Suplementary information for "Transition metal atoms embedded in monolayer $C_{13}N_3$ as OER/ORR bifunctional electrocatalysts"

Xiaoxue Yu[1], Junkai Xu[1], Yunhao Wang[1], Jianjun Fang[1],* Xianfang Yue[2],† Breno R. L. Galvão[3],‡ and Jing Li[1§]
[1] *School of Physics and Physical Engineering, Qufu Normal University, Qufu, Shandong 273165, China*
[2] *Department of Physics and Information Engineering, Jining University, Qufu 273155, China and*
[3] *Centro Federal de Educação Tecnológica de Minas Gerais, CEFET-MG, Av. Amazonas 5253, 30421-169 Belo Horizonte, Minas Gerais, Brazil*

(Dated: December 25, 2024)

* Corresponding author: jian-junfang@163.com
† Corresponding author: xfyuejnu@jnxy.edu.cn
‡ Corresponding author: brenogalvao@gmail.com
§ Corresponding author: jli@qfnu.edu.cn

TABLE S1. The total energy of TM-$C_{13}N_3$($E_{TM-C_{13}N_3}$), total energy of $C_{13}N_3$ with metal vacancies($E_{C_{13}N_3}$), total energy of the isolated metal atoms ($E_{TM-single}$), and binding energy (E_{bind}). All values are in eV.

	$E_{TM-C_{13}N_3}$	$E_{C_{13}N_3}$	$E_{TM-single}$	E_{bind}
Cr	-295.05	-284.95	-5.45	-4.65
Mn	-294.71	-284.95	-5.15	-4.61
Fe	-292.93	-284.95	-3.30	-4.68
Co	-291.37	-284.95	-1.73	-4.705
Ni	-290.32	-284.95	-0.29	-5.08
Cu	-288.82	-284.95	-0.25	-3.63
Ru	-292.52	-284.95	-2.00	-5.57
Rh	-291.46	-284.95	-1.26	-5.25
Pd	-289.94	-284.95	-1.48	-3.51
Ag	-288.29	-284.95	-0.20	-3.14
Os	-293.06	-284.95	-2.90	-5.21
Ir	-291.91	-284.95	-1.50	-5.46
Pt	-289.79	-284.95	-0.50	-4.34
Au	-287.56	-284.95	0.19	-2.42

TABLE S2. The adsorption energies (in eV) of *OH, *O and *OOH ($\Delta G_{*_{OH}}$, ΔG_{*_O} and $\Delta G_{*_{OOH}}$).

	$\Delta G_{*_{OH}}$	ΔG_{*_O}	$\Delta G_{*_{OOH}}$
Cr	0.20	1.43	3.49
Mn	0.00	2.19	3.37
Fe	0.03	1.43	3.29
Co	0.07	2.37	3.35
Ni	0.44	2.51	3.84
Cu	0.89	3.17	4.19
Ru	0.44	0.99	3.43
Rh	0.50	1.67	3.47
Pd	1.30	3.55	4.76
Ag	2.36	4.52	5.11
Os	-0.14	0.03	2.95
Ir	0.35	1.31	3.48
Pt	0.83	2.27	3.77
Au	1.59	3.52	4.76

TABLE S3. The free energy changes of each elementary step (ΔG_1, ΔG_2, ΔG_3 and ΔG_4) and the overpotential of OER and ORR (η_{OER} and η_{ORR}).

	ΔG_1(eV)	ΔG_2(eV)	ΔG_3(eV)	ΔG_4(eV)	η_{OER}(V)	η_{ORR}(V)
Cr	0.20	1.23	2.06	1.43	0.83	1.03
Mn	0.00	2.19	1.18	1.55	0.96	1.23
Fe	0.03	1.40	1.86	1.63	0.63	1.20
Co	0.07	2.30	0.98	1.57	1.07	1.16
Ni	0.44	2.06	1.34	1.08	0.74	0.79
Cu	0.89	2.29	1.01	0.73	1.06	0.50
Ru	0.44	0.55	2.44	1.49	1.21	0.79
Rh	0.50	1.16	1.80	1.45	0.57	0.73
Pd	1.30	2.25	1.21	0.16	1.02	1.07
Ag	2.36	2.16	0.59	-0.19	1.13	1.42
Os	-0.14	0.17	2.92	1.97	1.69	1.37
Ir	0.35	0.96	2.17	1.44	0.94	0.88
Pt	0.83	1.44	1.50	1.15	0.27	0.39
Au	1.59	1.93	1.24	0.16	0.70	1.07

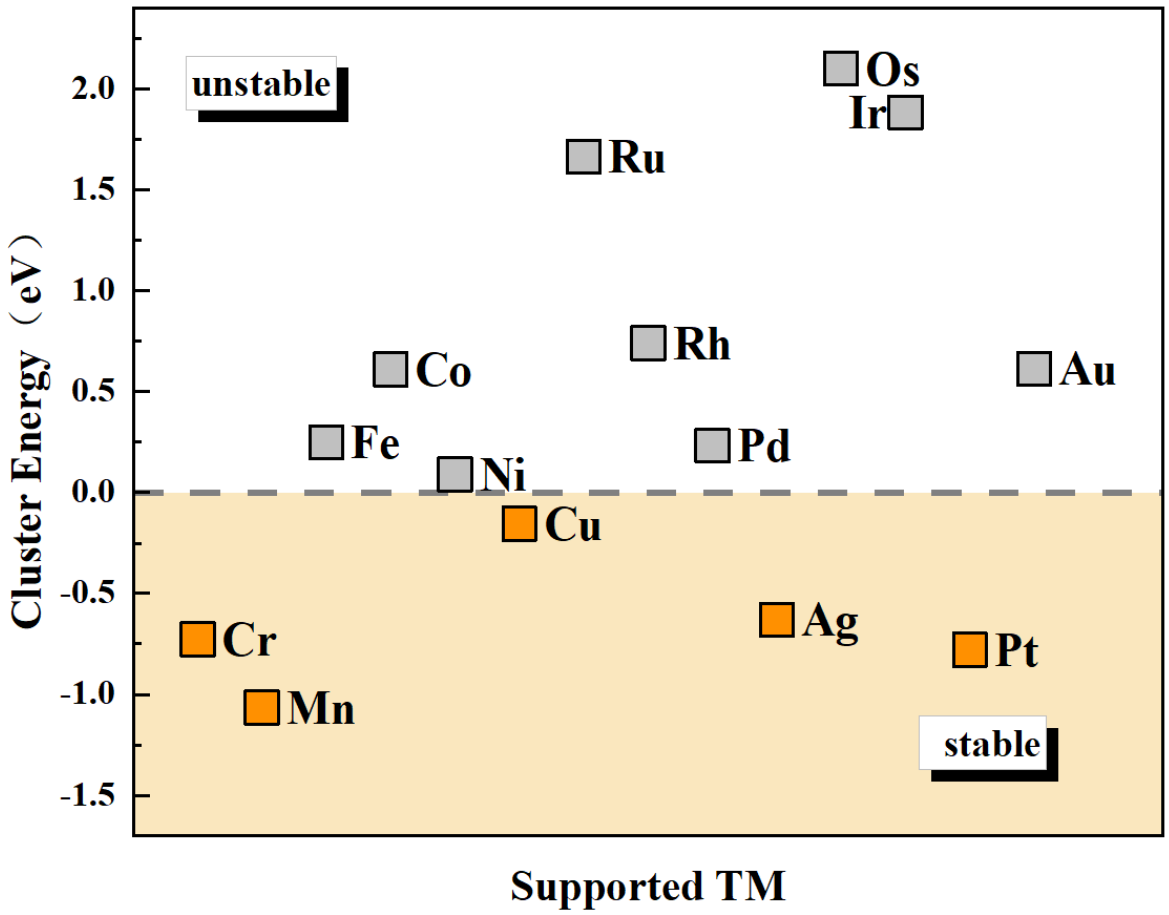

FIG. S1. $E_{cluster}$ energy calculated on TM-$C_{13}N_3$ system.

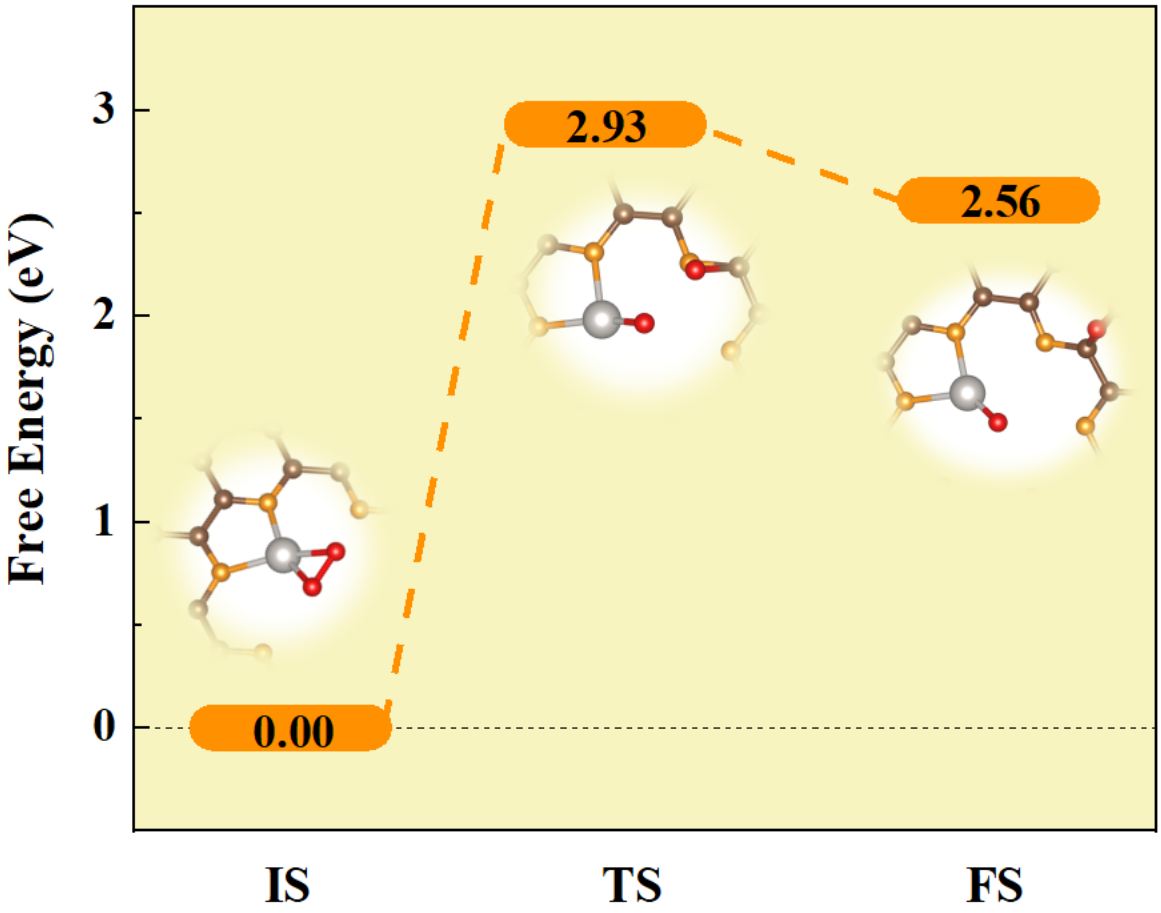

FIG. S2. Reaction pathways for O2 dissociation on C13N3 surfaces anchored by Pt atoms. IS, TS, FS represent the initial, transition, and final state along the reaction path.

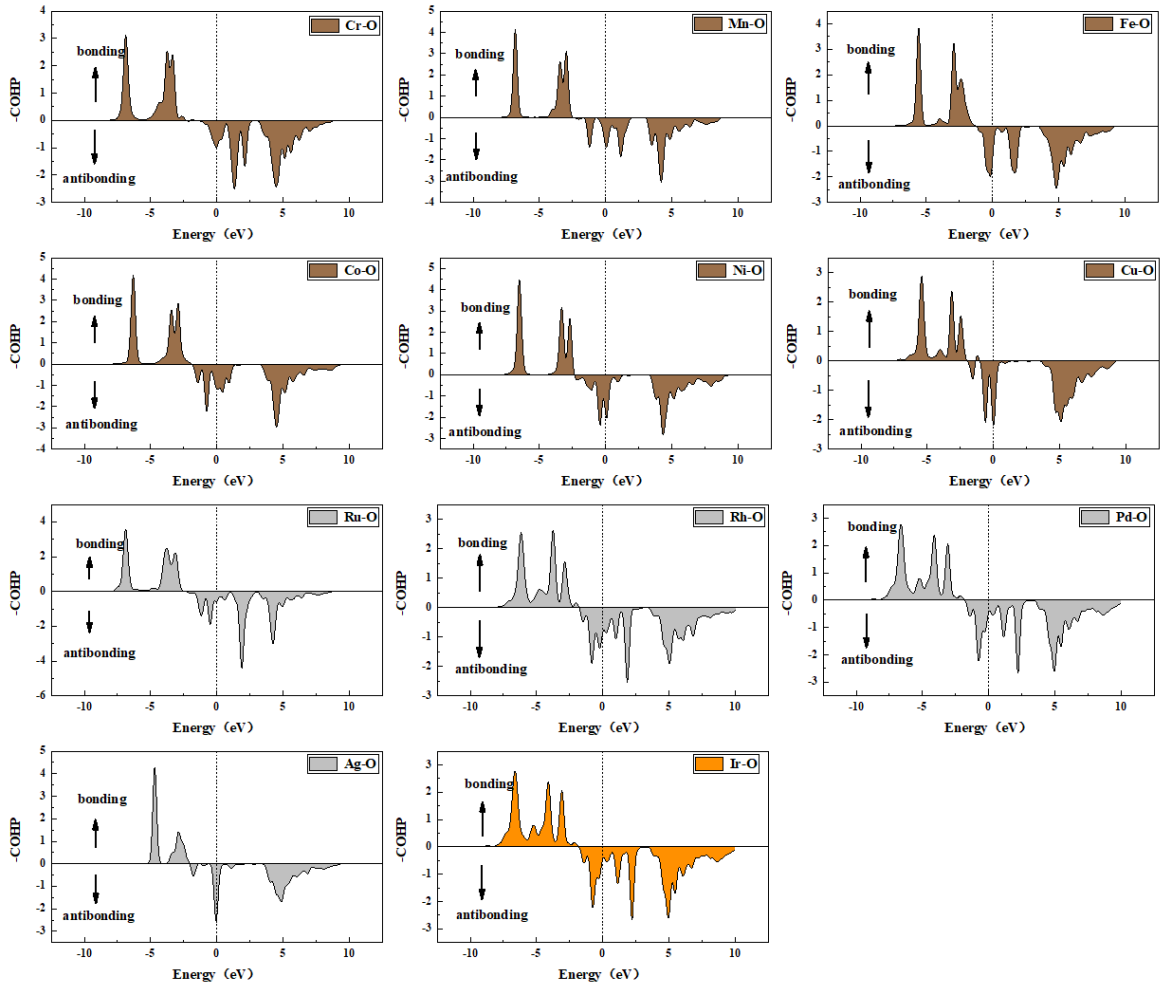

FIG. S3. -COHP of Cr,Mn,Fe,Co,Ni,Cu,Ru,Rh,Pd,Ag,Ir and Au-$C_{13}N_3$ with the reaction intermediate *OH ,where the Fermi level is set to zero.