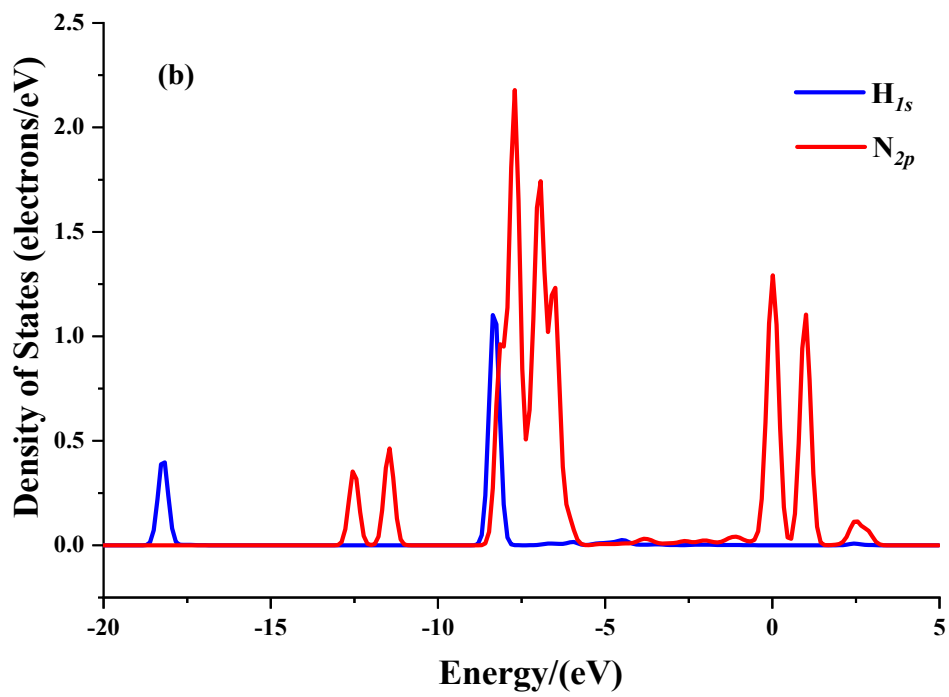
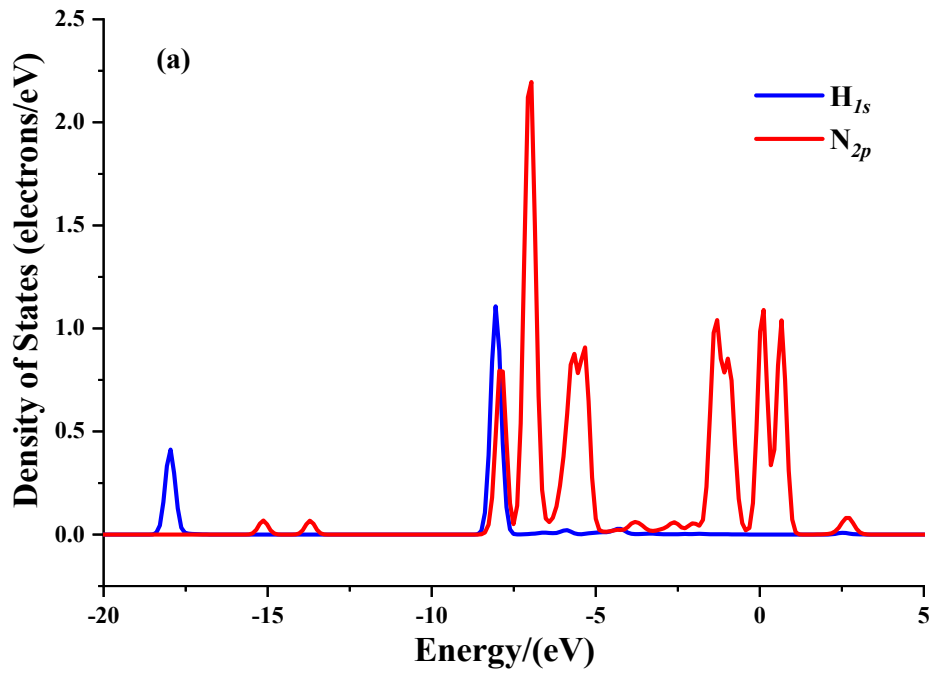


Table S1 E_{ads} and Bader charge changes for double molecules on α -Fe₂O₃ (001) surface

Gas molecules	$E_{ads}/(\text{kJ mol}^{-1})$	Bader charge changes
O ₂ +NH ₃	-248	¹ O: +0.21; ² O: +0.05; Fe: -0.01
		N: +0.03; 3×H: -0.06; Fe: -0.03
NH ₃ +NO	-184	N: +0.08; 3×H: -0.08; Fe: -0.02
		N: +0.37; O: -0.20; Fe: +0.02
NO+O ₂	-403	N: +0.25; O: -0.16; Fe: +0.04
		¹ O: +0.20; ² O: +0.01; Fe: -0.03



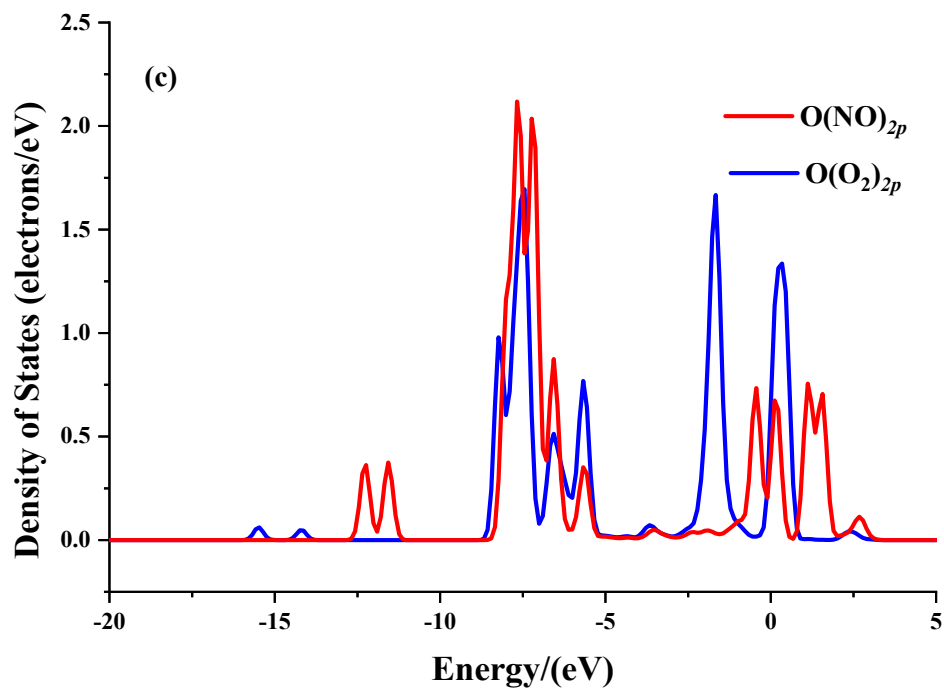


Figure S1 PDOS of double-molecule molecules adsorbed on the $\alpha\text{-Fe}_2\text{O}_3$ (001) surface. (a) NH_3+O_2 , (b) NH_3+NO , (c) $\text{NO}+\text{O}_2$