

Electronic Supplementary Material

Heterometallic cluster-based organic frameworks as highly active electrocatalysts for oxygen reduction and oxygen evolution reaction: a density functional theory study

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Table S1 Substitution energy for the substitution of Ni atom by M atom in the Fe₂Ni

	Fe ₂ Ti	Fe ₂ V	Fe ₂ Cr	Fe ₂ Mn	Fe ₂ Co	Fe ₂ Cu	Fe ₂ Zn
E_{sub} (eV)	-3.78	-2.78	-1.89	-2.85	-1.07	-0.34	-1.73

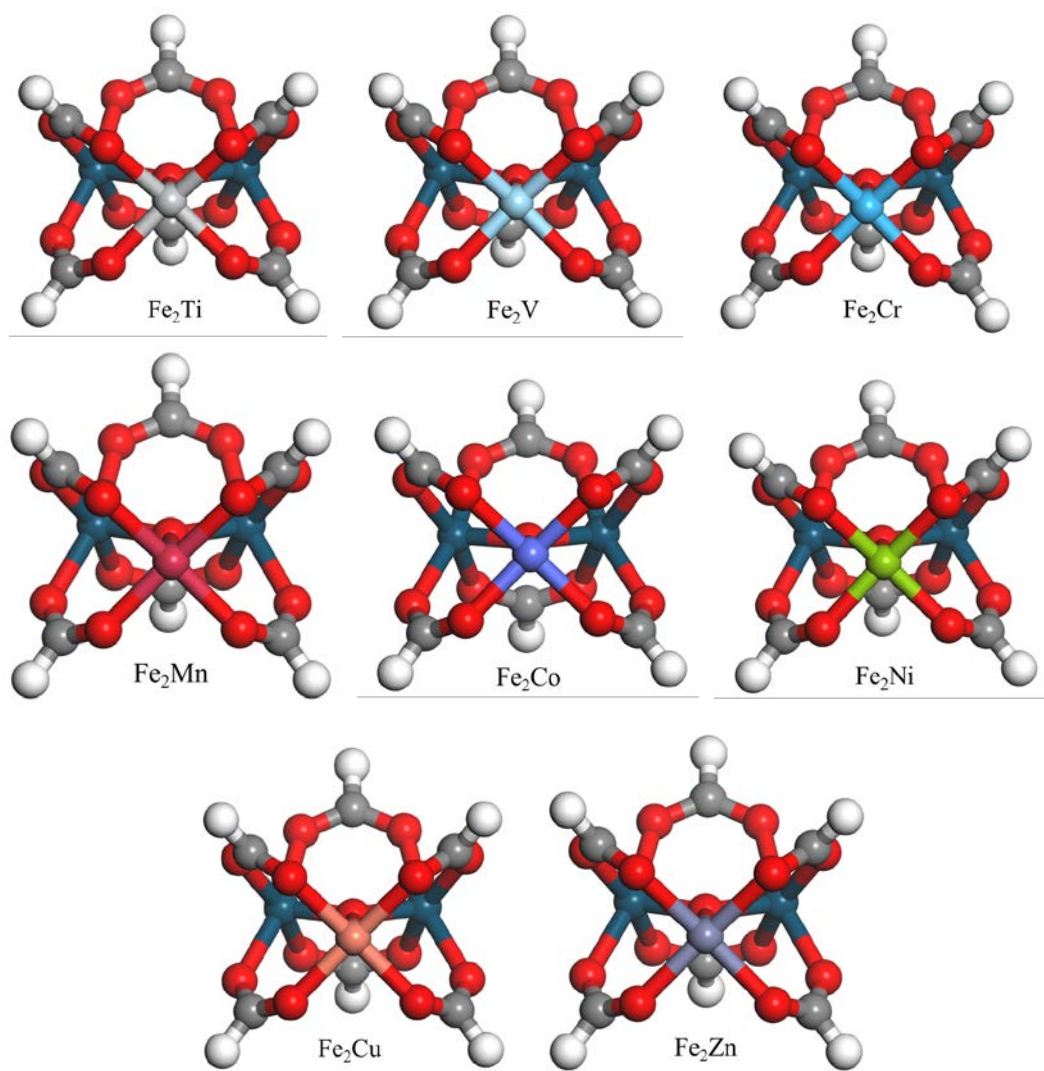
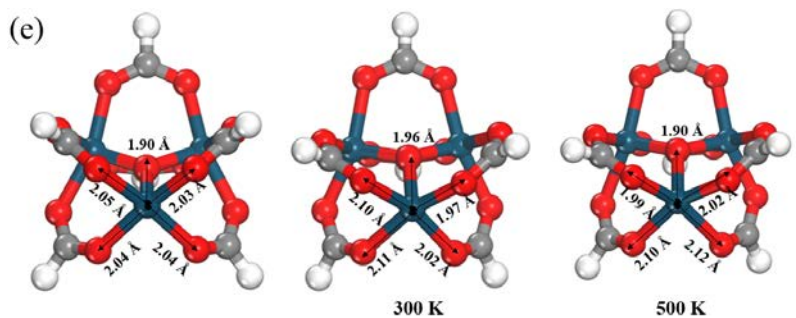
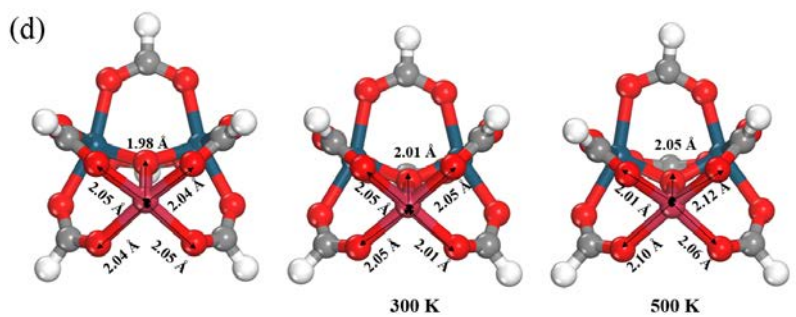
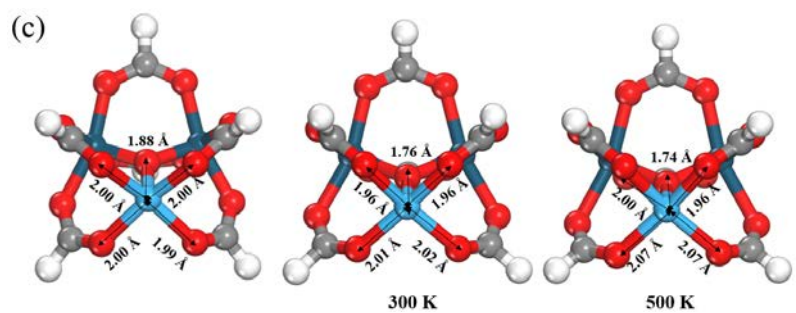
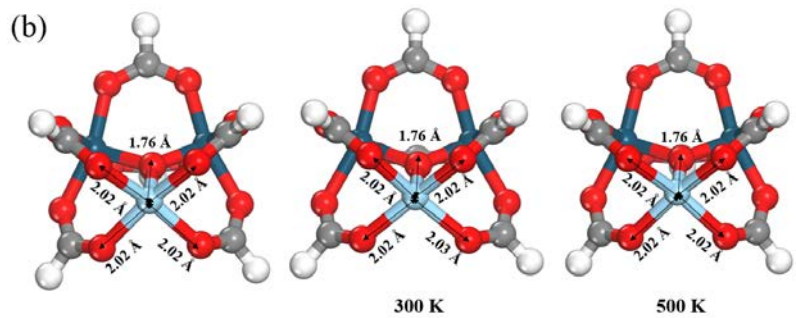
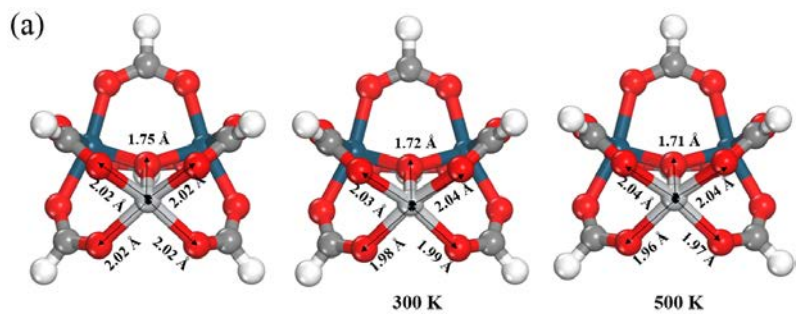


Fig. S1 Optimized configurations of Fe₂M clusters.



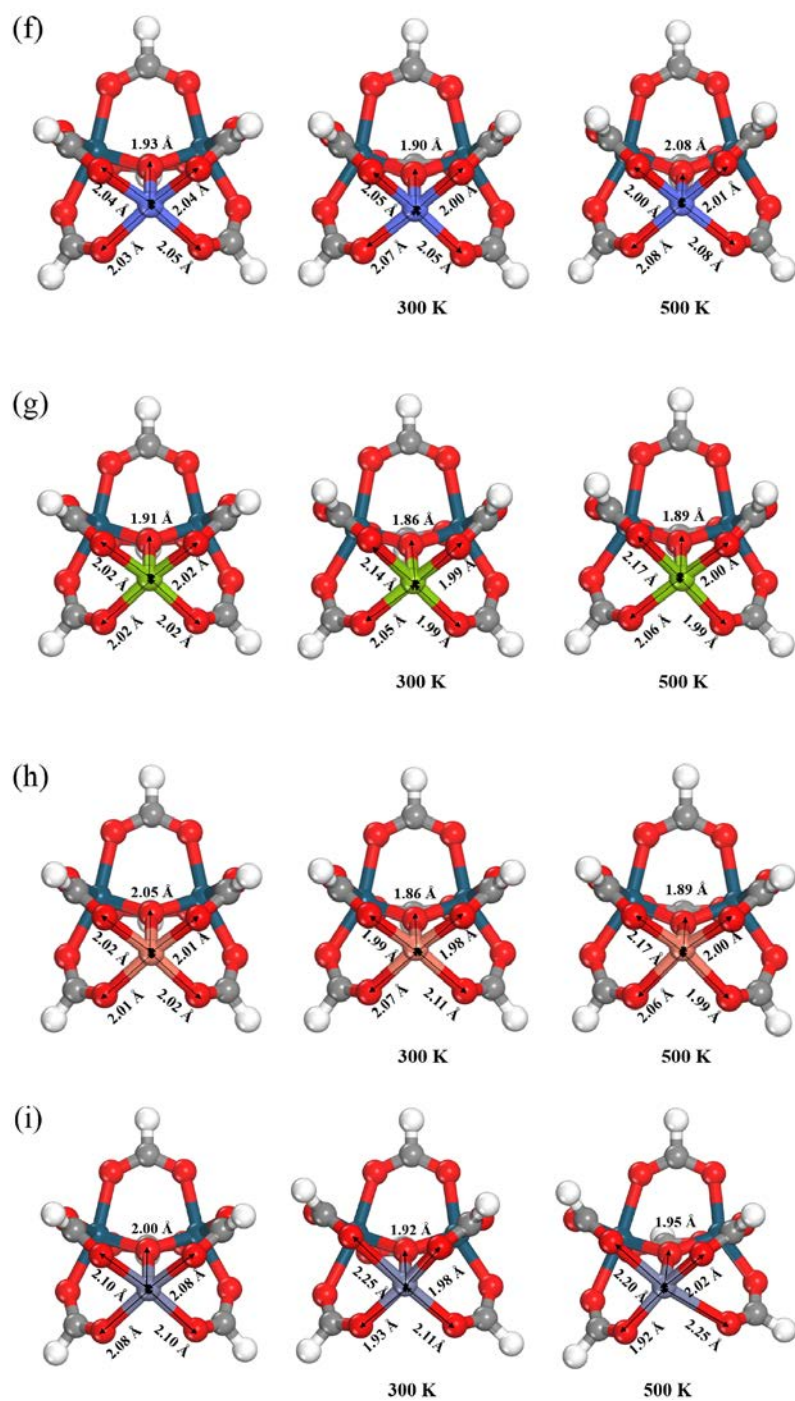


Fig. S2 Final structures and M–O bond lengths of (a) Fe₂Ti, (b) Fe₂V, (c) Fe₂Cr, (d) Fe₂Mn, (e) Fe₃, (f) Fe₂Co, (g) Fe₂Ni, (h) Fe₂Cu, and (i) Fe₂Zn after dynamics calculations at the temperatures of 300 K and 500 K.

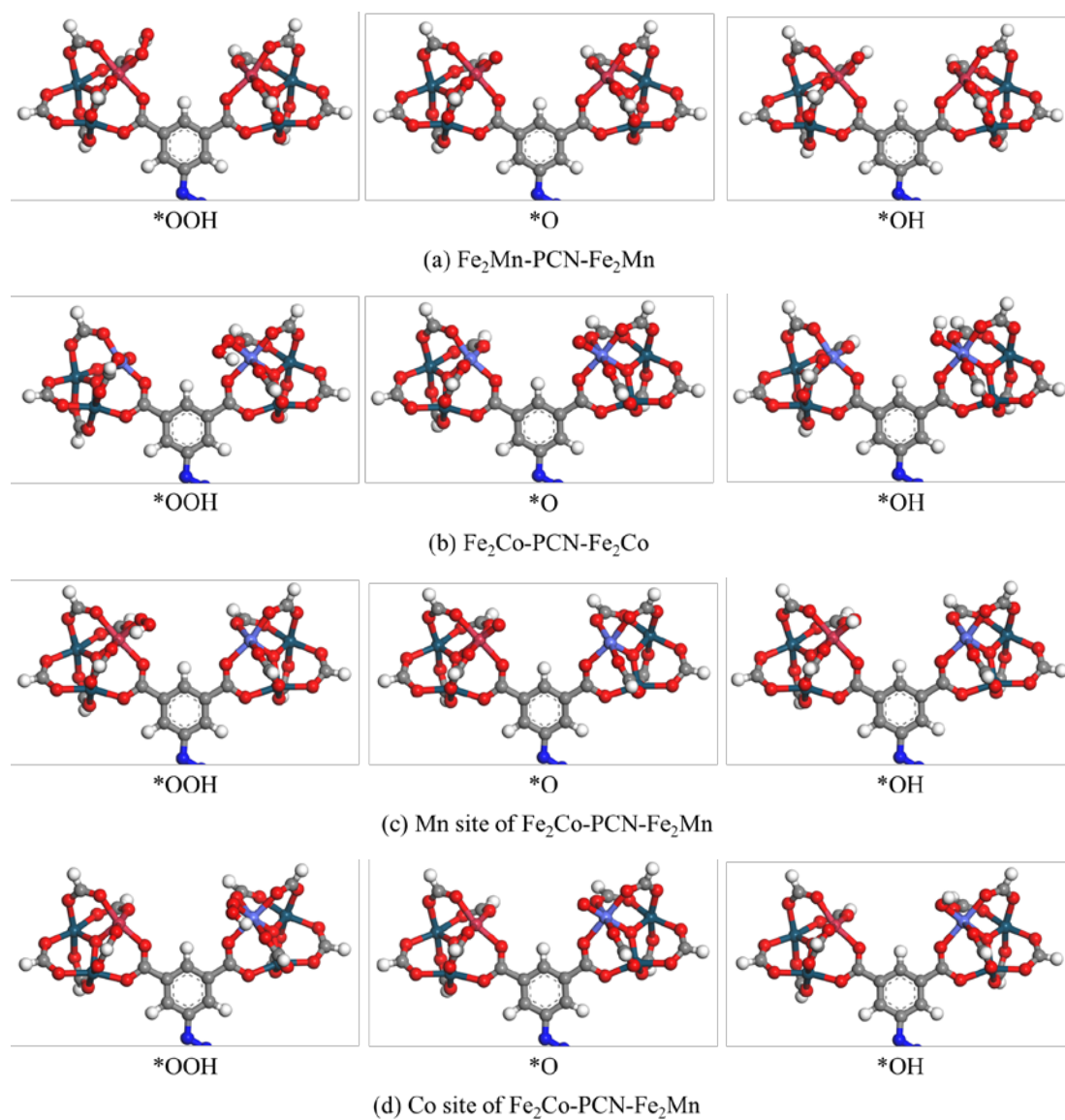


Fig. S3 Optimized configurations of reaction intermediates on (a) $\text{Fe}_2\text{Mn-PCN-Fe}_2\text{Mn}$, (b) $\text{Fe}_2\text{Co-PCN-Fe}_2\text{Co}$, (c) Mn site of $\text{Fe}_2\text{Co-PCN-Fe}_2\text{Mn}$, and (d) Co site of $\text{Fe}_2\text{Co-PCN-Fe}_2\text{Mn}$.