

Supplementary Materials

Efficient and reusable graphene- γ - Fe_2O_3 magnetic nano-composite for selective oxidation and one-pot synthesis of 1,2,3-triazole using green solvent

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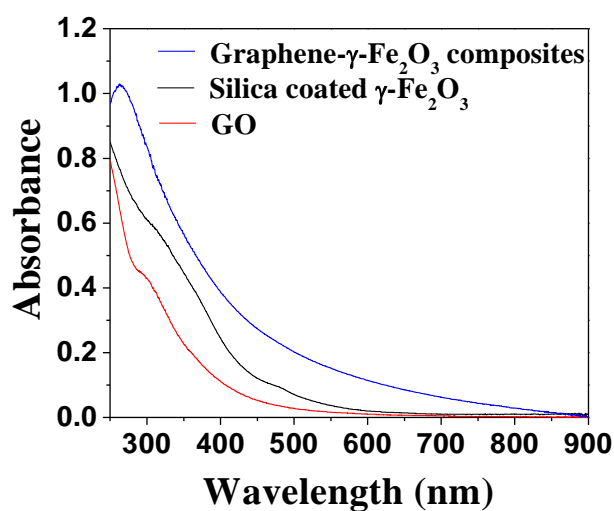


Figure S1. UV-Visible absorption spectra of graphene- γ - Fe_2O_3 composites, silica coated γ - Fe_2O_3 and graphene oxide.

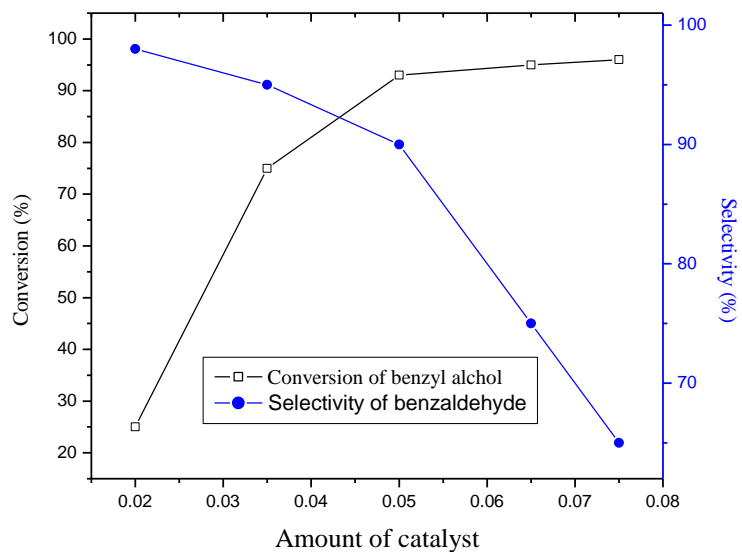


Figure S2. Effect of amount of catalyst on oxidation of benzyl alcohol as a function of time using graphene- γ - Fe_2O_3 composite

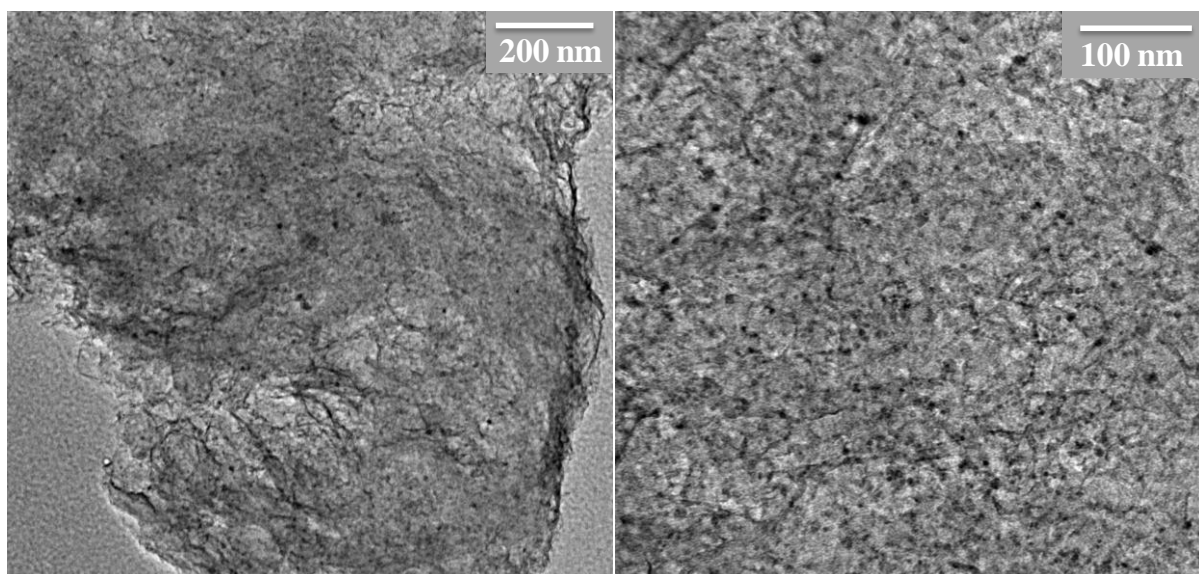


Figure S3: TEM image of reused Graphene- γ - Fe_2O_3 composite materials.

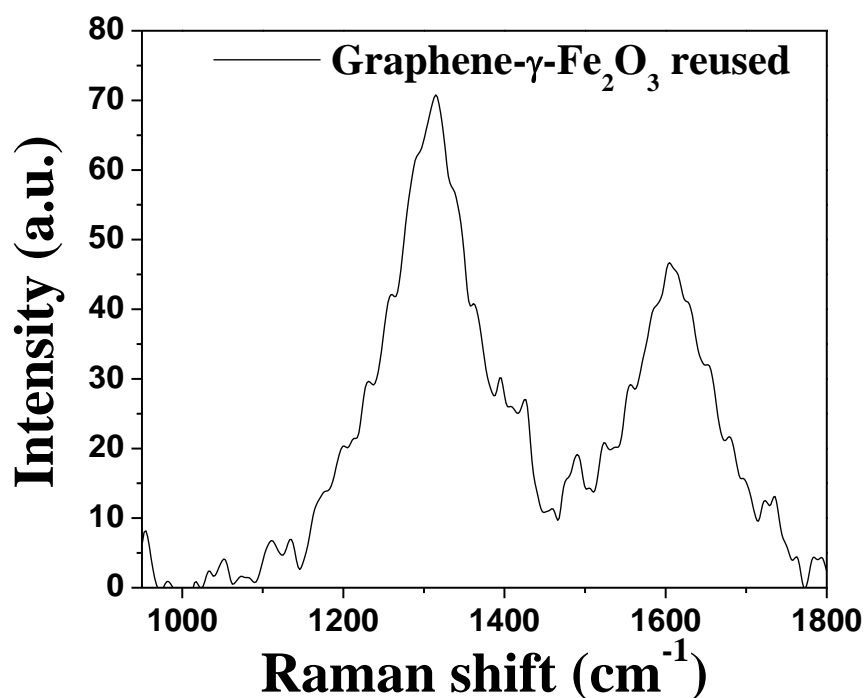


Figure S4: Raman spectra of Graphene- γ -Fe₂O₃ composite materials after reused showing two well documented D and G band at 1314 and 1604 cm⁻¹.

(c) Spectral data of the products

Spectral data of Bromination products

- 1. 5-Bromo-2-hydroxy benzaldehyde¹:** ¹H NMR (CDCl₃) δ (ppm) 10.80 (s, 1H, OH), 9.84 (s, 1H, CHO), 7.67 (d, 1H, ArH), 7.56 (dd, 1H, ArH), 6.88 (d, 1H, ArH); ¹³C NMR (CDCl₃) δ 195.6, 160.6, 139.6, 136.0, 121.8, 120.1, 111.7 ppm.
- 2. 4-Bromophenol²:** ¹H NMR (CDCl₃) δ (ppm) 5.4 (s, 1H, OH), 6.75 (d, 2H, ArH), 7.34 (d, 2H, ArH); ¹³C NMR (CDCl₃) δ 154.5, 132.8, 117.7, 112.5 ppm.

3. **4-Bromo-1, 3-dihydroxybenzene¹**: ¹H NMR (CDCl₃) δ (ppm) 7.24 (d, 1H, ArH), 6.51 (d, 1H, ArH), 6.36 (dd, 1H, ArH), 5.49 (brs, 1H, OH), 4.80 (brs, 1H, OH); ¹³C NMR (CDCl₃) δ 156.8, 154.1, 132.5, 110.1, 103.4, 98.3 ppm.
4. **2-Bromo-4-methylphenol²**: ¹H NMR (CDCl₃) δ (ppm) 2.31 (s, 3H), 5.31 (s, 1H), 6.80 (d, 1H, ArH), 7.02 (d, 1H, ArH), 7.26 (d, 1H, ArH); ¹³C NMR (CDCl₃) δ 20.4, 110.1, 115.5, 118.1, 129.5, 132.7, 133.1, 150.1 ppm.
5. **2-Bromo-4-nitrophenol³**: ¹H NMR (CDCl₃) δ (ppm) 6.19 (s, 1H, OH), 7.11 (d, 1H, ArH), 8.09 (dd, 1H, ArH), 8.44 (d, 1H, ArH); ¹³C NMR (CDCl₃) δ 159.4, 140.5, 126.1, 125.0, 118.8, 111.7 ppm.
6. **2-Bromo-4-aminophenol⁴**: ¹H NMR (CDCl₃) δ (ppm) 5.11 (s, 1H, OH), 4.14 (s, 2H, NH₂), 6.43-6.54 (m, 3H, ArH).
7. **4-Bromoanisole¹**: ¹H NMR (CDCl₃) δ (ppm) 3.81 (s, 3H, OCH₃), 7.35 (d, 2H, ArH), 6.80 (d, 2H, ArH); ¹³C NMR (CDCl₃) δ 159.1, 132.4, 116.4, 113.8, 55.7 ppm.
8. **2-Bromo-4-methylanisole⁵**: ¹H NMR (CDCl₃) δ (ppm) 2.28 (s, 3H, CH₃), 3.86 (s, 3H, OCH₃), 6.82 (d, 1H, ArH), 7.03 (dd, 1H, ArH), 7.36 (d, 1H, ArH).
9. **4-Bromoaniline²**: ¹H NMR (CDCl₃) δ (ppm) 3.70 (brs, 2H, NH₂), 6.58 (d, 2H, ArH), 7.25 (d, 2H, ArH); ¹³C NMR (CDCl₃) δ 110.1, 116.5, 132.3, 146.1 ppm.
10. **2-Bromo-4-nitroaniline⁷**: ¹H NMR (CDCl₃) δ (ppm) 4.90 (brs, 2H, NH₂), 6.71 (d, 1H, ArH), 8.01 (dd, 1H, ArH), 8.35 (d, 1H, ArH); ¹³C NMR (CDCl₃) δ 150.1, 138.4, 129.3, 124.6, 113.6, 107.1 ppm.
11. **2-Bromo-4-methylaniline⁸**: ¹H NMR (CDCl₃) δ (ppm) 2.24 (s, 3H, CH₃), 3.93 (brs, 2H, NH₂), 6.64 (d, 1H, ArH), 6.90 (d, 1H, ArH), 7.18 (s, 1H, ArH); ¹³C NMR (CDCl₃) δ 20.0, 108.8, 115.5, 129.3, 128.8, 132.7, 142.0 ppm.

- 12. 2-Bromo-4-chloroaniline⁹:** ¹H NMR (CDCl₃) δ (ppm) 4.08 (s, 2H, NH₂), 6.64 (d, 1H, ArH), 7.07 (dd, 1H, ArH), 7.38 (d, 1H, ArH); ¹³C NMR (CDCl₃) δ 144.7, 130.8, 128.5, 123.6, 119.7, 115.4 ppm.
- 13. 4-Bromo-2-methylaniline⁸:** ¹H NMR (CDCl₃) δ (ppm) 2.07 (s, 3H, CH₃), 3.56 (brs, 2H, NH₂), 6.47 (d, 1H, ArH), 7.09 (d, 1H, ArH), 7.14 (s, 1H, ArH); ¹³C NMR (CDCl₃) δ 17.7, 110.6, 116.4, 124.7, 129.5, 133.1, 143.8 ppm.
- 14. 4-Bromo-2-chloroaniline:** ¹H NMR (CDCl₃) δ (ppm) 6.44 (s, 2H, NH₂), 6.67 (d, 1H, ArH), 7.44 (dd, 1H, ArH), 7.88 (d, 1H, ArH); ¹³C NMR (CDCl₃) δ 143.0, 133.3, 132.5, 128.2, 120.6, 111.4 ppm.
- 15. 4-Bromo-2-nitroaniline¹⁰:** ¹H NMR (CDCl₃) δ (ppm) 6.51 (s, 2H, NH₂), 6.70 (d, 1H, ArH), 7.44 (dd, 1H, ArH), 8.25 (d, 1H, ArH); ¹³C NMR (CDCl₃) δ 142.6, 138.7, 133.0, 128.10, 120.0, 109.5 ppm.
- 16. 4-Bromo-N, N-dimethylaniline¹¹:** ¹H NMR (CDCl₃) δ (ppm) 2.94 (s, 6H, CH₃), 6.67 (d, 2H, ArH), 7.16 (d, 2H, ArH); ¹³C NMR (CDCl₃) δ 40.1, 108.10, 115.2, 131.9, 149.7 ppm.

Spectral data of Sulfides oxidation products

- 1. Methylphenylsulfoxide¹²:** ¹H NMR (CDCl₃) δ (ppm) 2.72(s, 3H); 7.31-7.36(m, 1H); 7.41-7.48(m, 2H); 7.60-7.68(m, 2H); ¹³C NMR (CDCl₃) δ 43.91; 123.50; 128.66; 130.99; 145.48

- 2. Butylpropylsulfoxide¹³:** ¹H NMR (CDCl₃) δ (ppm) 2.59-2.70 (m, 4H, CH₂) 1.67-1.73 (m, 4H, CH₂), 1.40-1.47 (m, 4H, CH₂), 0.91 (t, 6H, CH₃); ¹³C NMR (CDCl₃) δ (ppm) 51.8, 24.6, 22.3, 13.7
- 3. Diphenyl sulfoxide¹⁴:** ¹H NMR (CDCl₃) δ (ppm) 7.58-7.63 (m, 4H), 7.38-7.43 (m, 6H); ¹³C NMR (CDCl₃) δ (ppm), 145.7, 131.3, 129.0, 124.1
- 4. Ethylphenyl sulfoxide¹⁴:** ¹H NMR (CDCl₃) δ (ppm) 7.40-7.56 (m, 5H) 2.86-2.90 (m, 1H), 2.67-2.76 (m, 1H), 1.65 (t, 3H) ; ¹³C NMR (CDCl₃) δ (ppm) 143.7, 131.6, 128.9, 124.6, 49.4, 7.0
- 5. Cyclohexylphenyl sulfoxide¹³:** ¹H NMR (CDCl₃) δ (ppm) 7.52-7.58 (m, 2H), 7.41-7.50 (m, 3H), 2.78 (t, 2H), 1.66-1.73 (m, 1H), 1.50-1.57 (m, 1H), 1.27-1.40 (m, 2H), 1.20-1.25 (m, 4H), 0.91 (t, 3H) ; ¹³C NMR (CDCl₃) δ (ppm) 142.9, 130.3, 129.1, 123.7, 57.0, 31.3, 28.6, 22.4, 21.8, 14.1
- 6. Benzylphenyl sulfoxide¹³:** ¹H NMR (CDCl₃) δ (ppm) 7.386-7.42 (m, 5H) 7.17-7.23 (m, 3H), 6.90 (d, 2H), 4.11 (d, 1H), 3.98 (d, 1H); ¹³C NMR (CDCl₃) δ (ppm) 143.1, 131.6, 130.2, 129.5, 128.4, 128.1, 127.8, 124.1, 63.5
- 7. Phenyl (prop-1-ene) sulfoxide¹³:** ¹H NMR (CDCl₃) δ (ppm) 7.86-7.91 (m, 2H), 7.58-7.62 (m, 1H), 7.47-7.52 (m, 2H), 5.70-5.80 (m, 1H), 5.28 (d, 1H), 5.14 (d, 1H), 3.75 (d, 2H) ; ¹³C NMR (CDCl₃) δ (ppm) 138.5, 133.7, 129.4, 128.4, 124.6, 124.0, 60.2
- 8. 4-Methanesulfinyl benzonitrile¹⁵:** ¹H NMR (CDCl₃) δ(ppm) 2.74 (s, 3H), 7.73 (d, 2H), 7.80(d, 2H); ¹³C NMR (CDCl₃) δ(ppm) 151.3, 132.8, 124.3, 117.5, 114.6, 43.6
- 9. Methyl p-tolyl sulfoxide¹⁵:** ¹H NMR (CDCl₃) δ(ppm) 2.40 (s, 3H) , 2.72 (s, 3H) , 7.30 (d, 2H), 7.52 (d, 2H); ¹³C NMR (CDCl₃) δ(ppm) 142.2, 141.4, 130.0, 123.5, 43.7, 21.4

10. **Dimethyl sulfoxide**¹⁶: ¹H NMR (CDCl₃) δ (ppm) 2.56 (s, 6H); ¹³C NMR (CDCl₃) δ (ppm) 40.2
11. **Methyl(4-methoxyphenyl) sulfoxide**¹⁷: ¹H NMR (CDCl₃) δ (ppm) 7.58 (d, 2H), 6.98 (d, 2H), 3.82 (s, 3H), 2.72 (s, 3H); ¹³C NMR (CDCl₃) δ (ppm) 162.1, 136.3, 125.3, 114.7, 55.9, 39.8
12. **Di(n-propyl) sulfoxide**¹⁸: ¹H NMR (CDCl₃) δ (ppm) 2.69–2.76 (m, 2H), 2.52–2.59(m, 2H), 1.81 (m, 4H), 1.12 (t, 6H); ¹³C NMR (CDCl₃) δ (ppm) 54.4, 16.13, 13.46
13. **4-Nitro-methylphenyl sulfoxide**¹²: ¹H NMR (CDCl₃) δ (ppm) 2.54 (s, 3H), 7.83 (d, 2H), 8.32(d 2H); ¹³C NMR (CDCl₃) δ (ppm) 47.72, 124.4, 149.28, 153.2.
14. **2-Phenylsulfinylethanol**¹⁹: ¹H NMR (CDCl₃) δ (ppm) 2.31 (s, 1H), 2.80-2.87 (m, 1H), 3.15-3.20 (m, 1H), 4.0-4.05(m, 1H), 4.15-4.21 (m, 1H), 7.50-7.55 (m, 3H), 7.62-7.65 (m, 2H) ¹³C NMR (CDCl₃) δ (ppm) 142.69, 130.7, 129.1, 123.6, 59.0, 55.8

Spectral data of Alcohol oxidation products

1. **Benzaldehyde**²⁰: ¹H NMR (CDCl₃) δ (ppm) 10.13 (s, 1H), 7.91 (d, 2H), 7.63 (m, 1H), 7.50 (m, 2H); ¹³C NMR (CDCl₃) δ (ppm) 192.3, 136.0, 134.0, 130.2, 129.5.
2. **4-methoxy benzaldehyde**²¹: ¹H NMR (CDCl₃) δ (ppm) 9.80 (s, 1H), 7.77 (d, 2H), 7.01 (d, 2H), 3.80 (s, 3H); ¹³C NMR (CDCl₃) δ (ppm) 190.6, 164.4, 131.5, 129.8, 114.1, 55.4
3. **4-methyl benzaldehyde**²¹: ¹H NMR (CDCl₃) δ (ppm) 9.98 (s, 1H), 7.73 (d, 2H), 7.31 (d, 2H), 2.40 (s, 3H); ¹³C NMR (CDCl₃) δ (ppm) 192.1, 145.4, 134.0, 129.7, 129.6, 21.9
4. **4-bromo benzaldehyde**²¹: ¹H NMR (CDCl₃) δ (ppm) 9.97 (s, 1H), 7.76 (d, 2H), 7.66 (d, 2H); ¹³C NMR (CDCl₃) δ (ppm) 191.1, 135.2, 132.2, 130.9, 129.6

5. **2-methoxy benzaldehyde**²¹: ¹H NMR (CDCl₃) δ (ppm) 10.45 (s, 1H), 7.80 (dd, 1H), 7.56 (td, 1H), 7.00-6.97 (m, 2H), 3.92 (s, 3H); ¹³C NMR (CDCl₃) δ (ppm) 188.9, 161.4, 136.1, 128.4, 124.5, 120.5, 111.3, 55.8
6. **2,2-dimethyl-1-phenyl-1-propanone**²²: ¹H NMR (CDCl₃) δ (ppm) 7.57 (d, 2H), 7.20-7.48 (m, 3H), 1.25 (s, 9H); ¹³C NMR (CDCl₃) δ (ppm) 209.8, 138.4, 131.0, 127.3, 127.61, 44.7, 28.3
7. **4-nitro benzaldehyde**²³: ¹H NMR (CDCl₃) δ (ppm) 10.16 (s, 1H), 8.39 (d, 2H), 8.07 (d, 2H); ¹³C NMR (CDCl₃) δ (ppm) 192.4, 154.0, 143.7, 130.2, 124.1
8. **4-chloro benzaldehyde**²⁰: ¹H NMR (CDCl₃) δ (ppm) 10.14 (s, 1H), 7.80 (d, 2H), 7.63 (d, 2H); ¹³C NMR (CDCl₃) δ (ppm) 191.1, 141.0, 134.6, 131.3, 129.9.
9. **1,2-diphenylethane-1,2-dione**²⁴: ¹H NMR (CDCl₃) δ (ppm) 7.92 (d, 4H), 7.65-7.70 (m, 2H), 7.50-7.54 (m, 4H); ¹³C NMR (CDCl₃) δ (ppm) 194.6, 134.5, 132.9, 130.0, 128.8
10. **Acetophenone**: ¹H NMR (CDCl₃) δ (ppm) 2.15 (s, 6H); ¹³C NMR (CDCl₃) δ (ppm) 206.9, 31.1
11. **Benzophenone**²²: ¹H NMR (CDCl₃) δ (ppm) 7.85 (d, 4H), 7.73 (m, 2H), 7.53 (m, 4H); ¹³C NMR (CDCl₃) δ (ppm) 196.8, 138.1, 132.2, 129.9, 128.1.

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