Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Oxo transition metal anchored on C_3N_4 with constructing high-activity bifunctional electrocatalyst for rechargeable metal–air batteries

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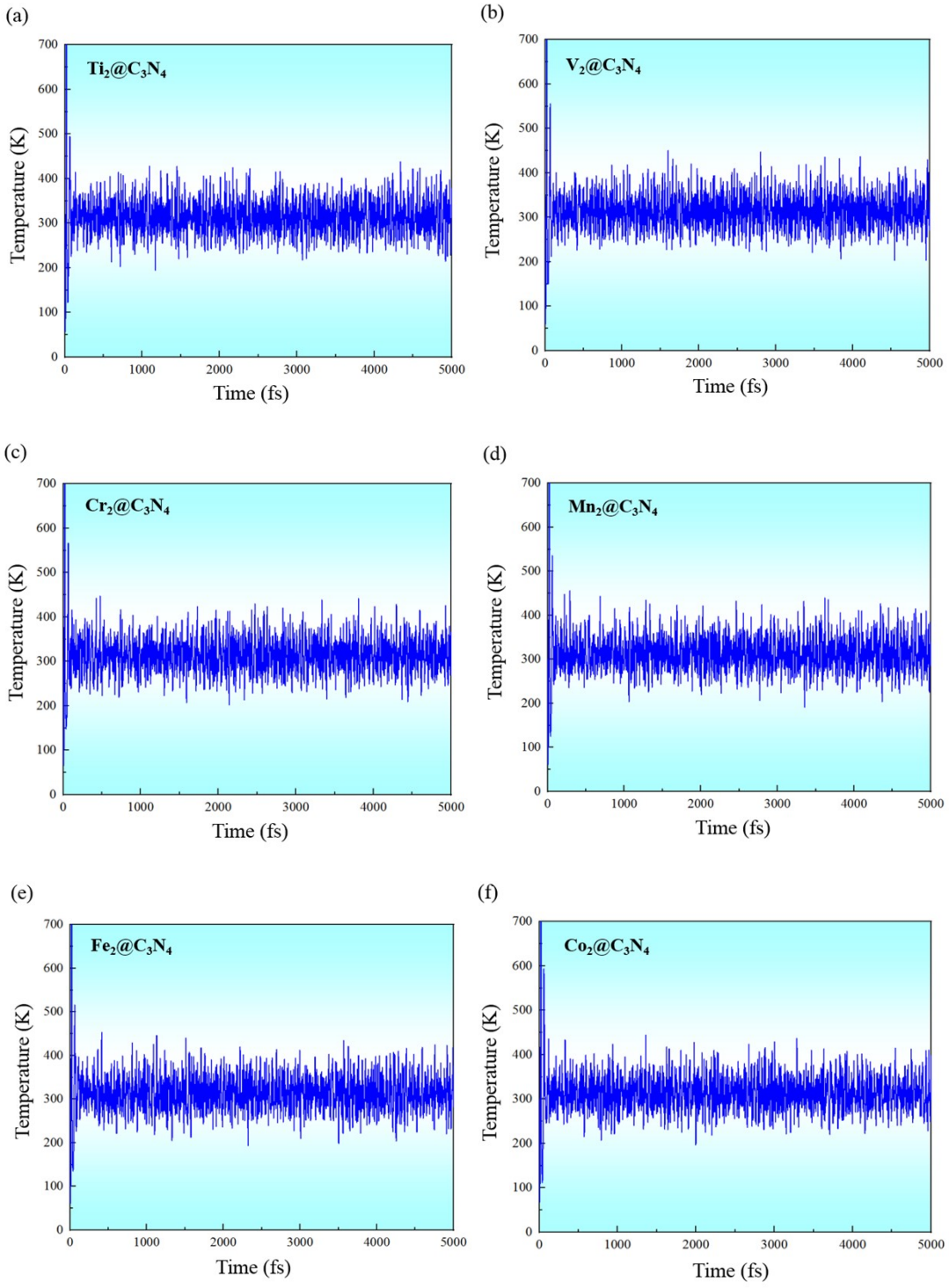
(a)
Ti2@C3N4
(b)
V2@C3N4
(c)
Cr2@C3N4
(d)
Mn2@C3N4
(e)
Fe2@C3N4
(f)
Co2@C3N4
Temperature (K)
Time (fs)
0
100
200
300
400
500
600
700
1000
2000
3000
4000
5000

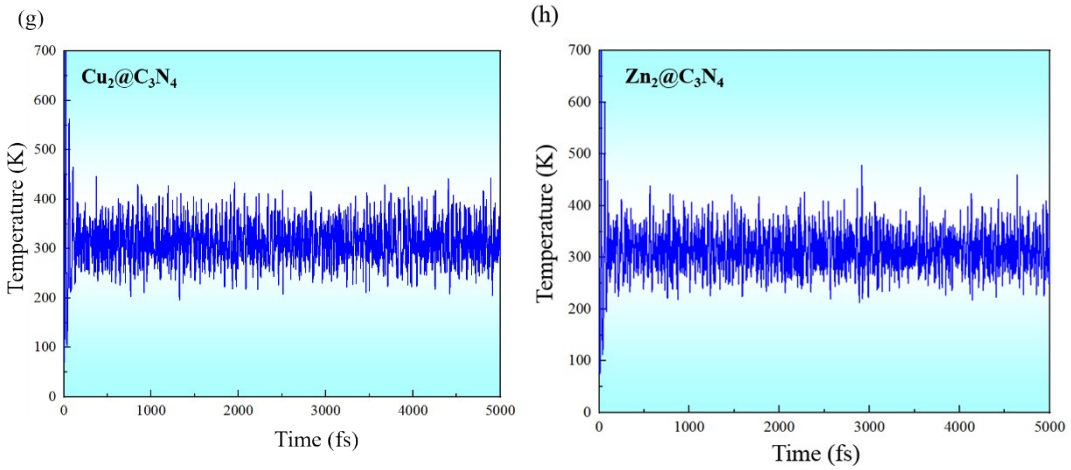

Fig. S1. FPMD of (a)$Ti_2@C_3N_4$, (b)$V_2@C_3N_4$, (c)$Cr_2@C_3N_4$, (d)$Mn_2@C_3N_4$, (e)$Fe_2@C_3N_4$, (f)$Co_2@C_3N_4$, (g)$Cu_2@C_3N_4$, and (h)$Zn_2@C_3N_4$.

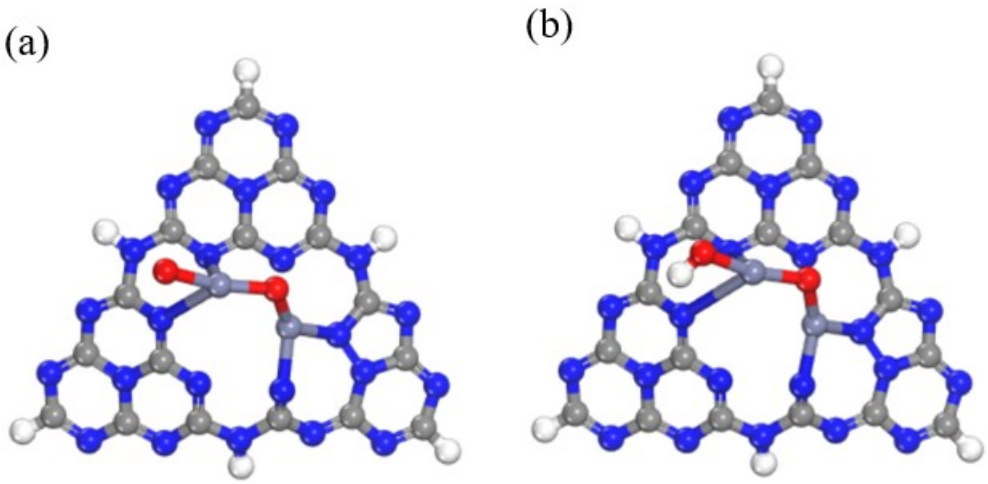

Fig. S2. Configurations of (a) *O and (b) *OH adsorbed at β site on $Zn_2@C_3N_4$.

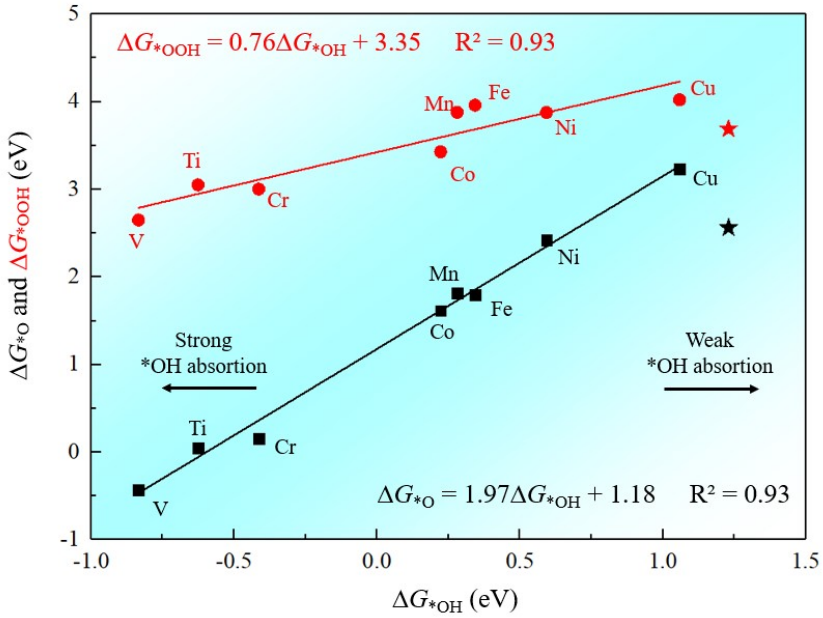

Fig. S3. Scaling relationships of ΔG_{*OH} with ΔG_{*OOH} and ΔG_{*O} at β site on $M_2@C_3N_4$.

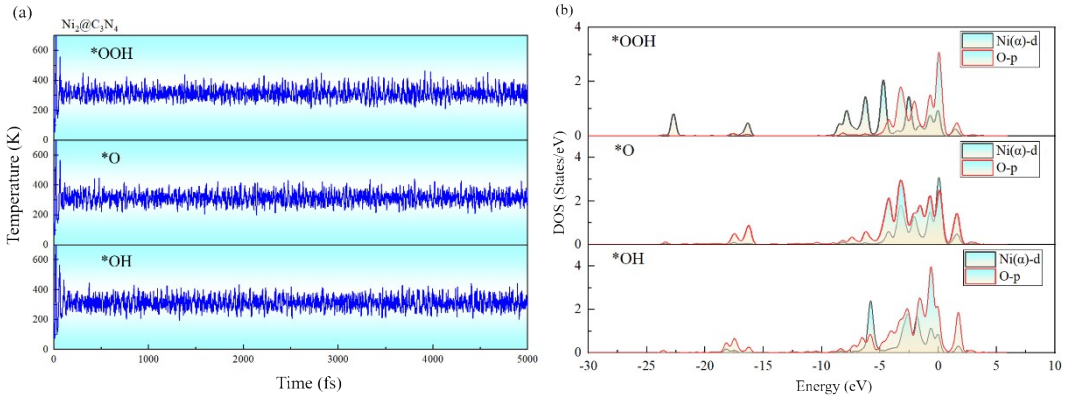

Fig. S4 (a) FPMD of *OOH, *O, and *OH at α site on $Ni_2@C_3N_4$. (b) DOS of *OOH, *O, and *OH at α site on $Ni_2@C_3N_4$. O-p orbitals represents the p orbital of O atom on *OOH, *O, or *OH directly connected to Ni(α) for $Ni_2@C_3N_4$.

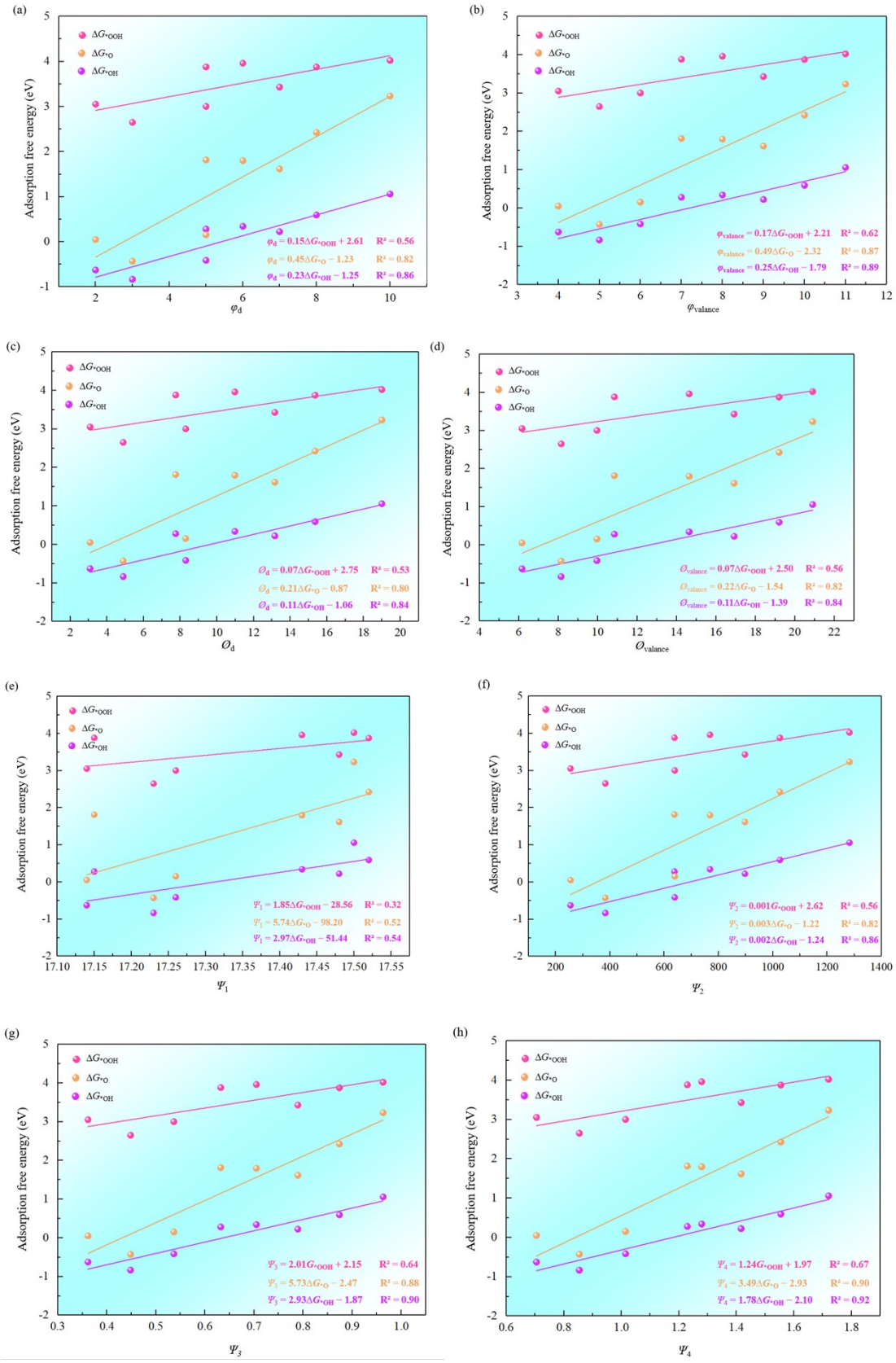

Fig. S5. Relationship of $\Delta G_{species}$ with (a) the φ_d, (b) $\varphi_{valence}$, (c) $\mathcal{O}_d$, (d) $\mathcal{O}_{valance}$, (e) Ψ_1, (f) Ψ_2, (g) Ψ_3, and (h) Ψ_4 at α site β site on $M_2@C_3N_4$.

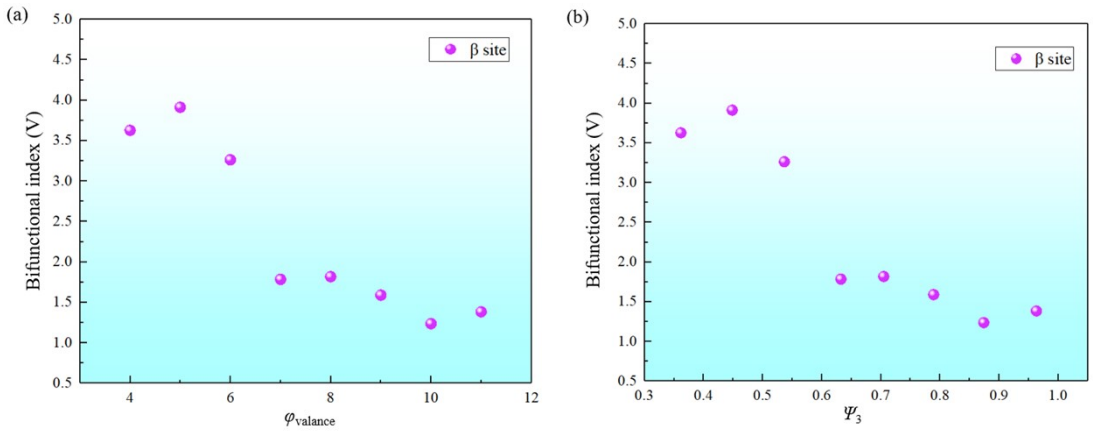

Fig. S6. (a) $\varphi_{valence}$ and (b) Ψ_3 versus bifunctional index at β site on $M_2@C_3N_4$.

Table S1 ICOHP of Cu(α)−O, Cu(β)−O, Cu(α)−N1, Cu(α)−N2, Cu(β)−N3, Cu(β)−N4 in $Cu_2@C_3N_4$.

Bonds	ICOHP (eV)
Cu(α)−O	−1.31
Cu(β)−O	−1.40
Cu(α)−N1	−1.59
Cu(α)−N2	−2.65
Cu(β)−N3	−0.67
Cu(β)−N4	−2.04

Table S2 Adsorption energy (E_{ads}, eV) of the O_2 molecule on $M_2@C_3N_4$.

		end-on	side-on
$Ti_2@C_3N_4$	α site	−2.03	−3.48
	β site	−2.45	−2.45
$V_2@C_3N_4$	α site	−2.45	−3.33
	β site	−2.84	−2.24
$Cr_2@C_3N_4$	α site	−1.75	−2.44
	β site	−1.40	−1.98
$Mn_2@C_3N_4$	α site	−1.56	−1.56
	β site	−1.08	−1.08
$Fe_2@C_3N_4$	α site	−0.35	−1.24
	β site	−0.53	−0.97
$Co_2@C_3N_4$	α site	−0.80	−1.32
	β site	−0.84	−0.84
$Ni_2@C_3N_4$	α site	−0.10	−0.58
	β site	−0.54	−0.68
$Cu_2@C_3N_4$	α site	−0.53	−0.53
	β site	−0.33	−0.37
$Zn_2@C_3N_4$	α site	——	−0.42
	β site	——	−0.35