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DFT Study of Oxygen Reduction Reaction Catalyzed by Single Fe Atom Catalyst Decorated with Axial Ligand

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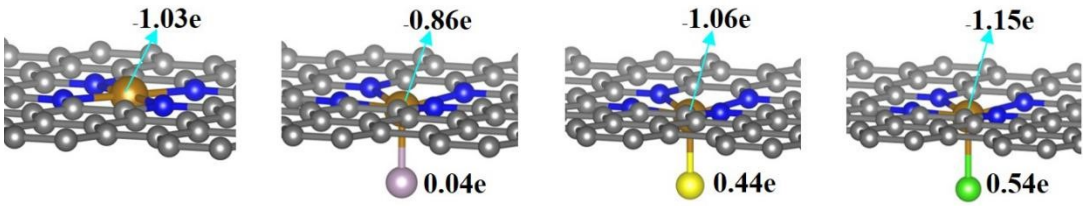

Figure S1 The Bader charge analysis of FeN_4, FeN_4P, FeN_4S, and FeN_4Cl, respectively.

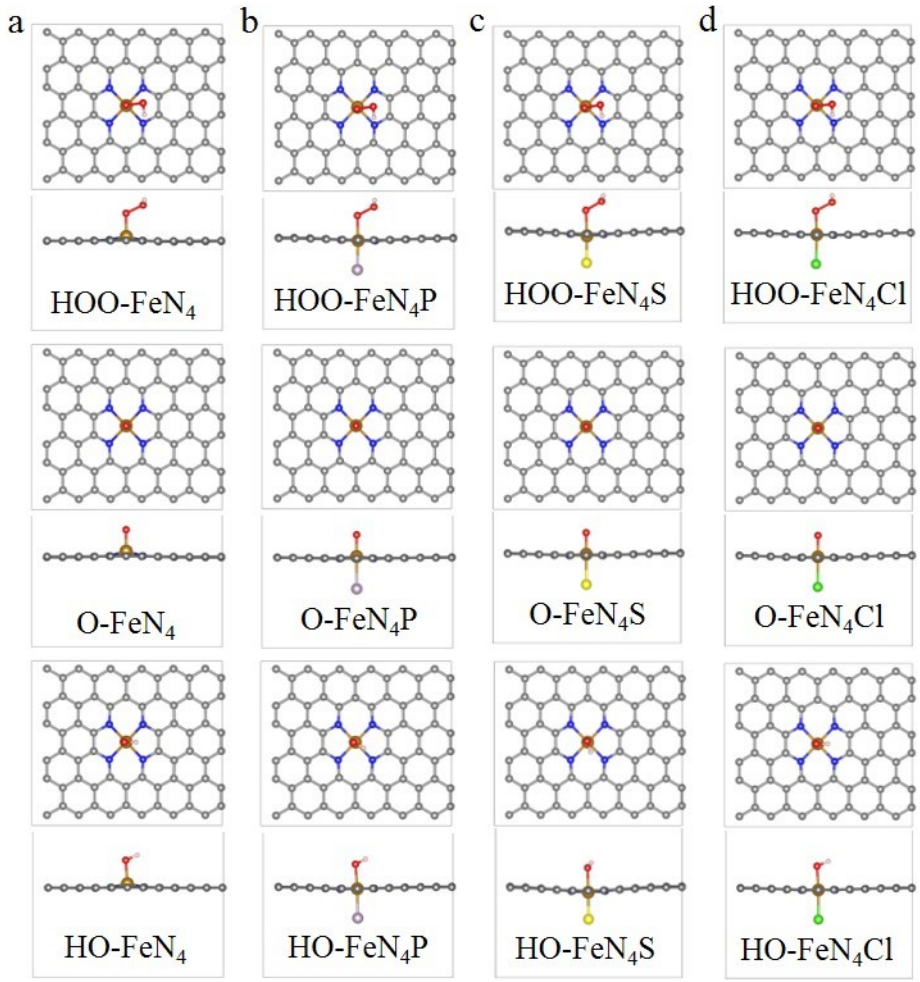

Figure S2 The geometric arrangements of OOH, O, and OH adsorbed on the surfaces of (a) FeN_4, (b) FeN_4P, (c) FeN_4S, and (d) FeN_4Cl during catalytic ORR.

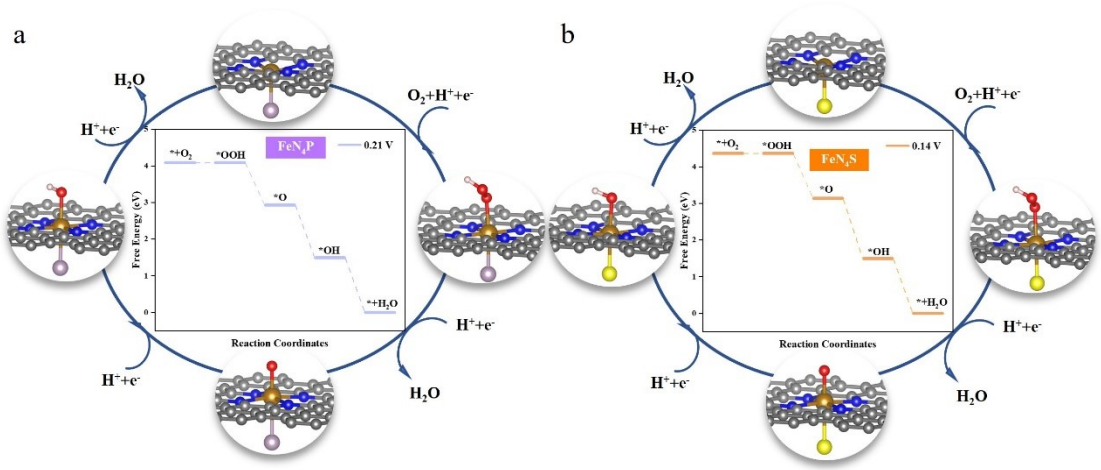

Figure S3 Schematic of the ORR. The inset in the cycle shows the free energy diagram for oxygen reduction reaction on (a) FeN_4P and (b) FeN_4S.

Table S1 The adsorption free energy of ORR intermediates on various catalysts.

System	*Adsorption free energy (ΔG_{ads}) / eV*		
	*OOH	*O	*OH
FeN_4	3.62	1.45	0.65
FeN_4P	4.71	3.35	1.70
FeN_4S	4.78	3.42	1.63
FeN_4Cl	4.20	2.31	1.17