Supplementary Information

for

Multifunctional electrocatalysis on single-site metal catalysts: a computational perspective

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Table S1. Calculated DFT energies and overpotentials for CoN_4, FeN_4 and NiN_4 with single-site adsorption mechanism, and NiN4 with double-site adsorption mechanism. All energies are in eV.

Surface species with PCM

Species	Non-solv	ZPE corr	Cv corr	Entropy corr	TS09 corr	Energy
Co	-538.71	-	-	-	-2.71	-541.41
Co_ooh	-554.35	0.45	0.09	-0.17	-2.88	-556.86
Co_o	-544.24	0.08	0.02	-0.03	-2.77	-546.94
Co_oh	-549.53	0.35	0.05	-0.09	-2.82	-552.04
Fe	-539.33	-	-	-	-2.71	-542.03
Fe_ooh	-555.28	0.45	0.08	-0.14	-2.88	-557.77
Fe_o	-546.04	0.06	0.04	-0.08	-2.78	-548.80
Fe_oh	-550.41	0.34	0.06	-0.11	-2.82	-552.94
Ni	-538.00	-	-	-	-2.70	-540.70
Ni_ooh	-552.65	0.46	0.08	-0.13	-2.86	-555.11
Ni_o	-542.05	0.04	0.05	-0.12	-2.76	-544.85
Ni_oh	-547.77	0.32	0.07	-0.12	-2.81	-550.31
Ni_o_d	-543.00	0.09	0.02	-0.04	-2.75	-545.68
Ni_oh_d	-547.54	0.40	0.03	-0.05	-2.81	-549.97
Small molecule data						
H_2	-6.75	0.27	0.09	-0.40	0.00	-6.80
H_2O	-14.57	0.57	0.10	-0.58	0.00	-14.48
O_2	-	-	-	-	-	-10.44

Calculated energy levels

	Co	Fe	Ni	Ni_dual
$*+O_2+4(H^++e^-)$	0.00	0.00	0.00	0.00
$OOH*+3(H^++e^-)$	-1.61	-1.89	-0.57	-0.57
$O*+2(H^++e^-)+H_2O$	-2.76	-4.00	-1.40	-2.22
$OH*+(H^++e^-)+H_2O$	-4.47	-4.75	-3.46	-3.12
$*+2H_2O$	-4.92	-4.92	-4.92	-4.92

Calculated overpotentials

	Co	Fe	Ni	Ni_dual
ORR	0.78	1.06	0.66	0.66
OER	0.47	0.88	0.83	0.57