Investigation into NO_2 Gas Sensing Behaviour of Defect Induced Heteroatom (N, B) Doped Reduced Graphene Oxide Modified Mesopores $MgFe_2O_4$

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S1. Preparation of Graphene oxide (GO);

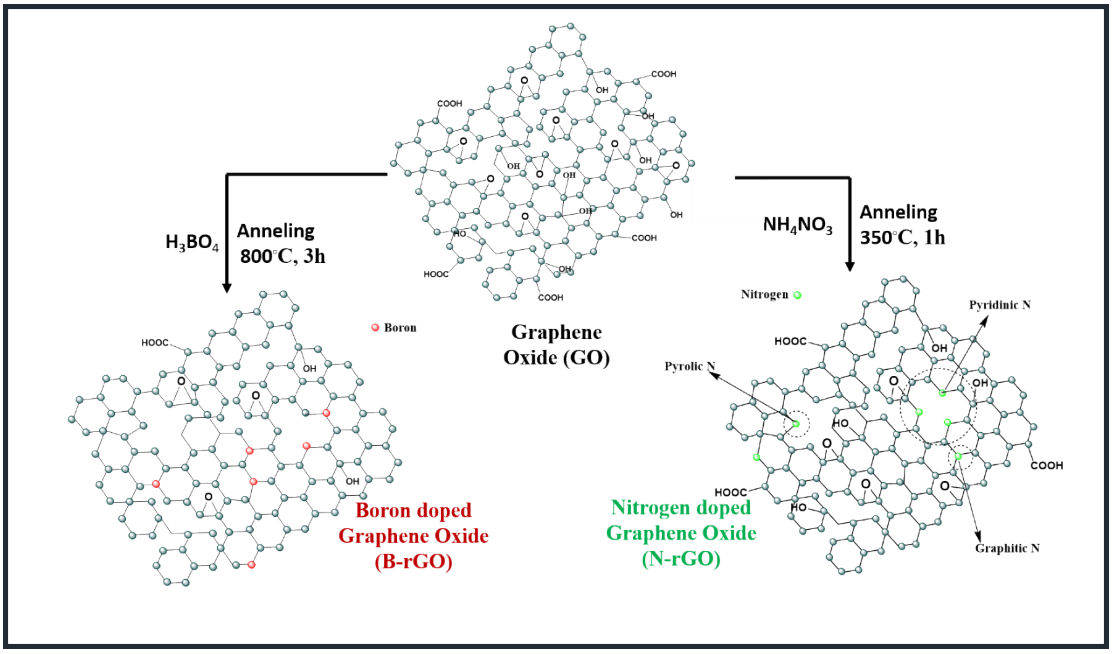
Primarily, GO was synthesized by following Improved Hummer's method.[1] Synthesis of GO was initiated by taking graphite powder (1.5 g) and mixture of H_2SO_4 and H_3PO_4(180:20 ml) as starting material at 50 °C. Then, 6 g of $KMnO_4$ was added pinch wise and let it stir for 12 h to oxidize the graphite flakes. Later, this mixture was worked up by adding 250 ml of ice water followed by addition of 3 ml of 30% H_2O_2. The obtained solution was centrifuged and washed with ethanol, deionized water and dilute HCl till neutral pH achieved and finally it was dried for 24 h to obtain GO powder. The obtained GO powder was thermally reduced at 350 °C to get reduced graphene oxide (rGO).

S2. Preparation of N-doped GO (N-rGO);

The synthesized GO and NH_4NO_3 was used as starting material to produce N-rGO as shown in scheme S1. 1:1 molar ratio of GO and NH_4NO_3 were poured onto a 250 ml beaker containing 50 ml ethanol. The mixture was stirred for 30 min and then after temperature was raised to 50 °C for evaporating ethanol while stirring. The dried sample mixture was calcined at 350 °C for 1 h with a ramp rate of 5 °C/min heating rate. After cooling synthesized N-rGO was washed with ethanol and ultrapure water several times. After drying in an oven for 80 °C overnight, N-rGO was obtained.[2]

S3. Preparation of B-doped GO (B-rGO);

B-rGO was synthesized by heating mixture of GO and H_3BO_3 at a weight ratio of 1:1, as shown in scheme S1. Typically, 1:1 mixture of GO and H_3BO_3 were mixed with 30 ml ultrapure water and sonicated for 2 h until a uniform suspension was obtained. The mixture was dried at 60 °C and further calcined at 800 °C with a heating rate of 10 °C/min for 3 h under pure Argon atmosphere to obtain B-rGO following previously reported literature.[3]



Scheme-S1: Synthesis of (N, B) rGO-$MgFe_2O_4$ nanocomposite

S4. Raman of MFO;

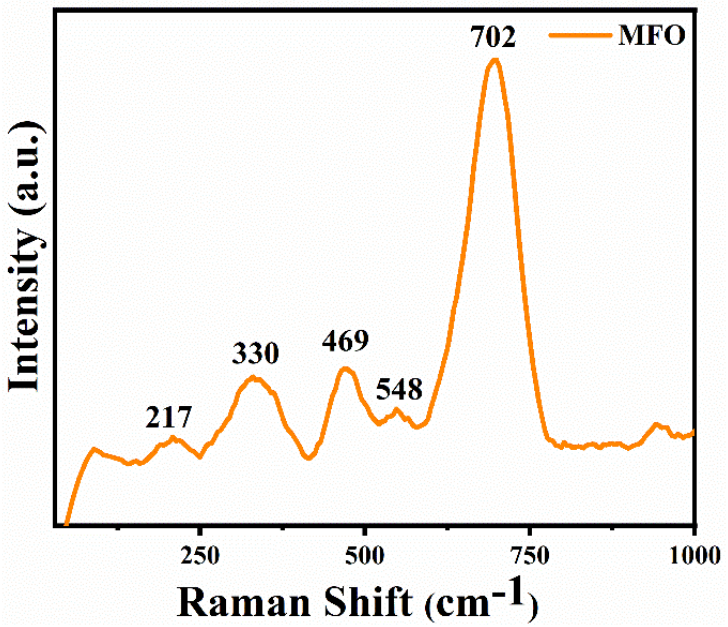


Figure S1: Raman of MFO.

S5. XPS of MFO;

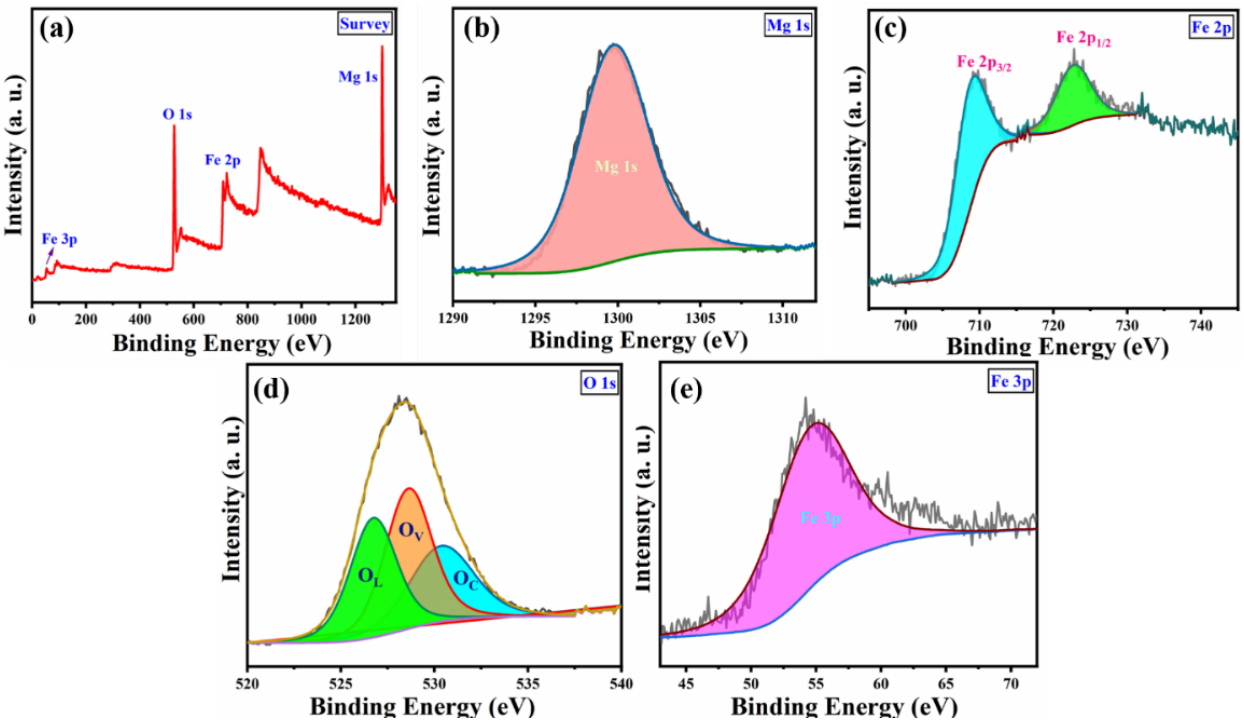


Figure S2: XPS (a) survey, (b) Mg 1s, (c) Fe 2p, (d) O 1s, and (e) Fe 3p of MFO.

S6. Gas sensing measurement of MFO;

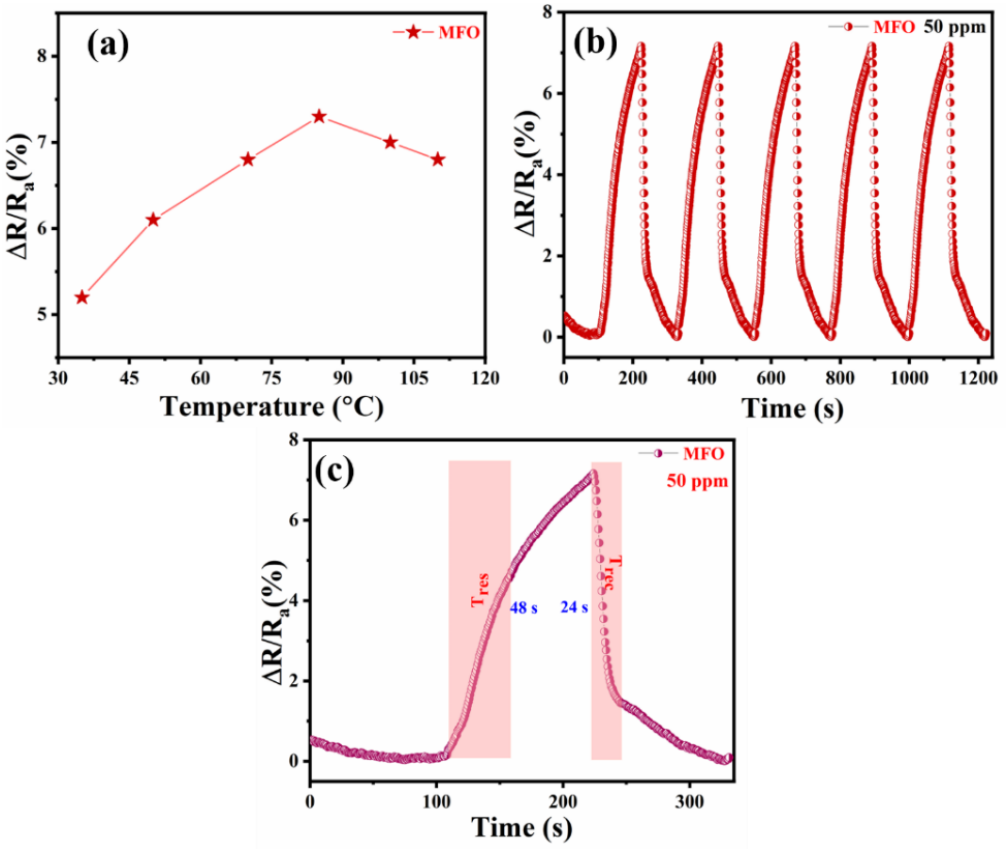


Figure S3: (a) Operating temperature varied response curve, (b) reproducibility, and (c) corresponding response and recovery curve of MFO towards 50 ppm NO_2.

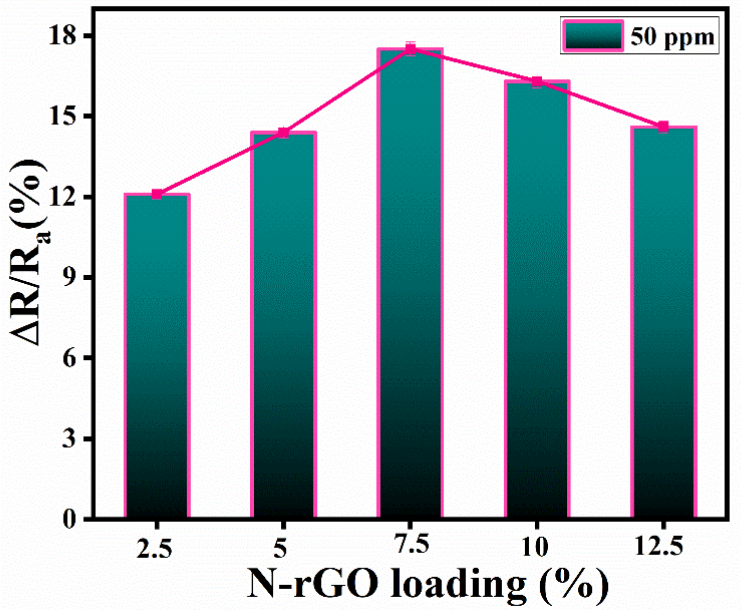


Figure S4: (a) Weight percentage variation responsive curve of N-rGO in N-rGO/MFO towards 50 ppm NO_2.

Table S1: Comparison table of gas sensing performance with other reported literature

Materials	NO_2 concentration (ppm)	S%	Operating Temperature (°C)	Response time	Recovery time	References
Fe_2O_3/Fe@N-GC	100	25.48[1]	RT	2.13s	11.73s	4
γ-Fe_2O_3@RGO	100	6.86	200	1.25s	--	5
ZnO-rGO	100	47.4	RT	6.2min	15.5min	6
ZnS NPs/N-rGO	10	2.16	RT	--	724s	7
Alumina-Pt/ZnO nanoparticles	100	18	300	45s	73s	8
rGO-Fe_3O_4	400	24.2	RT	276s	738s	9
Ag-PPy-pTSA	100	68	RT	148s	500s	10
In_2O_3 rod–rGO	97	2.45	RT	25s	-	11
N-rGO/MFO	**100**	**26.9**	**RT**	**15s**	**17s**	**This work**

1= R_a/R_g

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