

Supporting Information

Promotional effect of the electron donating functional groups on the gas sensing properties of graphene nanofakes

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Table S1. Adsorption energy (E_{ad}), and change in the band gap for the adsorption of O_2 molecule on the pristine (P-GNF), B-doped (B_D -GNF), N-doped (N_D -GNF), and functionalized GNFs: COOH-GNF, CN-GN, and NO_2 -GNF.

System	ΔE_g (%)	E_{ad} (kcal mol ⁻¹)
O_2 / P- GNF	8.30	0.127
O_2 / B_D -GNF	2.40	-40.45
O_2 / N_D -GNF	-14.30	-35.78
O_2 /COOH-GNF	0	-4.60
O_2 /CN-GNF	4	-2.80
O_2 / NO_2 -GNF	4.20	-6.30

Table S2. Adsorption energy (E_{ad}) and change in the band gap for the adsorption of NO molecule on the pristine (P-GNF), B-doped (B_D -GNF), N-doped (N_D -GNF), and functionalized GNFs: COOH-GNF, CN-GN, and NO_2 -GNF.

System	ΔE_g (%)	E_{ad} (kcal mol ⁻¹)
NO_N /P-GNF	508	-26.70
NO_N / B_D -GNF	-82	33.70
NO_N / N_D -GNF	-75	43.90
NO_N /COOH-GNF	550	-27.37
NO_N /CN-GNF	548	-27.08
NO_N / NO_2 -GNF	533	-29.58
NO_O /P-GNF	521	-27.00
NO_O / B_D -GNF	-77	46.50
NO_O / N_D -GNF	-75	45.28
NO_O /COOH-GNF	555	-27.67
NO_O /CN-GNR	512	-27.47
NO_O / NO_2 -GNF	529	-29.70

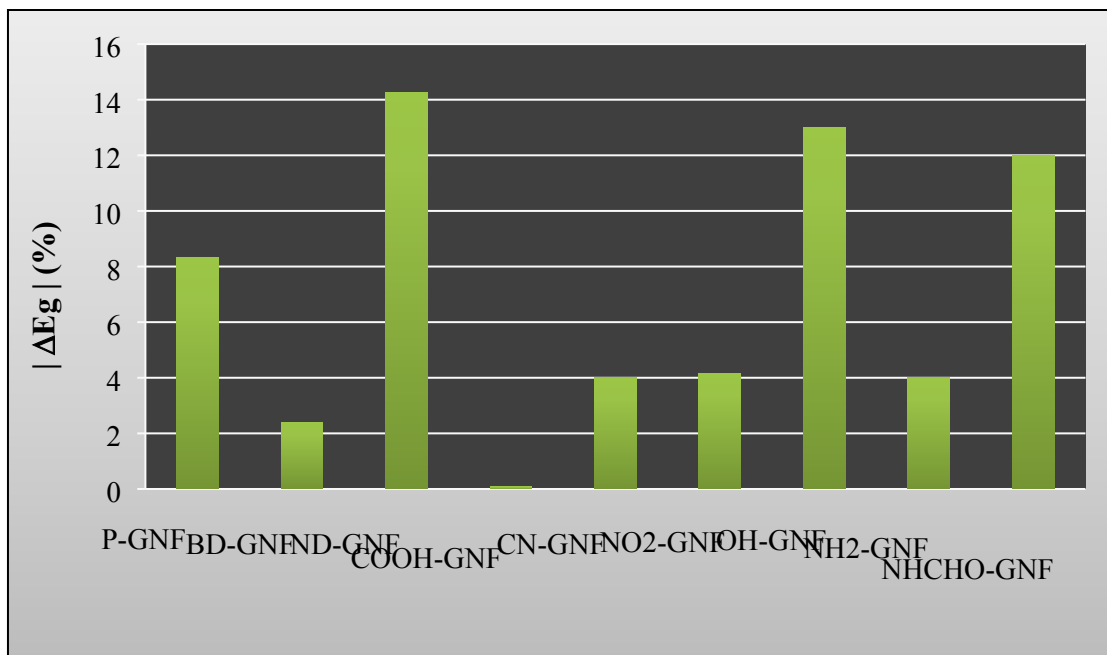


Figure S1. The absolute value of the change in the band gap as a result of O₂ adsorption on various GNFs studied in present and previous works.