Supporting Information

DFT screening of dual-atom catalysts on carbon nanotubes for enhanced oxygen reduction Reaction and oxygen evolution reaction: comparing dissociative and associative mechanisms

Xiangyi Zhou[1], Mohsen Tamtaji[2], Weijun Zhou[3], William A. Goddard III[4]*, Guanhua Chen[1,2,3]*

[1]*Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China*

[2]*Hong Kong Quantum AI Lab Limited, Pak Shek Kok, Hong Kong SAR, China*

[3]*QuantumFabless Limited, Pak Shek Kok, Hong Kong SAR, China*

[4]*Materials and Process Simulation Center (MSC), MC 139-74, California Institute of Technology, Pasadena CA, 91125, USA*

*Corresponding Authors, email: ghc@everest.hku.hk, and wag@caltech.edu

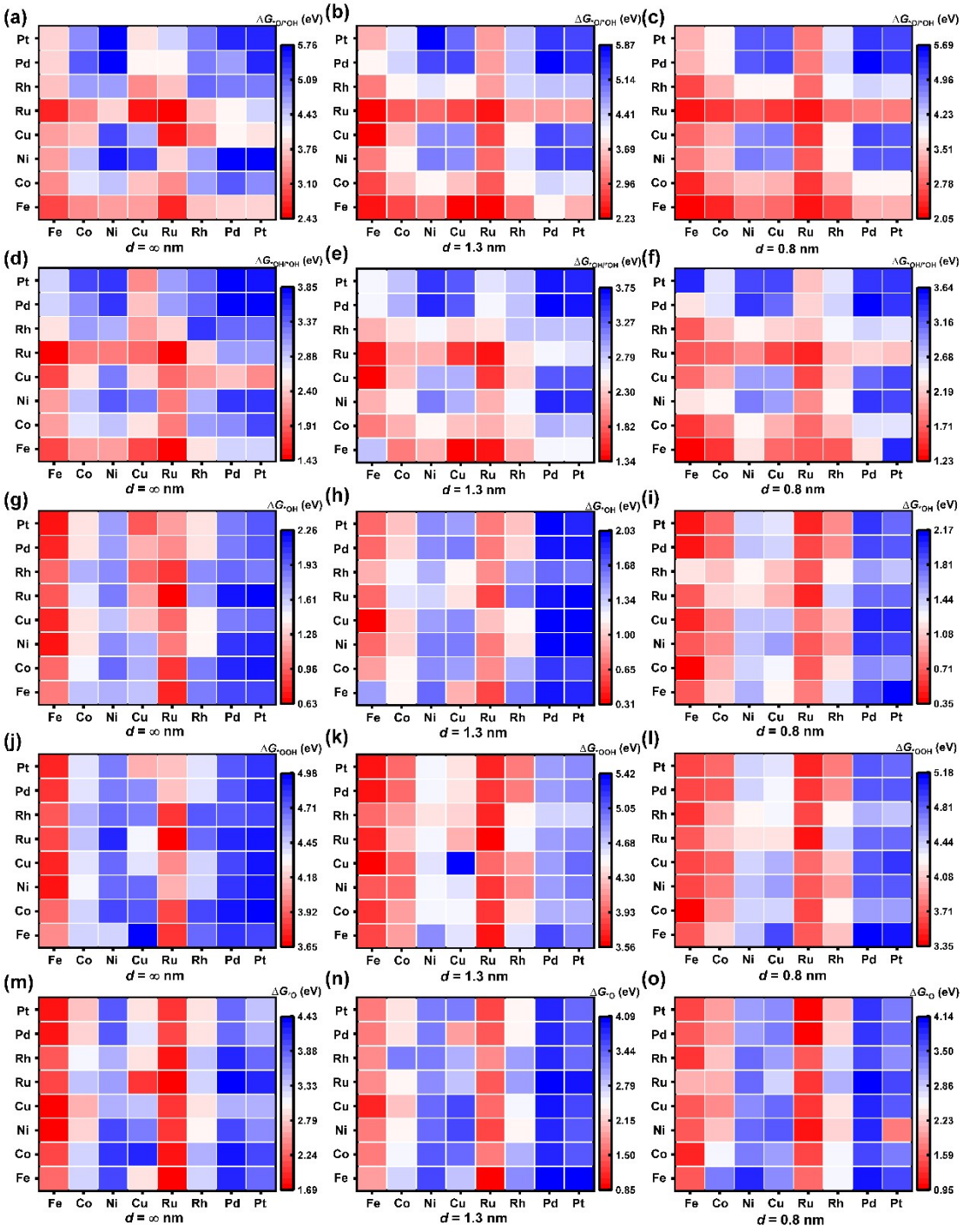

Fig S1. $\Delta G_{*O/*OH}$, $\Delta G_{*OH/*OH}$, ΔG_{*OH}, ΔG_{*OOH}, and ΔG_{*O} of $MM'N_6$-DACs at $d = \infty$ nm, $d = 1.3$ nm, and $d = 0.8$ nm, respectively. For ΔG_{*OH}, ΔG_{*OOH}, and ΔG_{*O}, intermediates adsorb on the metal site M (denoted by the horizontal axis), whereas for $\Delta G_{*O/*OH}$ and $\Delta G_{*OH/*OH}$, both metal sites contribute to the adsorption of intermediates.

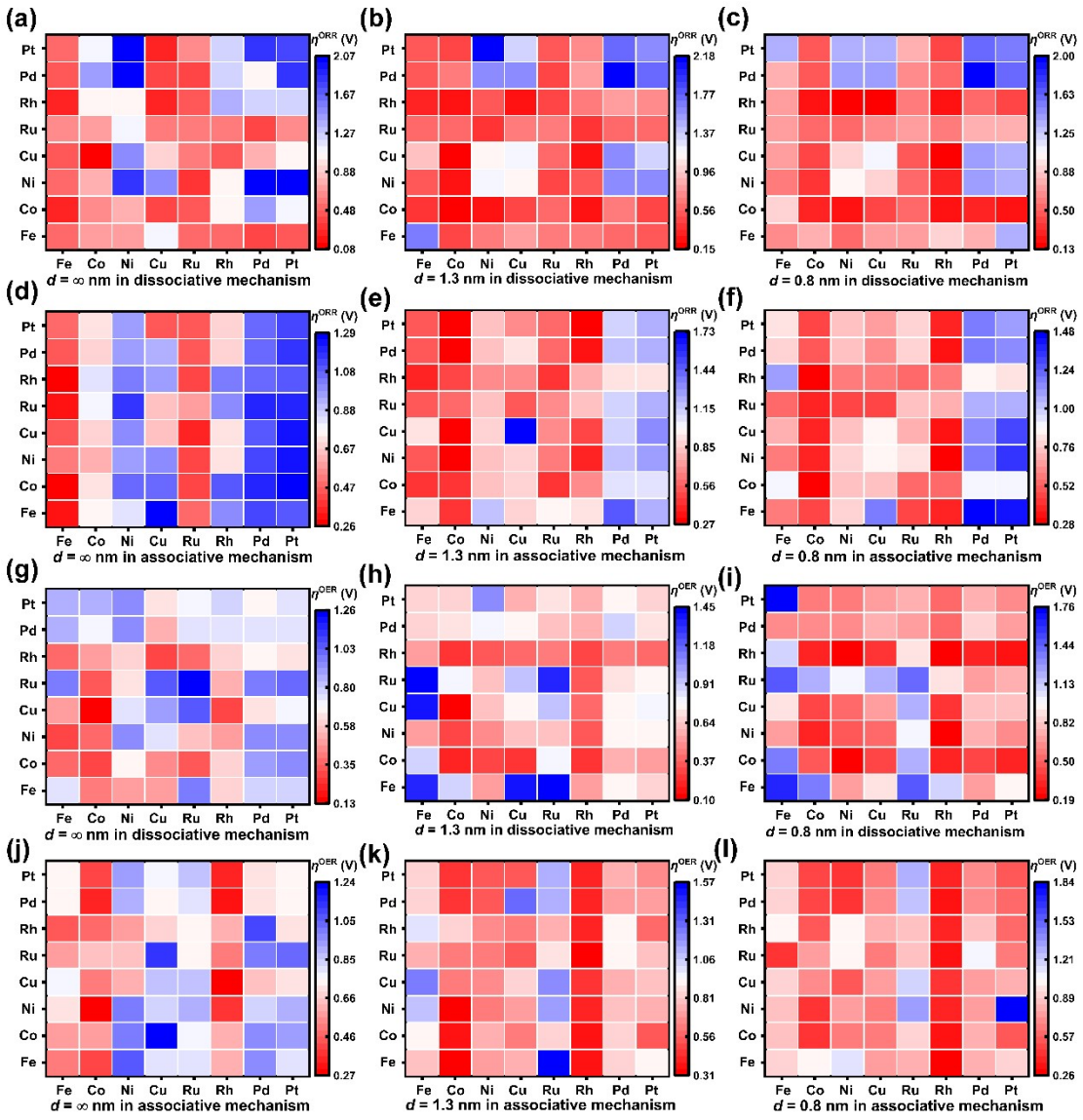

Fig S2. ORR and OER overpotential in two mechanisms for on MM′N_6-DACs at d = ∞ nm, d = 1.3 nm, and d = 0.8 nm, respectively. The overpotential denotes the activity on the metal site M (denoted by the horizontal axis). For associative mechanism, all intermediates adsorbed on the metal site M, whereas for dissociative mechanism, both metal sites contribute to the adsorption of *O/*OH and *OH/*OH.

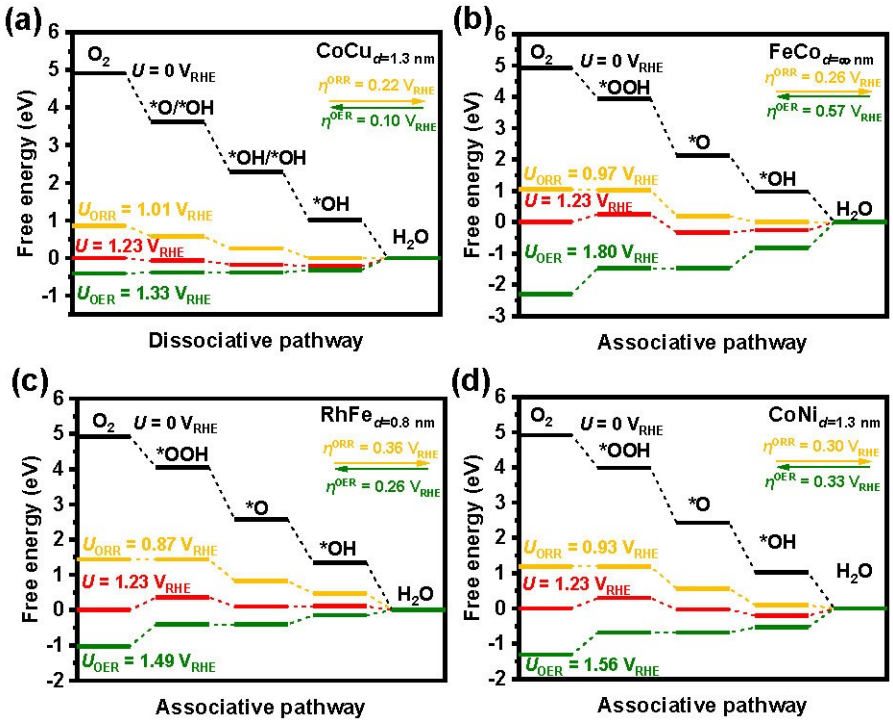

Fig S3. The Gibbs free energy diagrams for (a) CoCu-DAC at d = 1.3 nm in dissociative mechanism, (b) FeCo-DAC at the planar state in associative mechanism, (c) RhFe-DAC at d = 0.8 nm in associative mechanism, and (d) CoNi-DAC at d = 1.3 nm in associative mechanism.

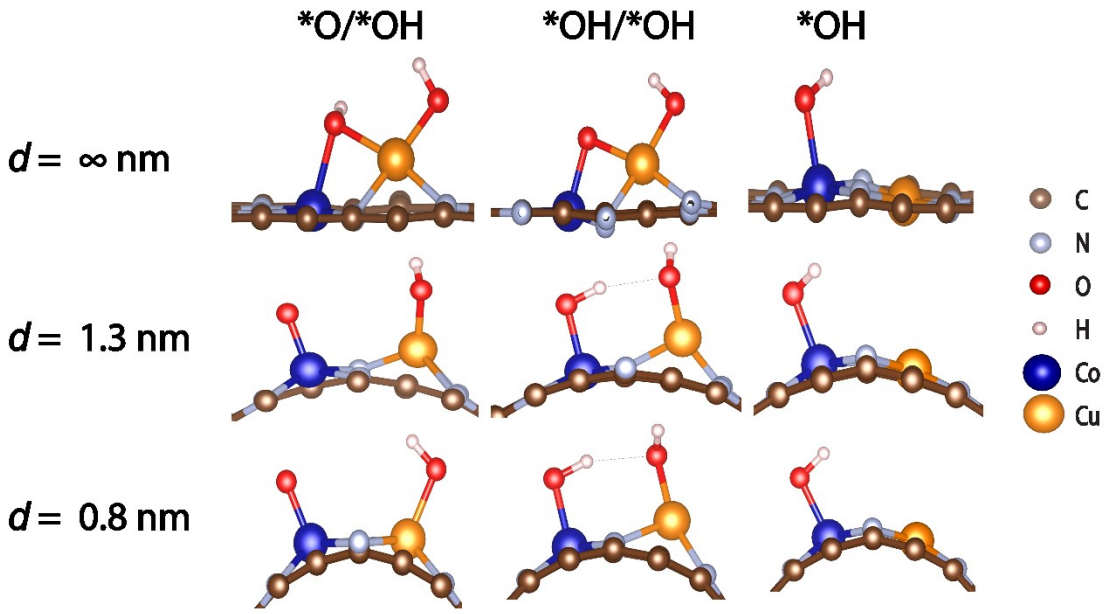

Fig S4. Adsorption configurations of intermediates in dissociative mechanism on CoCu-DACs under different curvature conditions.

Table S1. Computed formation energies (E_{form}) and dissolution potential (U_{diss}) of $MM'N_6$-DACs at $d = \infty$ nm. $E_{M'}$ and E_M are the atomic energies of metals M′ and M in their bulk phase, respectively. The number of electrons transferred during the dissolution (n) is 2 for eight metals in this work. [1,2] $U_{diss\_M'}^{o}$ and $U_{diss\_M}^{o}$ are the standard dissolution potential of the metals M′ and M, respectively. [3] U_{diss} is taken as the minimum of $U_{diss\_M'}$ and U_{diss_M}. The energy of the nitrogen-doped carbon substrate $E_{N\text{-}C}$ is -320.45 eV. The unit of all energies is eV, and the unit of all potential is V.

DACs	E_M	$E_{M'}$	E_{form}	$U_{diss\_M}^{o}$	$U_{diss\_M'}^{o}$	U_{diss_M}	$U_{diss\_M'}$	U_{diss}
FeFe	-8.24	-8.24	-2.16	-0.45	-0.45	0.63	0.63	0.63
CoFe	-7.02	-8.24	-3.17	-0.28	-0.45	1.30	1.13	1.13
NiFe	-5.47	-8.24	-3.03	-0.26	-0.45	1.25	1.06	1.06
CuFe	-3.73	-8.24	-2.46	0.34	-0.45	1.57	0.78	0.78
RuFe	-9.23	-8.24	-3.23	0.46	-0.45	2.08	1.17	1.17
RhFe	-7.26	-8.24	-3.06	0.60	-0.45	2.13	1.08	1.08
PdFe	-5.22	-8.24	-2.41	0.95	-0.45	2.15	0.75	0.75
PtFe	-6.10	-8.24	-1.80	1.18	-0.45	2.08	0.45	0.45
FeCo	-8.24	-7.02	-3.17	-0.45	-0.28	1.13	1.30	1.13
CoCo	-7.02	-7.02	-3.33	-0.28	-0.28	1.38	1.38	1.38
NiCo	-5.47	-7.02	-3.10	-0.26	-0.28	1.29	1.27	1.27
CuCo	-3.73	-7.02	-2.47	0.34	-0.28	1.57	0.95	0.95
RuCo	-9.23	-7.02	-3.09	0.46	-0.28	2.00	1.26	1.26
RhCo	-7.26	-7.02	-2.72	0.60	-0.28	1.96	1.08	1.08
PdCo	-5.22	-7.02	-2.72	0.95	-0.28	2.31	1.08	1.08
PtCo	-6.10	-7.02	-2.34	1.18	-0.28	2.35	0.89	0.89
FeNi	-8.24	-5.47	-3.03	-0.45	-0.26	1.06	1.25	1.06
CoNi	-7.02	-5.47	-3.10	-0.28	-0.26	1.27	1.29	1.27
NiNi	-5.47	-5.47	-2.49	-0.26	-0.26	0.98	0.98	0.98
CuNi	-3.73	-5.47	-2.39	0.34	-0.26	1.54	0.94	0.94
RuNi	-9.23	-5.47	-2.80	0.46	-0.26	1.86	1.14	1.14
RhNi	-7.26	-5.47	-2.78	0.60	-0.26	1.99	1.13	1.13
PdNi	-5.22	-5.47	-2.60	0.95	-0.26	2.25	1.04	1.04
PtNi	-6.10	-5.47	-2.68	1.18	-0.26	2.52	1.08	1.08
FeCu	-8.24	-3.73	-2.46	-0.45	0.34	0.78	1.57	0.78
CoCu	-7.02	-3.73	-2.47	-0.28	0.34	0.95	1.57	0.95
NiCu	-5.47	-3.73	-2.39	-0.26	0.34	0.94	1.54	0.94
CuCu	-3.73	-3.73	-1.91	0.34	0.34	1.29	1.29	1.29
RuCu	-9.23	-3.73	-2.18	0.46	0.34	1.55	1.43	1.43

DACs	E_M	$E_{M'}$	E_{form}	$U^{o}_{diss\_M}$	$U^{o}_{diss\_M'}$	U_{diss_M}	$U_{diss\_M'}$	U_{diss}
RhCu	-7.26	-3.73	-2.11	0.60	0.34	1.66	1.40	1.40
PdCu	-5.22	-3.73	-1.94	0.95	0.34	1.92	1.31	1.31
PtCu	-6.10	-3.73	-2.03	1.18	0.34	2.19	1.35	1.35
FeRu	-8.24	-9.23	-3.23	-0.45	0.46	1.17	2.08	1.17
CoRu	-7.02	-9.23	-3.09	-0.28	0.46	1.26	2.00	1.26
NiRu	-5.47	-9.23	-2.80	-0.26	0.46	1.14	1.86	1.14
CuRu	-3.73	-9.23	-2.18	0.34	0.46	1.43	1.55	1.43
RuRu	-9.23	-9.23	-2.73	0.46	0.46	1.82	1.82	1.82
RhRu	-7.26	-9.23	-2.86	0.60	0.46	2.03	1.89	1.89
PdRu	-5.22	-9.23	-2.43	0.95	0.46	2.16	1.67	1.67
PtRu	-6.10	-9.23	-2.51	1.18	0.46	2.44	1.72	1.72
FeRh	-8.24	-7.26	-3.06	-0.45	0.60	1.08	2.13	1.08
CoRh	-7.02	-7.26	-2.72	-0.28	0.60	1.08	1.96	1.08
NiRh	-5.47	-7.26	-2.78	-0.26	0.60	1.13	1.99	1.13
CuRh	-3.73	-7.26	-2.11	0.34	0.60	1.40	1.66	1.40
RuRh	-9.23	-7.26	-2.86	0.46	0.60	1.89	2.03	1.89
RhRh	-7.26	-7.26	-2.94	0.60	0.60	2.07	2.07	2.07
PdRh	-5.22	-7.26	-2.35	0.95	0.60	2.13	1.78	1.78
PtRh	-6.10	-7.26	-2.40	1.18	0.60	2.38	1.80	1.80
FePd	-8.24	-5.22	-2.41	-0.45	0.95	0.75	2.15	0.75
CoPd	-7.02	-5.22	-2.72	-0.28	0.95	1.08	2.31	1.08
NiPd	-5.47	-5.22	-2.60	-0.26	0.95	1.04	2.25	1.04
CuPd	-3.73	-5.22	-1.94	0.34	0.95	1.31	1.92	1.31
RuPd	-9.23	-5.22	-2.43	0.46	0.95	1.67	2.16	1.67
RhPd	-7.26	-5.22	-2.35	0.60	0.95	1.78	2.13	1.78
PdPd	-5.22	-5.22	-0.95	0.95	0.95	1.43	1.43	1.43
PtPd	-6.10	-5.22	-2.14	1.18	0.95	2.25	2.02	2.02
FePt	-8.24	-6.10	-1.80	-0.45	1.18	0.45	2.08	0.45
CoPt	-7.02	-6.10	-2.34	-0.28	1.18	0.89	2.35	0.89
NiPt	-5.47	-6.10	-2.68	-0.26	1.18	1.08	2.52	1.08
CuPt	-3.73	-6.10	-2.03	0.34	1.18	1.35	2.19	1.35
RuPt	-9.23	-6.10	-2.51	0.46	1.18	1.72	2.44	1.72
RhPt	-7.26	-6.10	-2.40	0.60	1.18	1.80	2.38	1.80
PdPt	-5.22	-6.10	-2.14	0.95	1.18	2.02	2.25	2.02
PtPt	-6.10	-6.10	-2.14	1.18	1.18	2.25	2.25	2.25

Table S2. Computed formation energies (E_{form}) and dissolution potential (U_{diss}) of $MM'N_6$-DACs at d = 1.3 nm. $E_{M'}$ and E_M are the atomic energies of metals M′ and M in their bulk phase, respectively. The number of electrons transferred during the dissolution (n) is 2 for eight metals in this work. [1,2] $U^{o}_{diss\_M'}$ and $U^{o}_{diss\_M}$ are the standard dissolution potential of the metals M′ and M, respectively. [3] U_{diss} is taken as the minimum of $U_{diss\_M'}$ and U_{diss_M}. The energy of the nitrogen-doped carbon substrate $E_{N\text{-}C}$ is -1134.42 eV. The unit of all energies is eV, and the unit of all potential is V.

DACs	E_M	$E_{M'}$	E_{form}	$U^{o}_{diss\_M}$	$U^{o}_{diss\_M'}$	U_{diss_M}	$U_{diss\_M'}$	U_{diss}
FeFe	-8.24	-8.24	-3.31	-0.45	-0.45	1.20	1.20	1.20
CoFe	-7.02	-8.24	-3.36	-0.28	-0.45	1.40	1.23	1.23
NiFe	-5.47	-8.24	-3.21	-0.26	-0.45	1.34	1.15	1.15
CuFe	-3.73	-8.24	-2.42	0.34	-0.45	1.55	0.76	0.76
RuFe	-9.23	-8.24	-3.15	0.46	-0.45	2.04	1.13	1.13
RhFe	-7.26	-8.24	-3.25	0.60	-0.45	2.23	1.18	1.18
PdFe	-5.22	-8.24	-2.97	0.95	-0.45	2.43	1.03	1.03
PtFe	-6.10	-8.24	-3.06	1.18	-0.45	2.71	1.08	1.08
FeCo	-8.24	-7.02	-3.36	-0.45	-0.28	1.23	1.40	1.23
CoCo	-7.02	-7.02	-3.19	-0.28	-0.28	1.31	1.31	1.31
NiCo	-5.47	-7.02	-3.05	-0.26	-0.28	1.26	1.24	1.24
CuCo	-3.73	-7.02	-2.43	0.34	-0.28	1.55	0.93	0.93
RuCo	-9.23	-7.02	-3.07	0.46	-0.28	2.00	1.26	1.26
RhCo	-7.26	-7.02	-3.08	0.60	-0.28	2.14	1.26	1.26
PdCo	-5.22	-7.02	-2.80	0.95	-0.28	2.35	1.12	1.12
PtCo	-6.10	-7.02	-2.89	1.18	-0.28	2.63	1.17	1.17
FeNi	-8.24	-5.47	-3.21	-0.45	-0.26	1.15	1.34	1.15
CoNi	-7.02	-5.47	-3.05	-0.28	-0.26	1.24	1.26	1.24
NiNi	-5.47	-5.47	-3.02	-0.26	-0.26	1.25	1.25	1.25
CuNi	-3.73	-5.47	-2.54	0.34	-0.26	1.61	1.01	1.01
RuNi	-9.23	-5.47	-2.81	0.46	-0.26	1.86	1.14	1.14
RhNi	-7.26	-5.47	-2.83	0.60	-0.26	2.02	1.16	1.16
PdNi	-5.22	-5.47	-2.76	0.95	-0.26	2.33	1.12	1.12
PtNi	-6.10	-5.47	-2.86	1.18	-0.26	2.61	1.17	1.17
FeCu	-8.24	-3.73	-2.42	-0.45	0.34	0.76	1.55	0.76
CoCu	-7.02	-3.73	-2.43	-0.28	0.34	0.93	1.55	0.93
NiCu	-5.47	-3.73	-2.54	-0.26	0.34	1.01	1.61	1.01
CuCu	-3.73	-3.73	-2.21	0.34	0.34	1.45	1.45	1.45
RuCu	-9.23	-3.73	-2.38	0.46	0.34	1.65	1.53	1.53
RhCu	-7.26	-3.73	-2.38	0.60	0.34	1.79	1.53	1.53
PdCu	-5.22	-3.73	-2.33	0.95	0.34	2.11	1.50	1.50

DACs	E_M	$E_{M'}$	E_{form}	$U^{o}_{diss\_M}$	$U^{o}_{diss\_M'}$	U_{diss_M}	$U_{diss\_M'}$	U_{diss}
PtCu	-6.10	-3.73	-2.42	1.18	0.34	2.39	1.55	1.55
FeRu	-8.24	-9.23	-3.15	-0.45	0.46	1.13	2.04	1.13
CoRu	-7.02	-9.23	-3.07	-0.28	0.46	1.26	2.00	1.26
NiRu	-5.47	-9.23	-2.81	-0.26	0.46	1.14	1.86	1.14
CuRu	-3.73	-9.23	-2.38	0.34	0.46	1.53	1.65	1.53
RuRu	-9.23	-9.23	-2.95	0.46	0.46	1.93	1.93	1.93
RhRu	-7.26	-9.23	-3.02	0.60	0.46	2.11	1.97	1.97
PdRu	-5.22	-9.23	-2.61	0.95	0.46	2.26	1.77	1.77
PtRu	-6.10	-9.23	-2.69	1.18	0.46	2.53	1.81	1.81
FeRh	-8.24	-7.26	-3.25	-0.45	0.60	1.18	2.23	1.18
CoRh	-7.02	-7.26	-3.08	-0.28	0.60	1.26	2.14	1.26
NiRh	-5.47	-7.26	-2.83	-0.26	0.60	1.16	2.02	1.16
CuRh	-3.73	-7.26	-2.38	0.34	0.60	1.53	1.79	1.53
RuRh	-9.23	-7.26	-3.02	0.46	0.60	1.97	2.11	1.97
RhRh	-7.26	-7.26	-3.04	0.60	0.60	2.12	2.12	2.12
PdRh	-5.22	-7.26	-2.58	0.95	0.60	2.24	1.89	1.89
PtRh	-6.10	-7.26	-2.70	1.18	0.60	2.53	1.95	1.95
FePd	-8.24	-5.22	-2.97	-0.45	0.95	1.03	2.43	1.03
CoPd	-7.02	-5.22	-2.80	-0.28	0.95	1.12	2.35	1.12
NiPd	-5.47	-5.22	-2.76	-0.26	0.95	1.12	2.33	1.12
CuPd	-3.73	-5.22	-2.33	0.34	0.95	1.50	2.11	1.50
RuPd	-9.23	-5.22	-2.61	0.46	0.95	1.77	2.26	1.77
RhPd	-7.26	-5.22	-2.58	0.60	0.95	1.89	2.24	1.89
PdPd	-5.22	-5.22	-2.53	0.95	0.95	2.21	2.21	2.21
PtPd	-6.10	-5.22	-1.23	1.18	0.95	1.80	1.57	1.57
FePt	-8.24	-6.10	-3.06	-0.45	1.18	1.08	2.71	1.08
CoPt	-7.02	-6.10	-2.89	-0.28	1.18	1.17	2.63	1.17
NiPt	-5.47	-6.10	-2.86	-0.26	1.18	1.17	2.61	1.17
CuPt	-3.73	-6.10	-2.42	0.34	1.18	1.55	2.39	1.55
RuPt	-9.23	-6.10	-2.69	0.46	1.18	1.81	2.53	1.81
RhPt	-7.26	-6.10	-2.70	0.60	1.18	1.95	2.53	1.95
PdPt	-5.22	-6.10	-1.23	0.95	1.18	1.57	1.80	1.57
PtPt	-6.10	-6.10	-2.65	1.18	1.18	2.50	2.50	2.50

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Table S3. Computed formation energies (E_{form}) and dissolution potential (U_{diss}) of $MM'N_6$-DACs at d = 0.8 nm. $E_{M'}$ and E_M are the atomic energies of metals M′ and M in their bulk phase, respectively. The number of electrons transferred during the dissolution (n) is 2 for eight metals in this work. [1,2] $U^{o}_{diss\_M'}$ and $U^{o}_{diss\_M}$ are the standard dissolution potential of the metals M′ and M, respectively. [3] U_{diss} is taken as the minimum of $U_{diss\_M'}$ and U_{diss_M}. The energy of the nitrogen-doped carbon substrate $E_{N\text{-}C}$ is -684.81 eV. The unit of all energies is eV, and the unit of all potential is V.

DACs	E_M	$E_{M'}$	E_{form}	$U^{o}_{diss\_M}$	$U^{o}_{diss\_M'}$	U_{diss_M}	$U_{diss\_M'}$	U_{diss}
FeFe	-8.24	-8.24	-2.59	-0.45	-0.45	0.85	0.85	0.85
CoFe	-7.02	-8.24	-3.01	-0.28	-0.45	1.23	1.06	1.06
NiFe	-5.47	-8.24	-3.03	-0.26	-0.45	1.25	1.06	1.06
CuFe	-3.73	-8.24	-2.56	0.34	-0.45	1.62	0.83	0.83
RuFe	-9.23	-8.24	-3.01	0.46	-0.45	1.97	1.06	1.06
RhFe	-7.26	-8.24	-3.02	0.60	-0.45	2.11	1.06	1.06
PdFe	-5.22	-8.24	-2.72	0.95	-0.45	2.31	0.91	0.91
PtFe	-6.10	-8.24	-2.46	1.18	-0.45	2.41	0.78	0.78
FeCo	-8.24	-7.02	-3.01	-0.45	-0.28	1.06	1.23	1.06
CoCo	-7.02	-7.02	-2.93	-0.28	-0.28	1.19	1.19	1.19
NiCo	-5.47	-7.02	-2.85	-0.26	-0.28	1.16	1.14	1.14
CuCo	-3.73	-7.02	-2.33	0.34	-0.28	1.50	0.88	0.88
RuCo	-9.23	-7.02	-2.82	0.46	-0.28	1.87	1.13	1.13
RhCo	-7.26	-7.02	-2.86	0.60	-0.28	2.03	1.15	1.15
PdCo	-5.22	-7.02	-2.66	0.95	-0.28	2.28	1.05	1.05
PtCo	-6.10	-7.02	-2.70	1.18	-0.28	2.53	1.07	1.07
FeNi	-8.24	-5.47	-3.03	-0.45	-0.26	1.06	1.25	1.06
CoNi	-7.02	-5.47	-2.85	-0.28	-0.26	1.14	1.16	1.14
NiNi	-5.47	-5.47	-2.87	-0.26	-0.26	1.17	1.17	1.17
CuNi	-3.73	-5.47	-2.47	0.34	-0.26	1.57	0.97	0.97
RuNi	-9.23	-5.47	-2.61	0.46	-0.26	1.76	1.04	1.04
RhNi	-7.26	-5.47	-2.68	0.60	-0.26	1.94	1.08	1.08
PdNi	-5.22	-5.47	-2.66	0.95	-0.26	2.28	1.07	1.07
PtNi	-6.10	-5.47	-2.75	1.18	-0.26	2.55	1.11	1.11
FeCu	-8.24	-3.73	-2.56	-0.45	0.34	0.83	1.62	0.83
CoCu	-7.02	-3.73	-2.33	-0.28	0.34	0.88	1.50	0.88
NiCu	-5.47	-3.73	-2.47	-0.26	0.34	0.97	1.57	0.97
CuCu	-3.73	-3.73	-2.19	0.34	0.34	1.44	1.44	1.44
RuCu	-9.23	-3.73	-2.28	0.46	0.34	1.60	1.48	1.48
RhCu	-7.26	-3.73	-2.30	0.60	0.34	1.75	1.49	1.49
PdCu	-5.22	-3.73	-2.30	0.95	0.34	2.10	1.49	1.49

DACs	E_M	$E_{M'}$	E_{form}	$U^{o}_{diss\_M}$	$U^{o}_{diss\_M'}$	U_{diss_M}	$U_{diss\_M'}$	U_{diss}
PtCu	-6.10	-3.73	-2.39	1.18	0.34	2.37	1.53	1.53
FeRu	-8.24	-9.23	-3.01	-0.45	0.46	1.06	1.97	1.06
CoRu	-7.02	-9.23	-2.82	-0.28	0.46	1.13	1.87	1.13
NiRu	-5.47	-9.23	-2.61	-0.26	0.46	1.04	1.76	1.04
CuRu	-3.73	-9.23	-2.28	0.34	0.46	1.48	1.60	1.48
RuRu	-9.23	-9.23	-2.73	0.46	0.46	1.82	1.82	1.82
RhRu	-7.26	-9.23	-2.81	0.60	0.46	2.00	1.86	1.86
PdRu	-5.22	-9.23	-2.45	0.95	0.46	2.18	1.69	1.69
PtRu	-6.10	-9.23	-2.50	1.18	0.46	2.43	1.71	1.71
FeRh	-8.24	-7.26	-3.02	-0.45	0.60	1.06	2.11	1.06
CoRh	-7.02	-7.26	-2.86	-0.28	0.60	1.15	2.03	1.15
NiRh	-5.47	-7.26	-2.68	-0.26	0.60	1.08	1.94	1.08
CuRh	-3.73	-7.26	-2.30	0.34	0.60	1.49	1.75	1.49
RuRh	-9.23	-7.26	-2.81	0.46	0.60	1.86	2.00	1.86
RhRh	-7.26	-7.26	-2.86	0.60	0.60	2.03	2.03	2.03
PdRh	-5.22	-7.26	-2.50	0.95	0.60	2.20	1.85	1.85
PtRh	-6.10	-7.26	-2.59	1.18	0.60	2.48	1.90	1.90
FePd	-8.24	-5.22	-2.72	-0.45	0.95	0.91	2.31	0.91
CoPd	-7.02	-5.22	-2.66	-0.28	0.95	1.05	2.28	1.05
NiPd	-5.47	-5.22	-2.66	-0.26	0.95	1.07	2.28	1.07
CuPd	-3.73	-5.22	-2.30	0.34	0.95	1.49	2.10	1.49
RuPd	-9.23	-5.22	-2.45	0.46	0.95	1.69	2.18	1.69
RhPd	-7.26	-5.22	-2.50	0.60	0.95	1.85	2.20	1.85
PdPd	-5.22	-5.22	-2.50	0.95	0.95	2.20	2.20	2.20
PtPd	-6.10	-5.22	-2.56	1.18	0.95	2.46	2.23	2.23
FePt	-8.24	-6.10	-2.46	-0.45	1.18	0.78	2.41	0.78
CoPt	-7.02	-6.10	-2.70	-0.28	1.18	1.07	2.53	1.07
NiPt	-5.47	-6.10	-2.75	-0.26	1.18	1.11	2.55	1.11
CuPt	-3.73	-6.10	-2.39	0.34	1.18	1.53	2.37	1.53
RuPt	-9.23	-6.10	-2.50	0.46	1.18	1.71	2.43	1.71
RhPt	-7.26	-6.10	-2.59	0.60	1.18	1.90	2.48	1.90
PdPt	-5.22	-6.10	-2.56	0.95	1.18	2.23	2.46	2.23
PtPt	-6.10	-6.10	-2.60	1.18	1.18	2.48	2.48	2.48

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Table S4. Adsorption free energies ΔG(eV) and overpotentials η (V) on $CoCuN_6$-DACs under three curvature conditions, $CoCoN_6$-DAC, $CuCuN_6$-DAC, CoN_4-SAC, and CuN_4-SAC at plane state.

□	□	□	□	□	□	□	Dissociative			Associative		
d **(nm)**	**samples**	$\Delta G_{*O/*OH}$	$\Delta G_{*OH/*OH}$	ΔG_{*OH}	ΔG_{*OOH}	ΔG_{*O}	η^{ORR}	η^{OER}	η^{bifunc}	η^{ORR}	η^{OER}	η^{bifunc}
∞	$CoCuN_6$	4.37	2.62	1.36	4.37	2.62	0.09	0.13	0.22	0.68	0.51	1.19
	CoN_4	4.12	2.93	0.85	3.79	2.38	0.43	0.84	1.27	0.38	0.30	0.68
	CuN_4	4.84	3.00	1.46	4.51	3.51	1.15	0.61	1.76	0.82	0.81	1.63
	$CoCoN_6$	4.41	3.28	1.48	4.41	3.28	0.61	0.30	0.91	0.72	0.57	1.29
	$CuCuN_6$	4.36	3.36	1.26	4.36	3.36	0.91	0.91	1.82	0.67	0.87	1.54
1.3	$CoCuN_6$	3.98	2.14	1.01	3.98	2.14	0.22	0.10	0.32	0.29	0.61	0.89
0.8	$CoCuN_6$	3.76	1.85	0.84	3.76	1.85	0.39	0.40	0.80	0.39	0.68	1.08

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