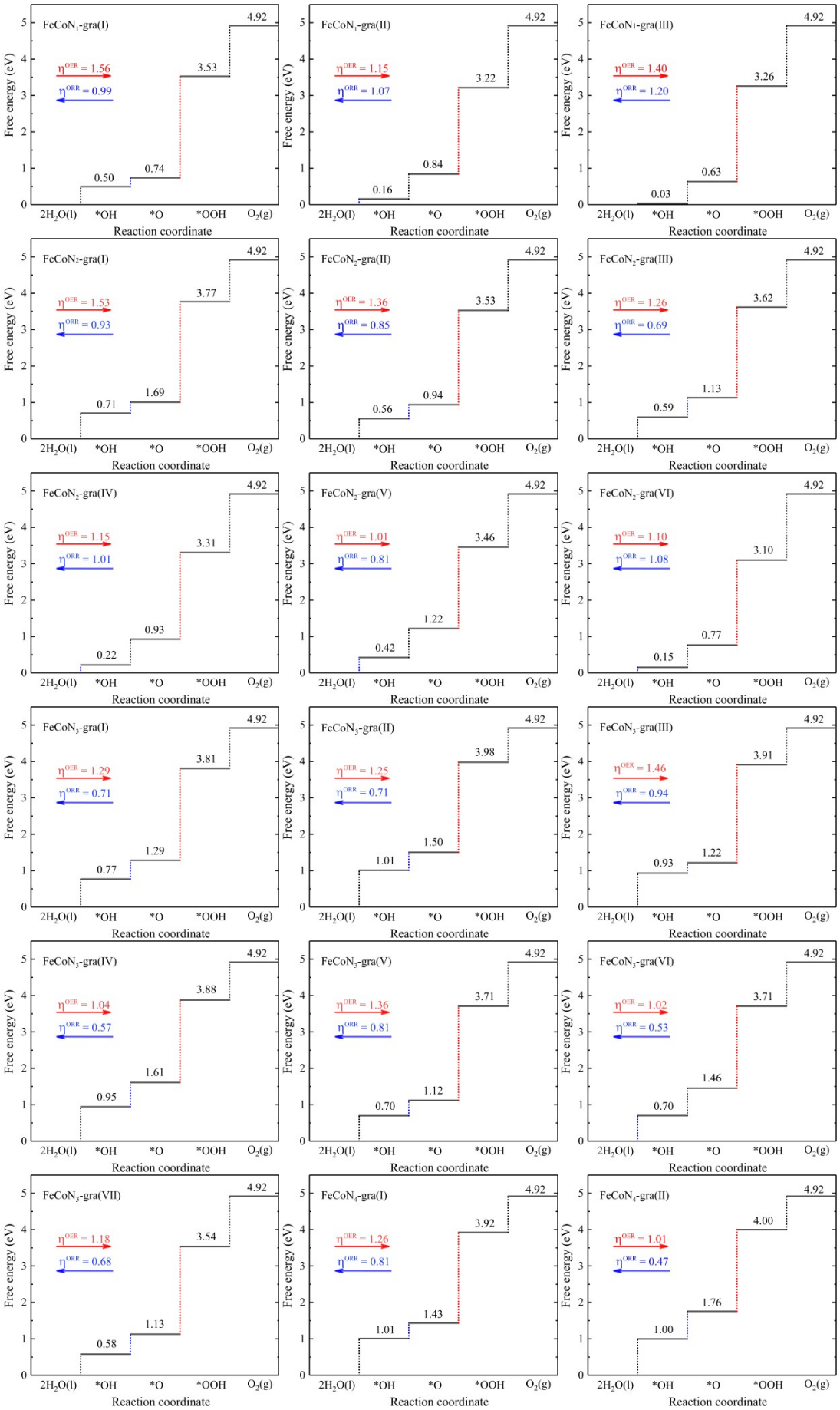

CoN4-gra
*O2
*OH
*H (0.00, -1.48)
*H (0.17, -1.74)
*OOH
H2O
FeFeN6-gra
*O2
*OH
*H (0.11, -0.91)
*H (0.11, -1.30)
*OOH
H2O
FeCoN4-gra(III)
*O2
*OH
*H (0.02, -1.91)
*H (0.14, -1.25)
*OOH
H2O
FeCoN5-gra(I)
*O2
*OH
*H (0.12, -1.78)
*H (0.03, -1.31)
*OOH
H2O

Figure S3.



To be continued

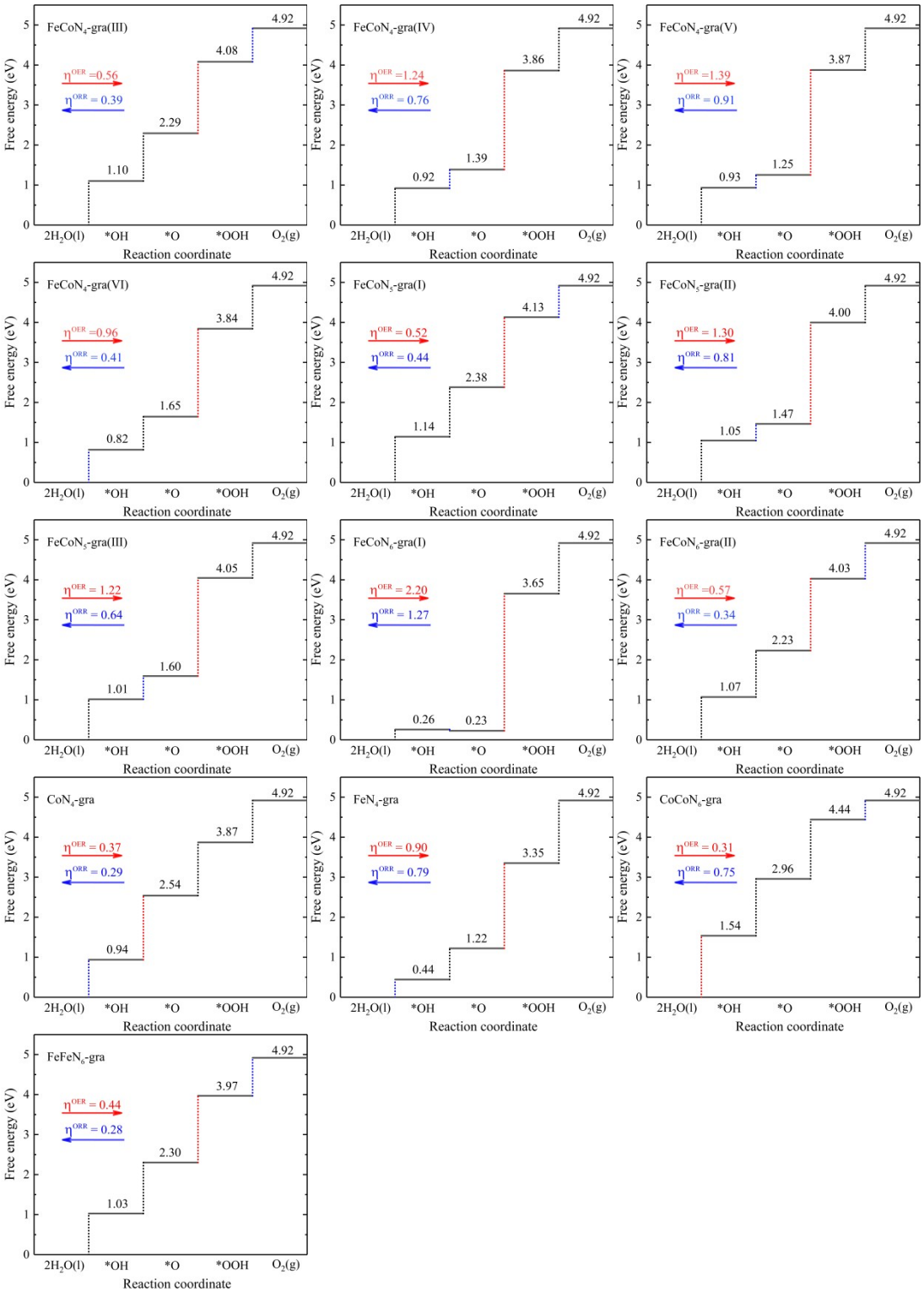

FeCoN4-gra(III)
ηOER =0.56
ηORR = 0.39
1.10
2.29
4.08
4.92
FeCoN4-gra(IV)
ηOER =1.24
ηORR = 0.76
0.92
1.39
3.86
4.92
FeCoN4-gra(V)
ηOER =1.39
ηORR = 0.91
0.93
1.25
3.87
4.92
FeCoN4-gra(VI)
ηOER =0.96
ηORR = 0.41
0.82
1.65
3.84
4.92
FeCoN5-gra(I)
ηOER = 0.52
ηORR = 0.44
1.14
2.38
4.13
4.92
FeCoN5-gra(II)
ηOER = 1.30
ηORR = 0.81
1.05
1.47
4.00
4.92
FeCoN5-gra(III)
ηOER = 1.22
ηORR = 0.64
1.01
1.60
4.05
4.92
FeCoN6-gra(I)
ηOER = 2.20
ηORR = 1.27
0.26
0.23
3.65
4.92
FeCoN6-gra(II)
ηOER =0.57
ηORR = 0.34
1.07
2.23
4.03
4.92
CoN4-gra
ηOER = 0.37
ηORR = 0.29
0.94
2.54
3.87
4.92
FeN4-gra
ηOER = 0.90
ηORR = 0.79
0.44
1.22
3.35
4.92
CoCoN6-gra
ηOER = 0.31
ηORR = 0.75
1.54
2.96
4.44
4.92
FeFeN6-gra
ηOER = 0.44
ηORR = 0.28
1.03
2.30
3.97
4.92
Free energy (eV)
Reaction coordinate
2H2O(l)
*OH
*O
*OOH
O2(g)

Figure S4.

Table S1.

	$E_{ads\text{-}O2}$	$d_{O\text{-}O}$	$d_{Fe\text{-}O}$	$d_{Co\text{-}O}$
$FeCoN_1$-gra(Ⅰ)	-1.10	1.36	1.81	1.90
$FeCoN_1$-gra(Ⅱ)	-1.09	1.29	1.72	-
$FeCoN_1$-gra(Ⅲ)	-1.12	1.36	1.77	1.89
$FeCoN_2$-gra(Ⅰ)	-0.85	1.35	1.84	2.03
$FeCoN_2$-gra(Ⅱ)	-1.04	1.28	1.73	-
$FeCoN_2$-gra(Ⅲ)	-1.09	1.36	1.83	1.92
$FeCoN_2$-gra(Ⅳ)	-1.39	1.37	1.81	1.90
$FeCoN_2$-gra(Ⅴ)	-1.34	1.38	1.83	1.89
$FeCoN_2$-gra(Ⅵ)	-1.41	1.29	1.71	-
$FeCoN_3$-gra(Ⅰ)	-0.74	1.36	1.84	2.03
$FeCoN_3$-gra(Ⅱ)	-0.66	1.29	1.84	-
$FeCoN_3$-gra(Ⅲ)	-0.68	1.28	1.83	-
$FeCoN_3$-gra(Ⅳ)	-0.74	1.36	1.84	2.00
$FeCoN_3$-gra(Ⅴ)	-0.92	1.29	1.74	-
$FeCoN_3$-gra(Ⅵ)	-0.97	1.38	1.84	1.92
$FeCoN_3$-gra(Ⅶ)	-1.06	1.29	1.75	-
$FeCoN_4$-gra(Ⅰ)	-0.72	1.29	1.86	-
$FeCoN_4$-gra(Ⅱ)	-0.71	1.29	1.87	-
$FeCoN_4$-gra(Ⅲ)	-0.64	1.29	1.89	-
$FeCoN_4$-gra(Ⅳ)	-0.77	1.29	1.84	-
$FeCoN_4$-gra(Ⅴ)	-0.73	1.29	1.82	-
$FeCoN_4$-gra(Ⅵ)	-0.79	1.30	1.84	-
$FeCoN_5$-gra(Ⅰ)	-0.63	1.29	1.88	-
$FeCoN_5$-gra(Ⅱ)	-0.60	1.29	1.79	-
$FeCoN_5$-gra(Ⅲ)	-0.62	1.29	1.88	-
$FeCoN_6$-gra(Ⅰ)	-1.60	1.38	1.86	1.88
$FeCoN_6$-gra(Ⅱ)	-0.62	1.29	1.88	-
CoN_4-gra	-0.89	1.29	-	1.88
$CoCoN_6$-gra	-0.19	1.28	-	1.99
$FeFeN_6$-gra	-0.75	1.36	1.85, 2.10	-
FeN_4-gra	-1.22	1.30	1.77	-

Table S2.

	Fe	Co
$FeCoN_1$-gra(Ⅰ)	2.01	0.67
$FeCoN_1$-gra(Ⅱ)	2.00	1.05
$FeCoN_1$-gra(Ⅲ)	2.11	0.78
$FeCoN_2$-gra(Ⅰ)	2.04	-0.36
$FeCoN_2$-gra(Ⅱ)	2.05	0.42
$FeCoN_2$-gra(Ⅲ)	1.87	0.72
$FeCoN_2$-gra(Ⅳ)	1.94	0.74
$FeCoN_2$-gra(Ⅴ)	1.82	1.04
$FeCoN_2$-gra(Ⅵ)	2.10	0.67
$FeCoN_3$-gra(Ⅰ)	1.85	0.27
$FeCoN_3$-gra(Ⅱ)	1.87	-0.42
$FeCoN_3$-gra(Ⅲ)	2.08	-0.51
$FeCoN_3$-gra(Ⅳ)	1.67	0.61
$FeCoN_3$-gra(Ⅴ)	2.10	-0.12
$FeCoN_3$-gra(Ⅵ)	1.76	0.67
$FeCoN_3$-gra(Ⅶ)	2.00	-0.03
$FeCoN_4$-gra(Ⅰ)	1.85	-0.63
$FeCoN_4$-gra(Ⅱ)	1.39	0.00
$FeCoN_4$-gra(Ⅲ)	1.35	0.15
$FeCoN_4$-gra(Ⅳ)	1.71	-0.38
$FeCoN_4$-gra(Ⅴ)	1.90	-0.55
$FeCoN_4$-gra(Ⅵ)	1.73	-0.29
$FeCoN_5$-gra(Ⅰ)	1.42	0.40
$FeCoN_5$-gra(Ⅱ)	1.84	0.12
$FeCoN_5$-gra(Ⅲ)	1.67	0.18
$FeCoN_6$-gra(Ⅰ)	2.35	1.04

Table S3.

	$*O_2$	***OOH**	***O**	***OH**
$FeCoN_1$-gra(Ⅰ)	-444.9887	-449.0913	-440.8283	-444.6682
$FeCoN_1$-gra(Ⅱ)	-444.9817	-448.9986	-440.3046	-444.5913
$FeCoN_1$-gra(Ⅲ)	-445.0027	-448.9026	-440.4794	-444.6373
$FeCoN_2$-gra(Ⅰ)	-445.4475	-449.5706	-441.2703	-445.1821
$FeCoN_2$-gra(Ⅱ)	-445.5308	-449.7231	-441.2247	-445.2241
$FeCoN_2$-gra(Ⅲ)	-445.5429	-449.5882	-440.9987	-445.1495
$FeCoN_2$-gra(Ⅳ)	-445.4373	-449.4954	-440.7907	-445.1008
$FeCoN_2$-gra(Ⅴ)	-445.2953	-449.235	-440.3799	-444.8115
$FeCoN_2$-gra(Ⅵ)	-445.3107	-449.5214	-440.8095	-445.0027
$FeCoN_3$-gra(Ⅰ)	-445.9511	-450.1546	-441.6033	-445.7422
$FeCoN_3$-gra(Ⅱ)	-445.8613	-449.9847	-441.3761	-445.4717
$FeCoN_3$-gra(Ⅲ)	-445.8379	-450.0259	-441.6260	-445.5249
$FeCoN_3$-gra(Ⅳ)	-445.7066	-449.8240	-441.0029	-445.3231
$FeCoN_3$-gra(Ⅴ)	-445.8214	-449.9101	-441.4557	-445.5022
$FeCoN_3$-gra(Ⅵ)	-445.6639	-449.7295	-440.8856	-445.2911
$FeCoN_3$-gra(Ⅶ)	-445.7206	-449.8607	-441.2117	-445.4396
$FeCoN_4$-gra(Ⅰ)	-446.2963	-450.4039	-441.8188	-445.8696
$FeCoN_4$-gra(Ⅱ)	-446.2242	-450.2846	-441.4058	-445.8171
$FeCoN_4$-gra(Ⅲ)	-446.1189	-450.1699	-440.7930	-445.6828
$FeCoN_4$-gra(Ⅳ)	-446.1977	-450.3155	-441.7177	-445.7967
$FeCoN_4$-gra(Ⅴ)	-446.0546	-450.2221	-441.7497	-445.6985
$FeCoN_4$-gra(Ⅵ)	-445.9080	-450.0031	-441.1231	-445.5956
$FeCoN_5$-gra(Ⅰ)	-446.4062	-450.42215	-440.9952	-445.9304
$FeCoN_5$-gra(Ⅱ)	-446.3158	-450.4321	-441.8741	-445.9141
$FeCoN_5$-gra(Ⅲ)	-446.2639	-450.3587	-441.6863	-445.9215
$FeCoN_6$-gra(Ⅰ)	-445.9368	-449.4509	-441.7595	-445.4090
$FeCoN_6$-gra(Ⅱ)	-446.4121	-450.4443	-441.0717	-445.9417
CoN_4-gra	-458.7990	-462.7659	-452.9111	-458.2405
$CoCoN_6$-gra	-444.2073	-448.3234	-438.7217	-443.7586
$FeFeN_6$-gra	-447.9625	-451.9855	-442.512	-447.4729
FeN_4-gra	-460.2559	-464.4192	-455.4095	-459.8889