Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Adsorption mechanism of NH_3, NO, and O_2 molecules over Fe_xO_y/AC catalyst surface: a DFT-D3 study

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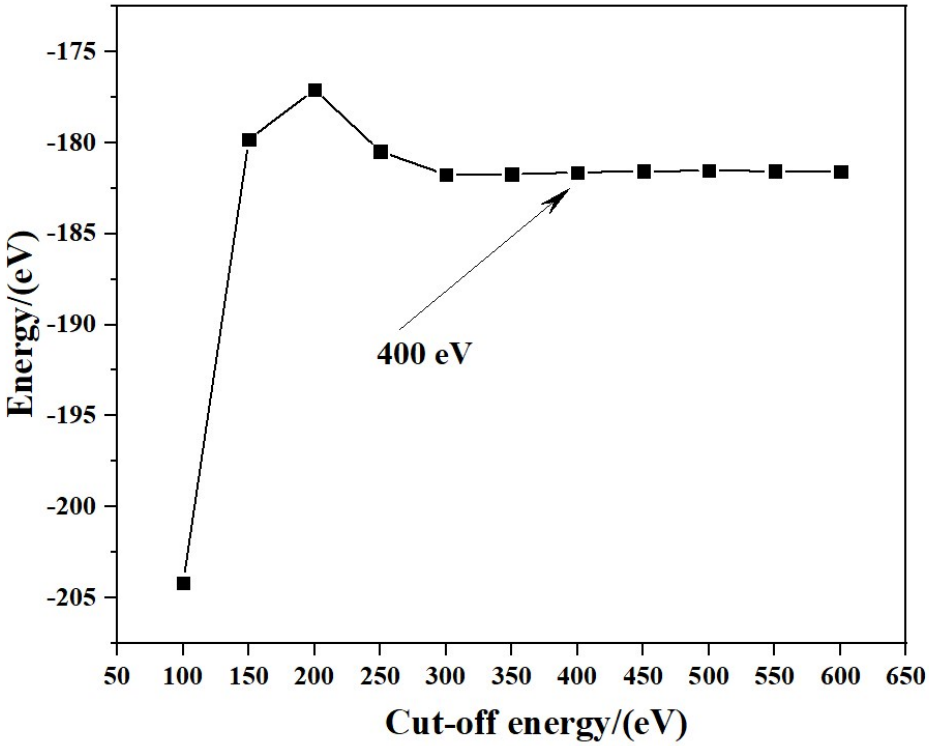

(a)

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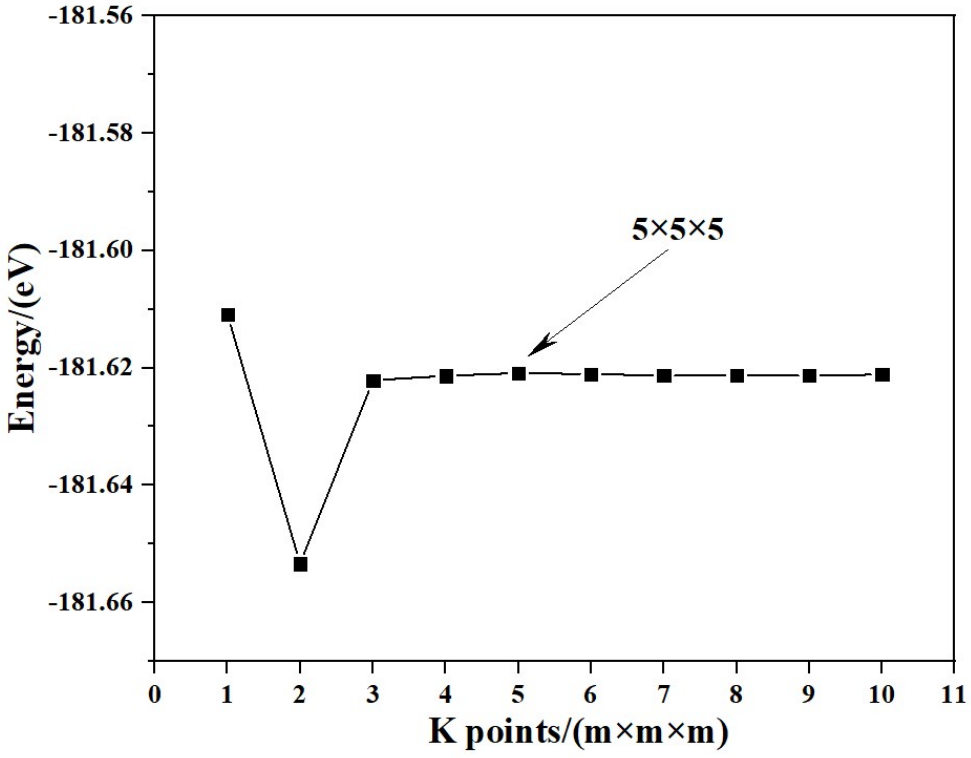


(b)

Figure S1 Convergence test (a) cut-off energy, (b) K points.

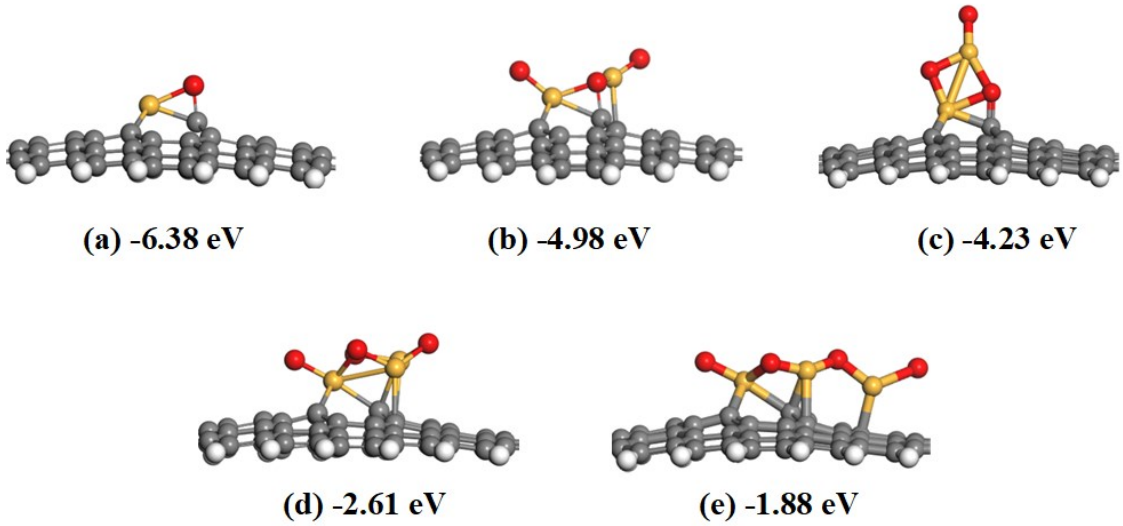


Figure S2 Configurations of Fe_xO_y clusters loaded on the AC surface (Fe: golden, O: red, C: gray, H: white).

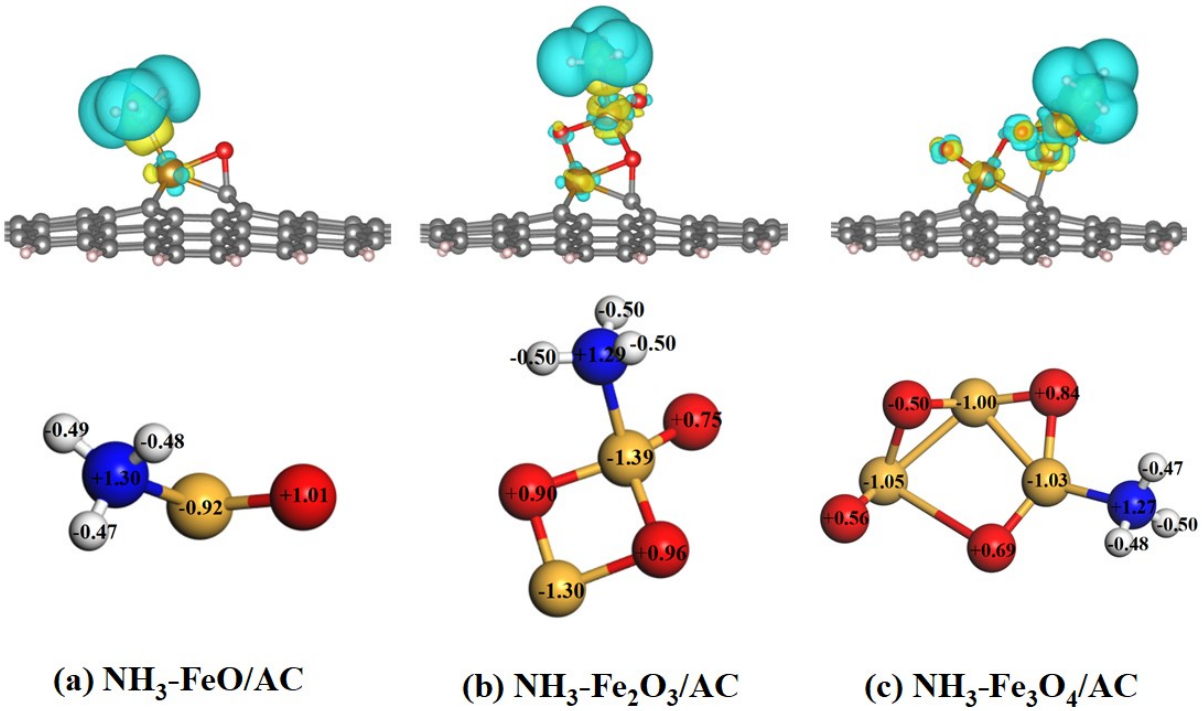
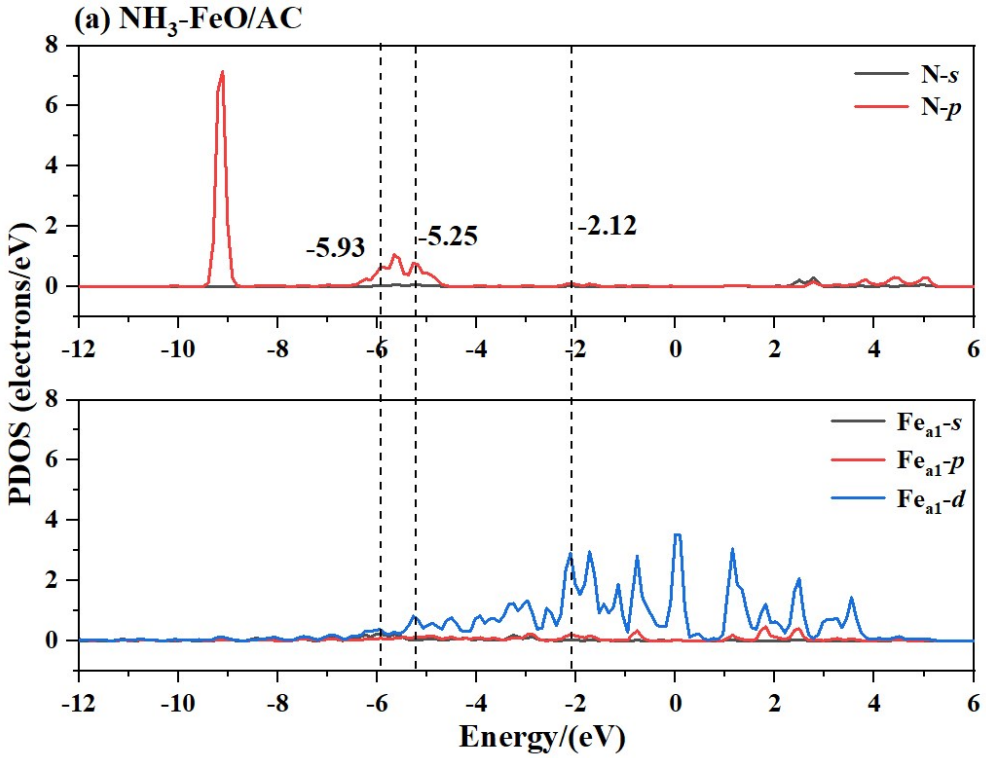


Figure S3 Electron density difference and Bader charge change of NH_3 adsorbed on the Fe_xO_y/AC surface.



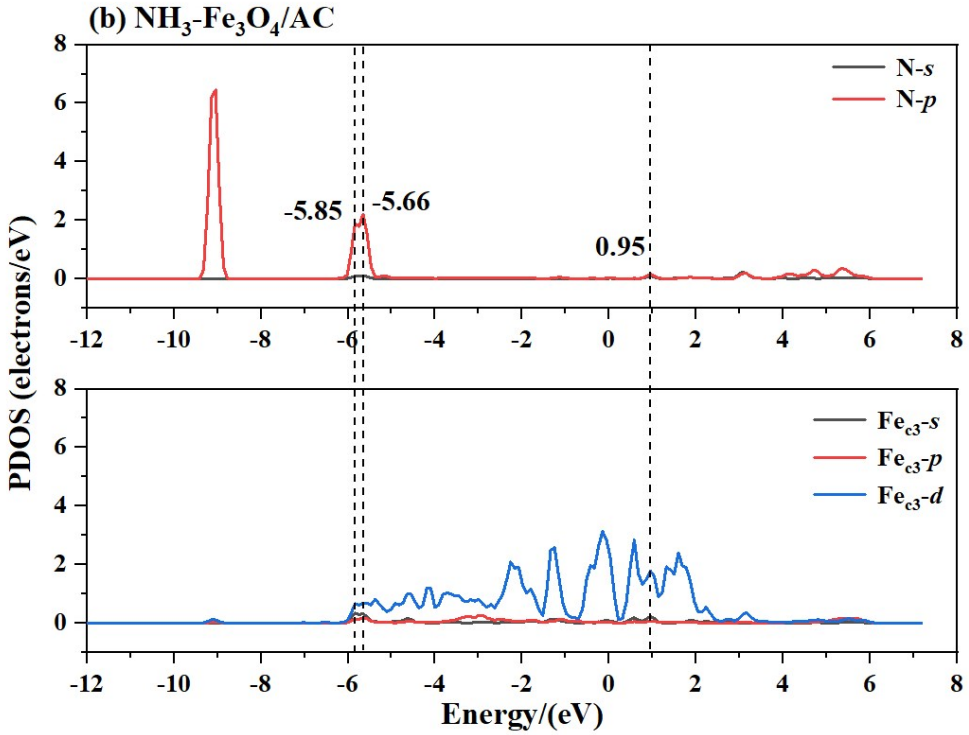


Figure S4 PDOS results of NH_3 adsorbed on the FeO/AC and Fe_3O_4/AC surfaces.

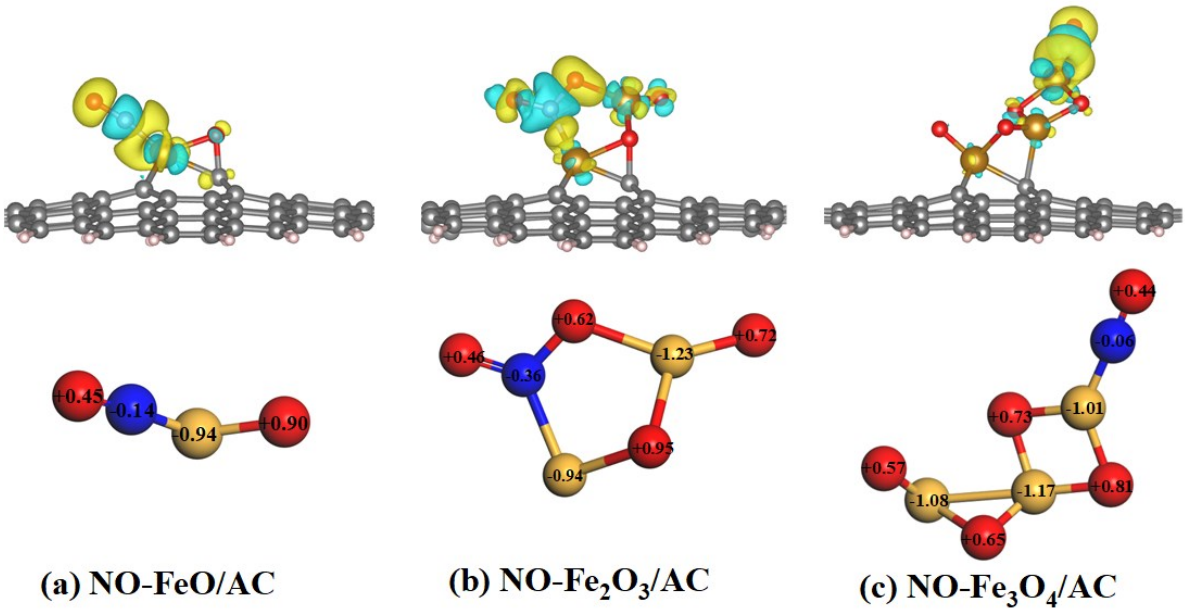


Figure S5 Electron density difference and Bader charge change of NO adsorbed on the Fe_xO_y/AC surface.

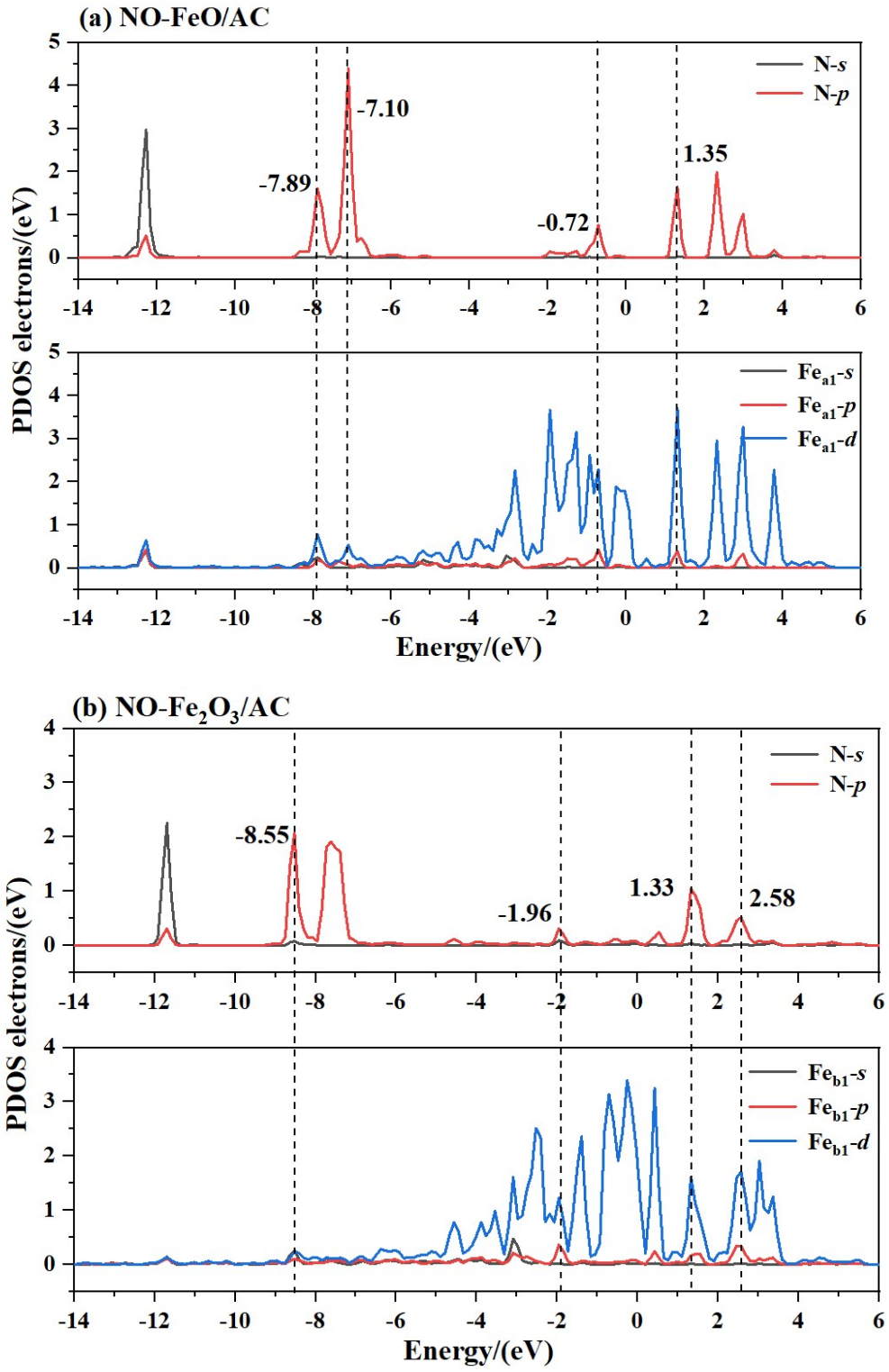


Figure S6 PDOS results of NO adsorbed on the FeO/AC and Fe_2O_3/AC surfaces.

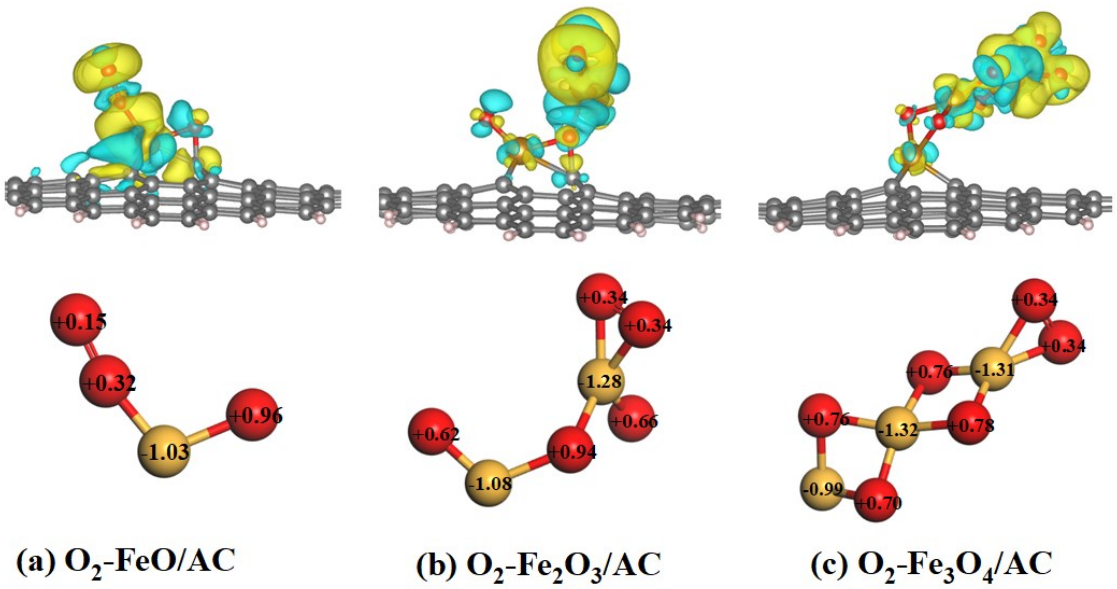
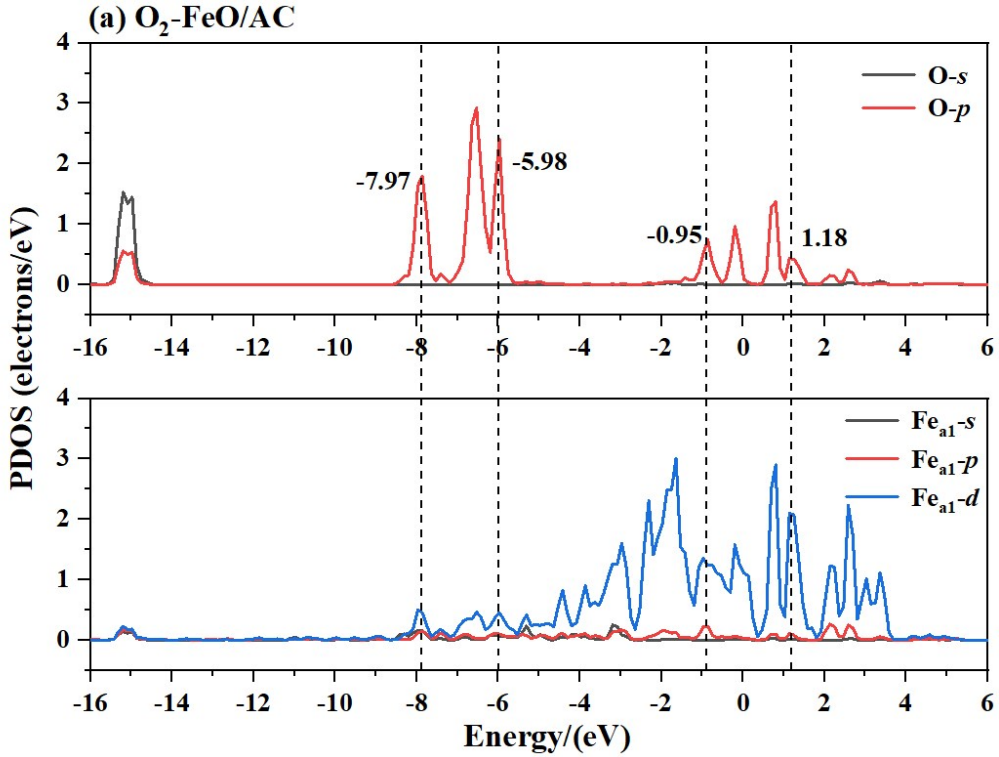


Figure S7 Electron density difference and Bader charge change of O_2 adsorbed on the Fe_xO_y/AC surface.



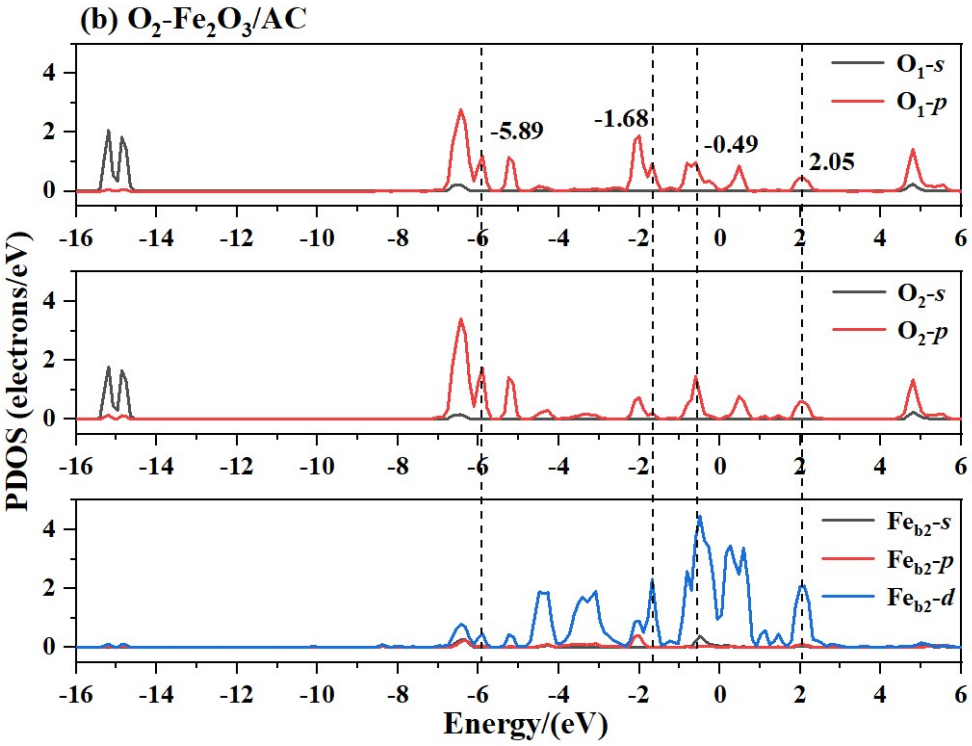


Figure S8 PDOS results of O_2 adsorbed on the FeO/AC and Fe_2O_3/AC surfaces.

Table S1 Comparison of gas adsorption energies between calculated values and experimental values for the Fe_xO_y/AC catalyst

Gas	Fe_xO_y/AC (eV)	Experimental value (eV)[1]
NH_3	-2.33	-1.23
NO	-3.58	-2.51
O2	-4.99	-2.25

Table S2 Comparison of adsorption energies between Fe_xO_y/AC catalyst and Fe_2O_3 catalyst.

Gas	Fe_xO_y/AC (eV)	α-Fe_2O_3 (eV) [2]	γ-Fe_2O_3 (eV)[3]
NH_3	-2.33	-1.20	-1.69
NO	-3.58	-1.08	-2.17
O_2	-4.99	-1.28	-2.01

Previous studies [4-6] have shown that the edges of two-dimensional carbon-based materials have the ability to bind to gas molecules or active groups. Hence, we studied the adsorption behaviors of NH_3, NO, and O_2 on the edge of AC model. The hydrogen-deficient AC surface is shown in Figure S9 and there are two exposed carbon sites (C_1 and C_2). We can see from the adsorption configurations in Fig. S10b-e that NH_3 and NO molecules can combine with C sites to form N-C bonds, while O_2 cannot bind to them. Table S3 shows that the adsorption energies are -0.59, -1.59, -0.79, and -0.16 eV, and the corresponding electron changes are -0.24, +0.21, +0.25, and -0.01e, respectively. By comparison, it can be found that the adsorption energies of gas molecules on C sites are lower than those of on Fe_xO_y/AC surface, suggesting that Fe_xO_y clusters loaded on AC surface have more excellent adsorption performance for these gas molecules.

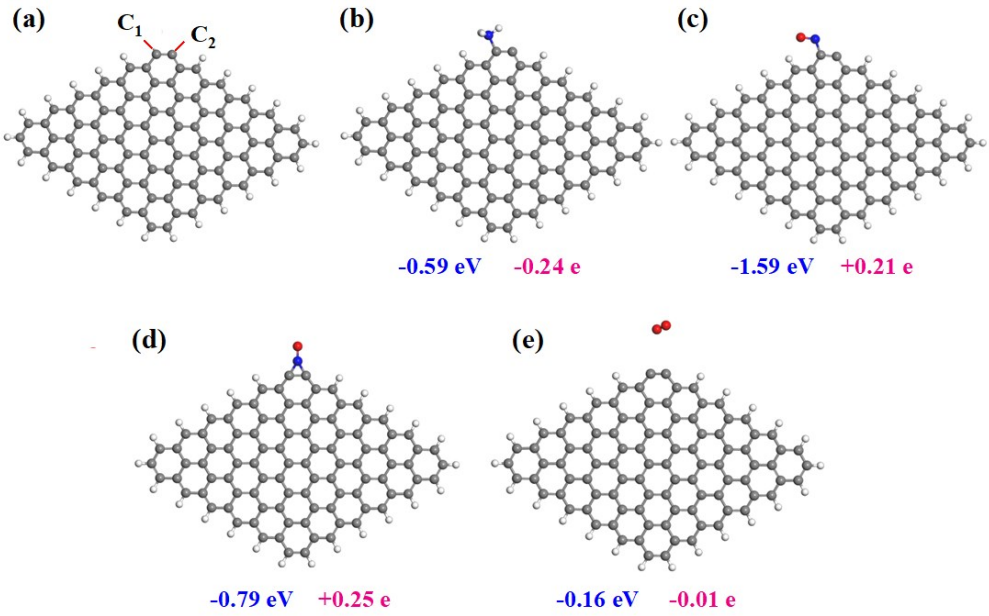


Figure S9 Gas adsorption configurations on the AC surface.

Table S3 Adsorption energies and electrons changes of gas molecules on the edge of AC surface.

Gas	Adsorption energy (eV)	Electron changes (e)
NH_3	-0.59	-0.24
NO	-1.59; -0.79	+0.21; +0.25
O_2	-0.16	-0.01

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