Supplementary materials

Exploring high-efficiency electrocatalysts of metal-doped two-dimensional C_4N for oxygen reduction, oxygen evolution, and hydrogen evolution by first principles screening

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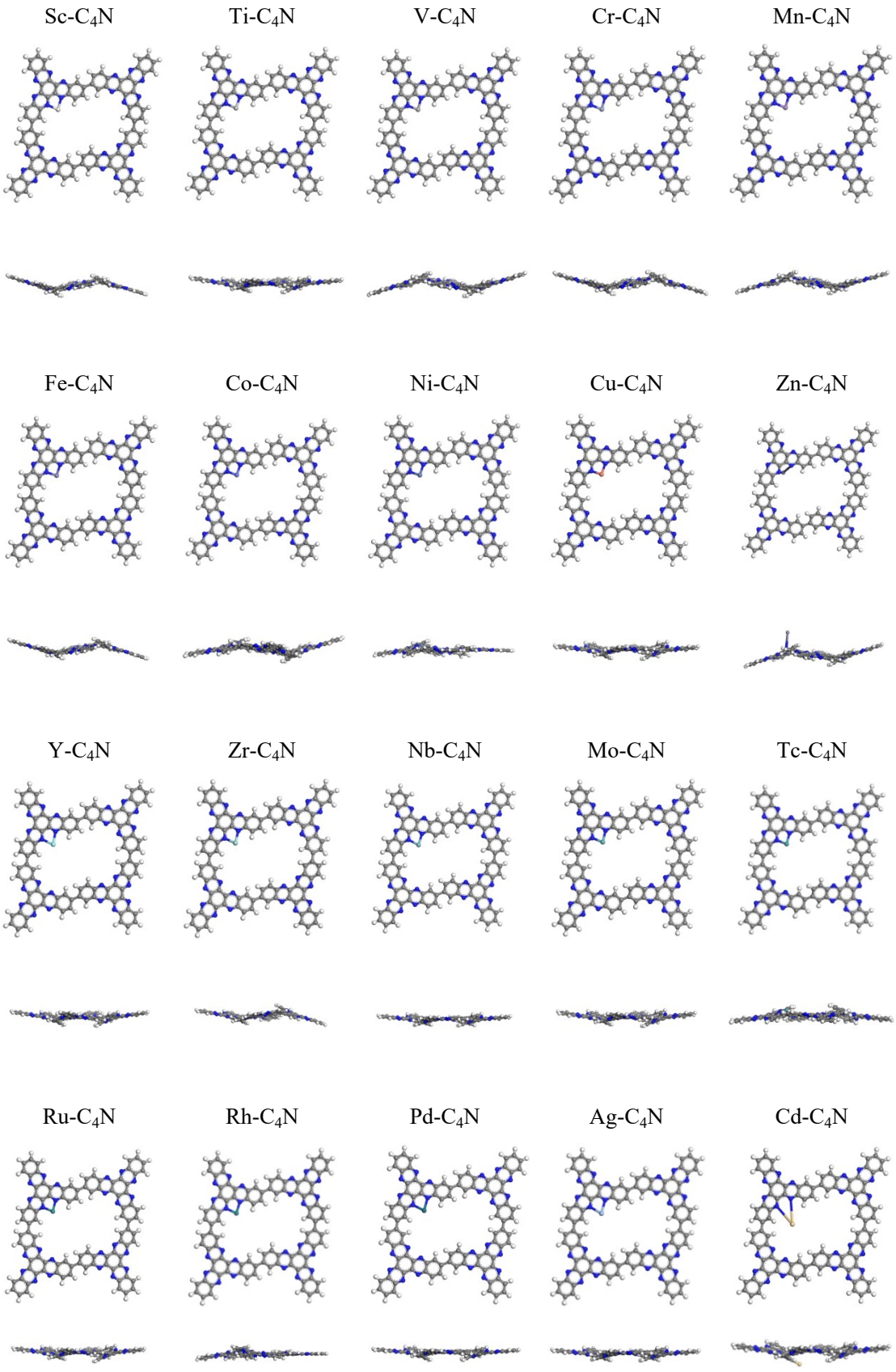

Sc-C4N
Ti-C4N
V-C4N
Cr-C4N
Mn-C4N
Fe-C4N
Co-C4N
Ni-C4N
Cu-C4N
Zn-C4N
Y-C4N
Zr-C4N
Nb-C4N
Mo-C4N
Tc-C4N
Ru-C4N
Rh-C4N
Pd-C4N
Ag-C4N
Cd-C4N

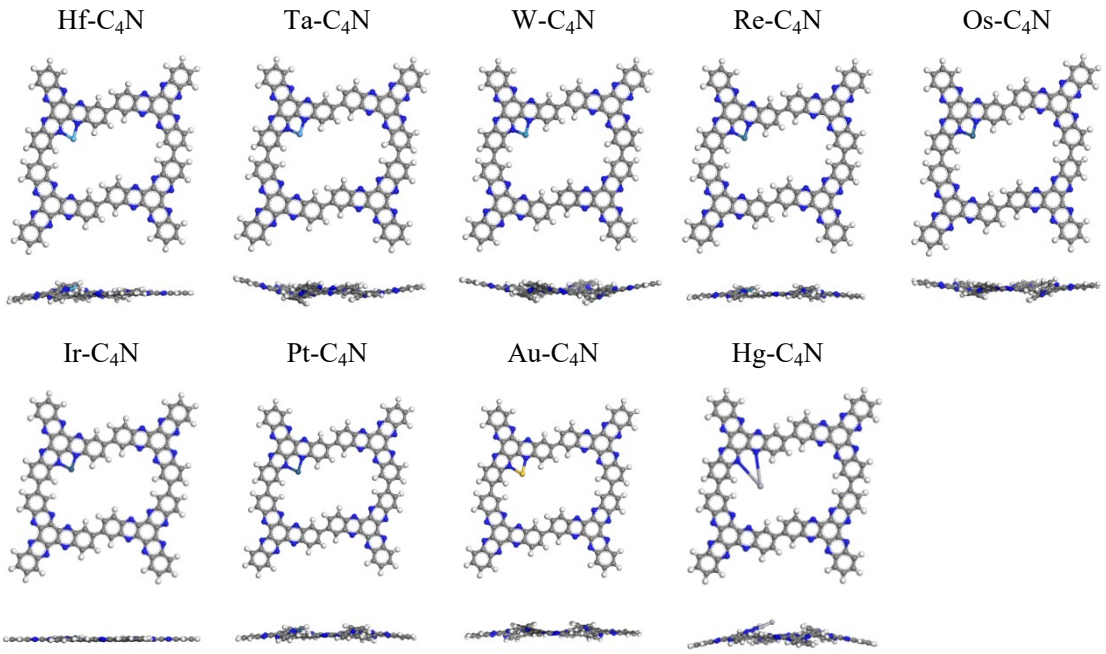


Fig. S1. Optimized geometries of all TM-C_4N.

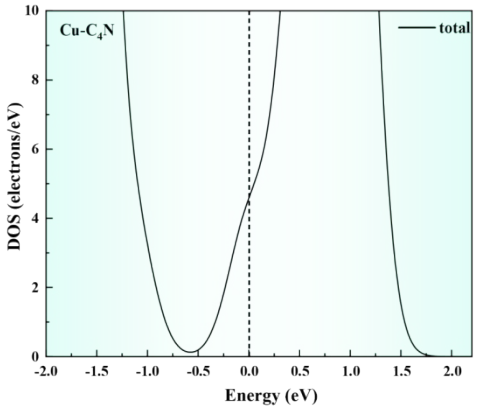


Fig. S2. Corresponding magnified pattern of DOS on Cu-C_4N near the Fermi level.

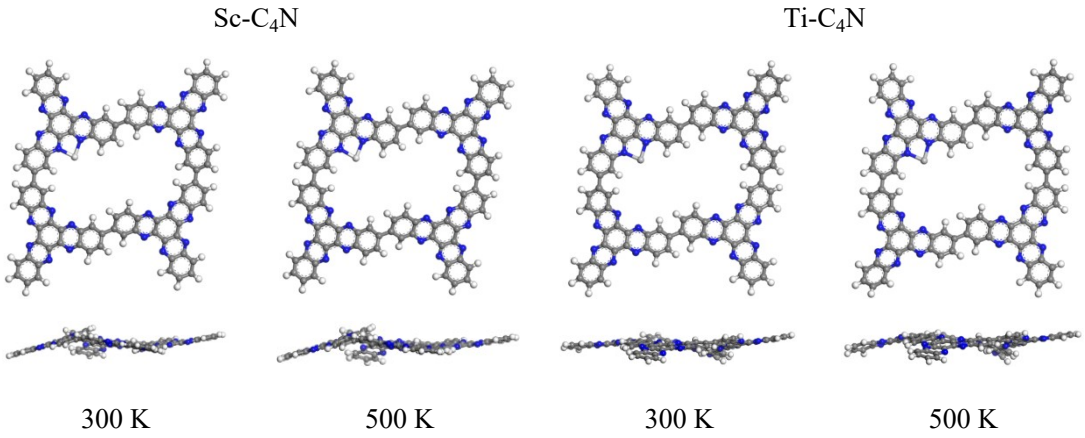


Fig. S3. Final structures of Sc-C_4N and Ti-C_4N after dynamics calculations.

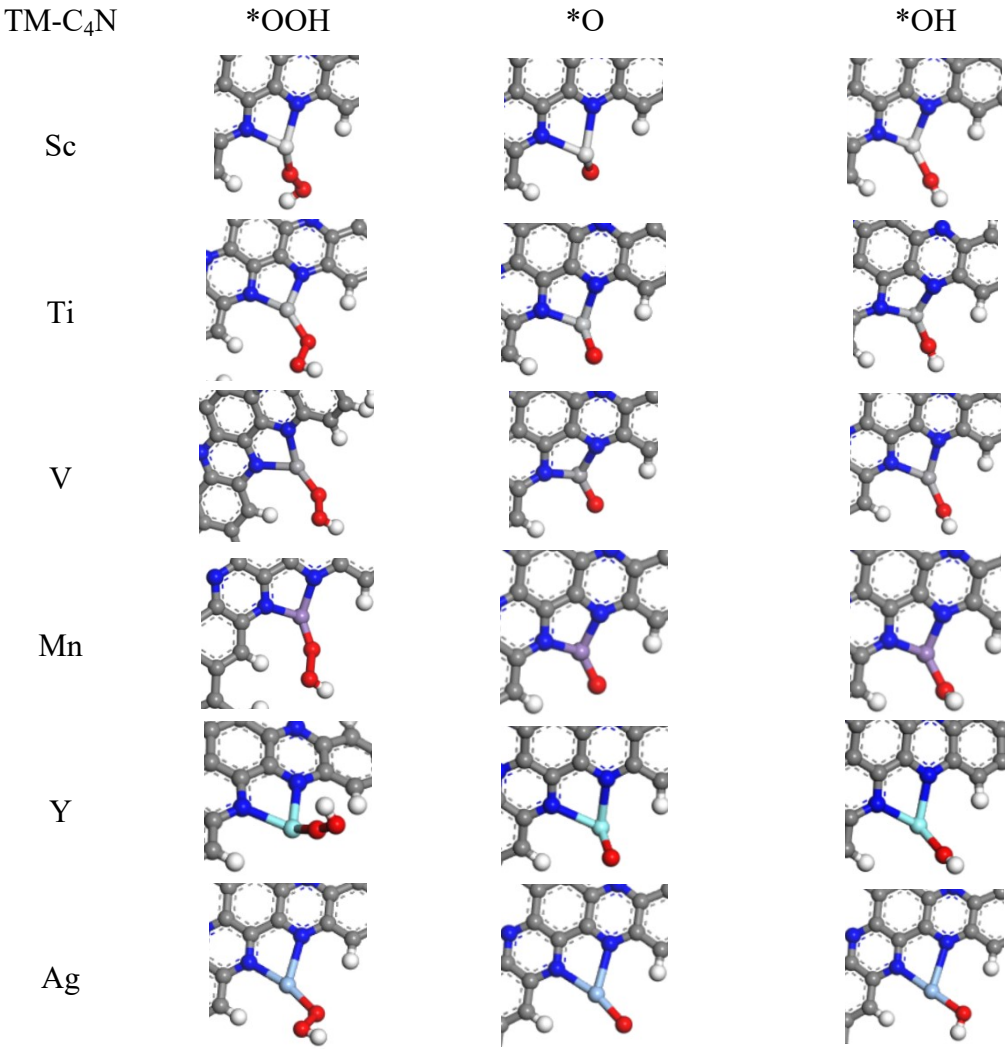


Fig. S4. Optimized structures of *OOH, *O, and *OH species on TM-C_4N.

TM-OH-C_4N *OOH *O *OH

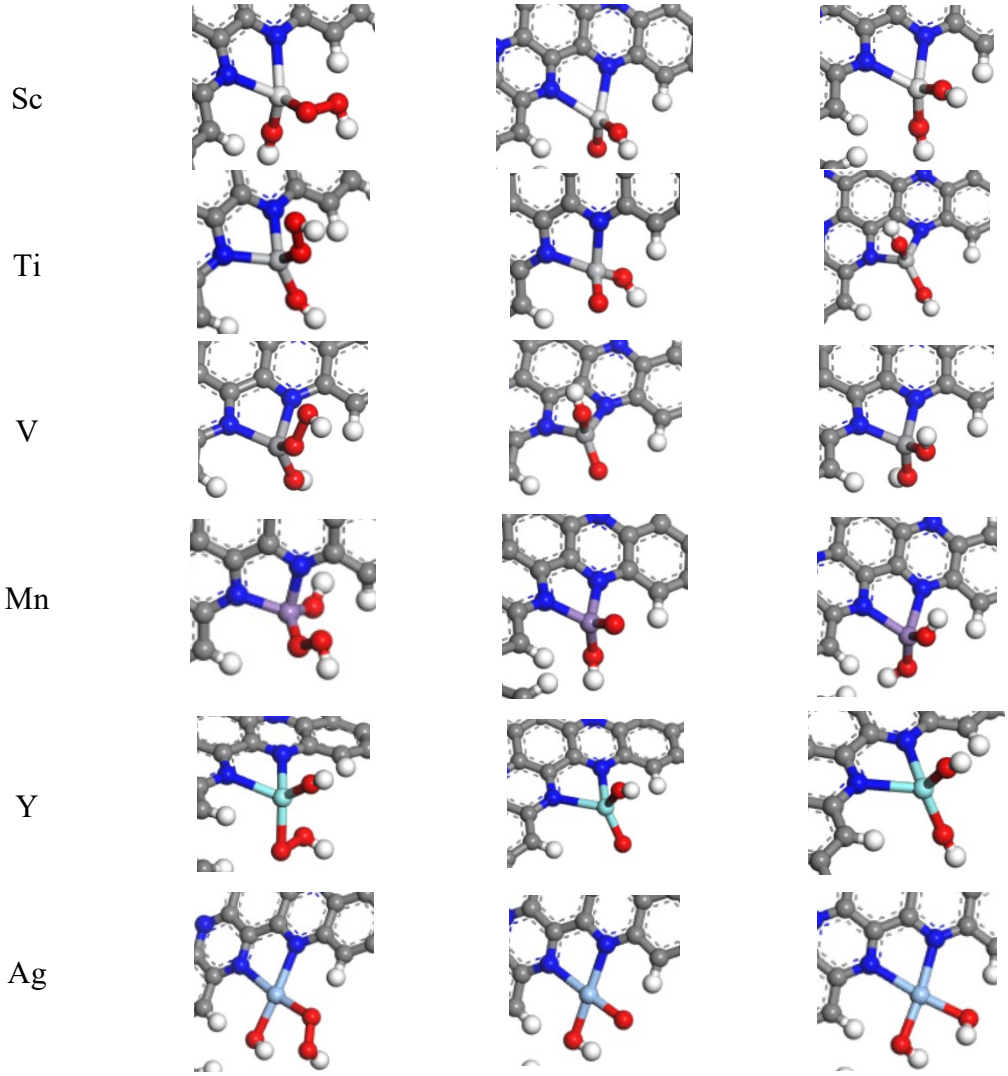
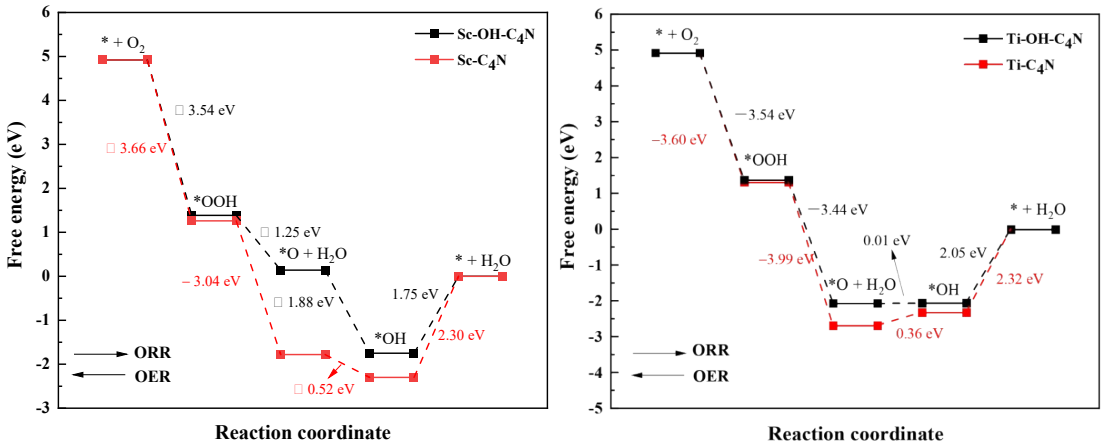


Fig. S5. Optimized structures of *OOH, *O, and *OH species on all TM-OH-C_4N.



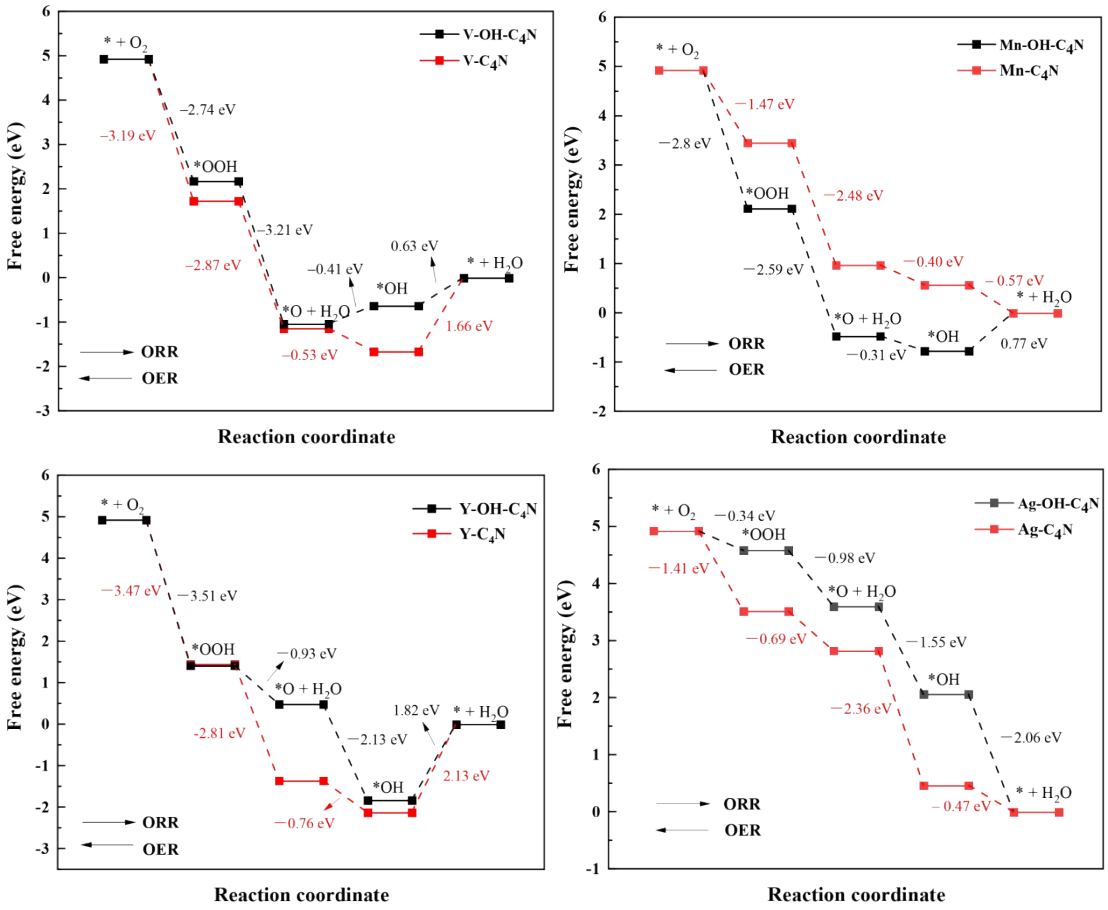


Fig. S6. Free energy profiles for OER/ORR on other TM-C_4N and TM-OH-C_4N.

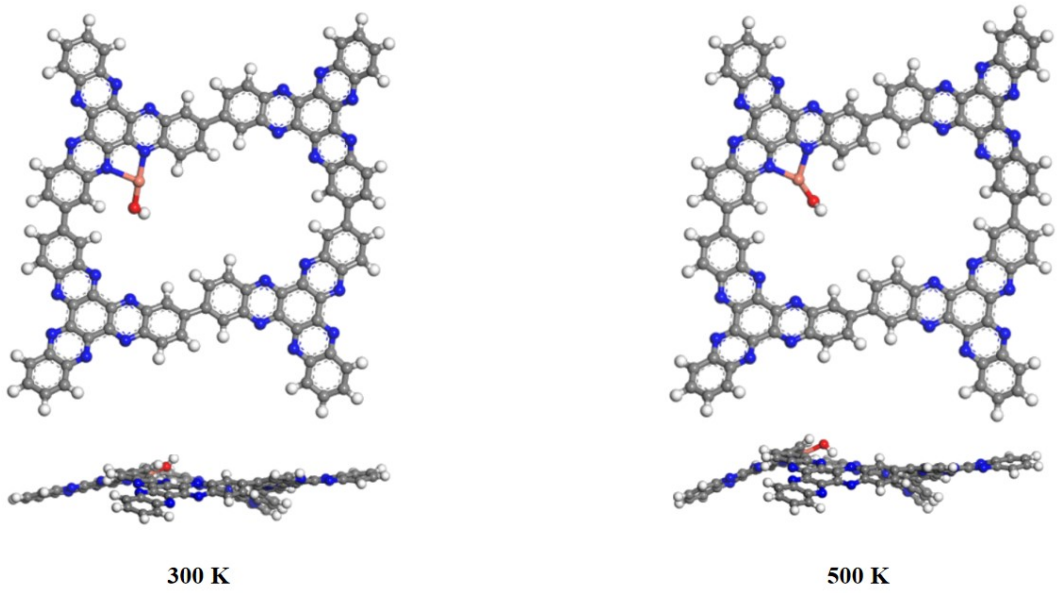


Fig. S7. Final structures of Cu-OH-C_4N after dynamics calculations.

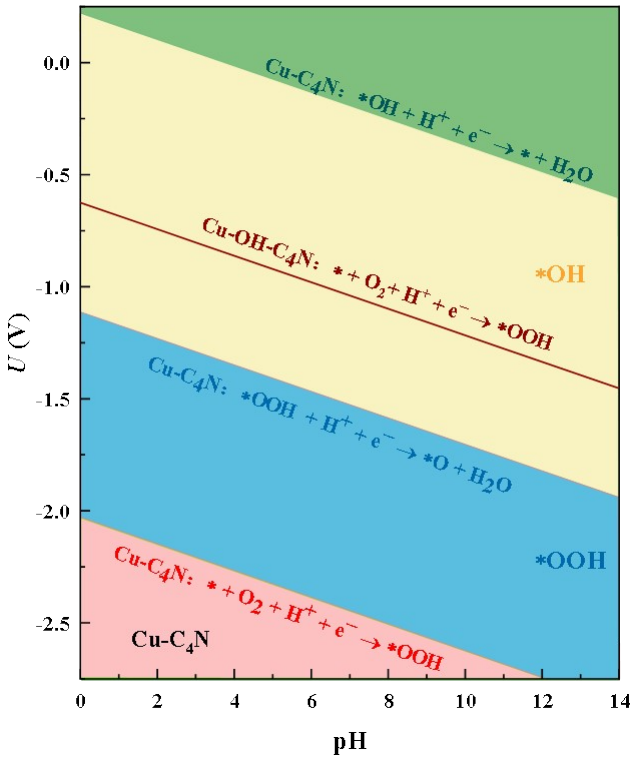


Fig. S8. Pourbaix plots of Cu-C_4N and Cu-OH-C_4N.

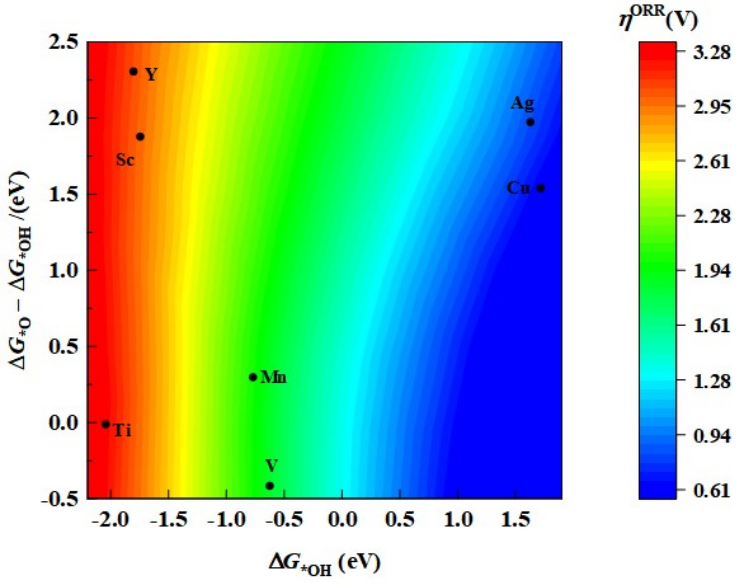


Fig. S9. Volcano diagram of ORR for TM-OH-C_4N.

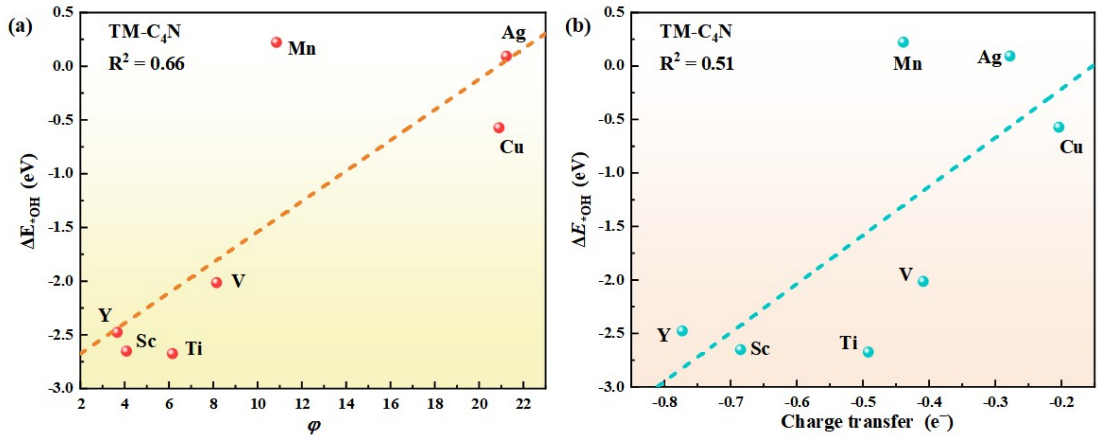


Fig. S10. Relationships between $\Delta E_{*\mathrm{OH}}$ and (a) descriptor φ as well as (b) charge transfer on TM-C_4N.

Table S1 Mulliken charge (e) of the metal atoms and the surrounding N atoms of TM-C_4N.

TM-C_4N	Sc-	Ti-	V-	Mn-	Cu-	Zn-	Y-	Ag-	Cd-	Hg-
TM atom	0.685	0.492	0.409	0.439	0.204	0.018	0.773	0.278	0.025	0.009
N atom	−0.60	−0.54	−0.4	−0.48	−0.39	−0.26	−0.63	−0.39	−0.26	−0.25

Table S2 E_f values (eV) of TM-C_4N and TM_2-C_4N.

Catalyst	Sc-	Ti-	Cu-
TM-C_4N	−1.44	−0.01	−0.54
TM_2-C_4N	−0.02	1.07	0.08

Table S3 Corresponding values of N_e and N_m of TM.

TM-C_4N	Sc-	Ti-	V-	Mn-	Cu-	Y-	Ag-
N_e	3	4	5	7	11	3	11
N_m	1.36	1.54	1.63	1.55	1.90	1.22	1.93