

Table S1. The distance between gas molecules and Co atom ($d_{\text{Co-gas}}/\text{\AA}$), the charge transferred to the gas molecules ($\Delta Q_{\text{gas}}/e$), adsorption energies (E_{ad}/eV), and the total magnetic moment of the systems (M/μ_{B}), after gas adsorption.

Gas	$d_{\text{Co-gas}} (\text{\AA})$	$\Delta Q_{\text{gas}} (e)$	$E_{\text{ad}} (\text{eV})$	$M (\mu_{\text{B}})$
C_2H_2	1.92	-0.38	-1.95	2.00
CO	1.76	-0.31	-2.27	2.00
NO_2	1.92	-0.70	-3.32	1.00
SO_2	1.93	-0.71	-1.85	0.14

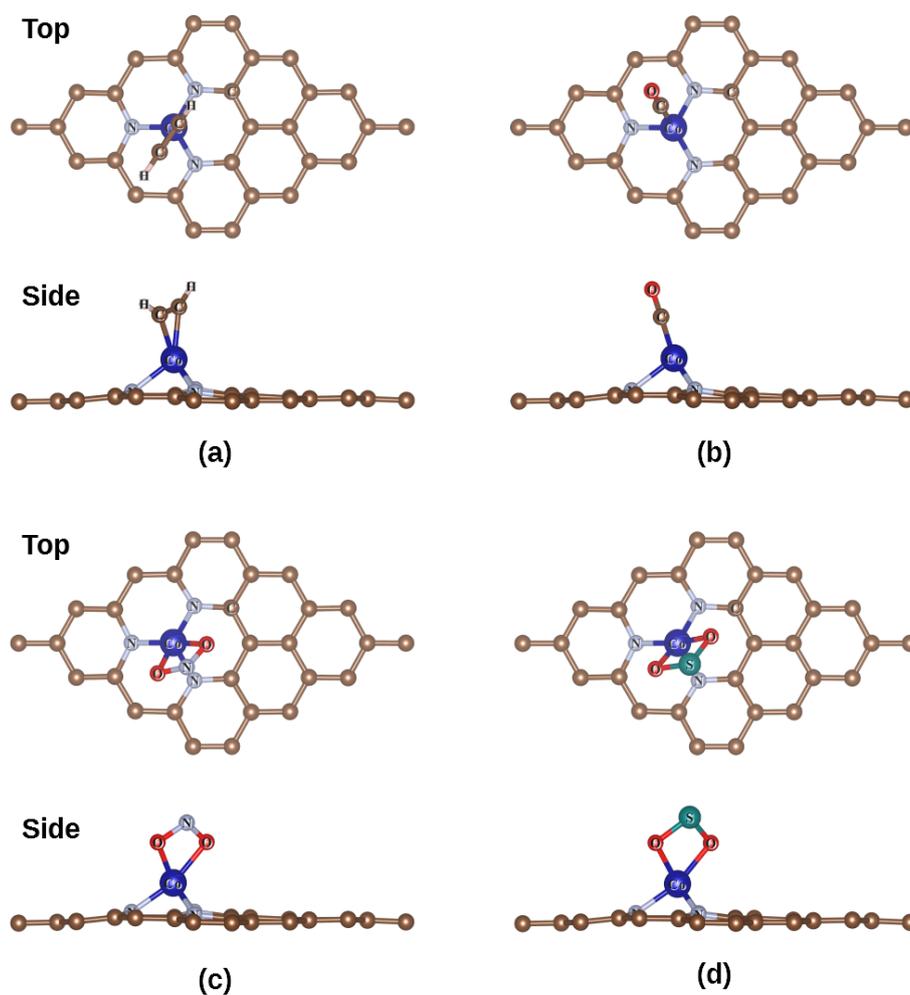


Figure S1. The top and side view of configurations of Co/N₃-gra with (a) C₂H₂, (b) CO, (c) NO₂, and (d) SO₂ adsorbed on it.

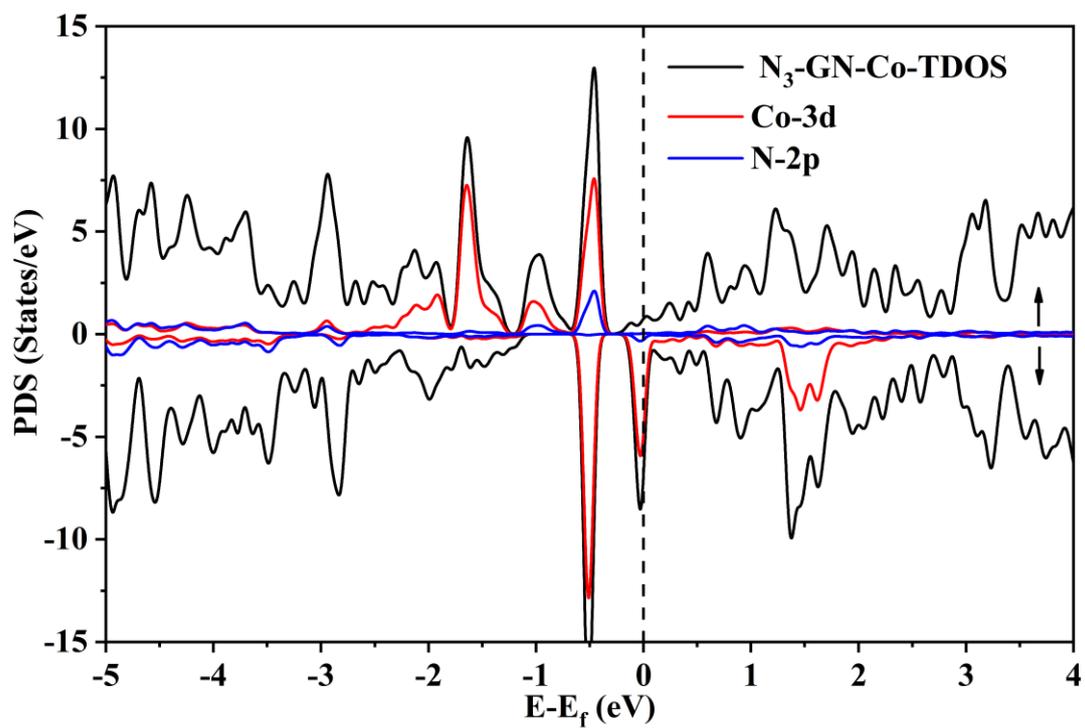


Figure S2. The density of states of Co/ N_3 -gra, with the up (down) spin denoted as \uparrow (\downarrow). The dotted line indicates the Fermi level.