Fe₃O₄-boosted MWCNT as an efficient sustainable catalyst for PET glycolysis

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Supplementary Materials

1. Identification of the main glycolysis product

UV-Visible Absorption Spectroscopy

Initially, UV-Visible analysis was carried out to identify the generated glycolysis product. The UV-Vis absorption spectrum (Fig. S1(a)) exhibits a single sharp peak at 298 nm, which corresponds to the λ_{max} of the generated product. The resemblance between the λ_{max} of BHET and the generated product emphasizes that the generated product is BHET.
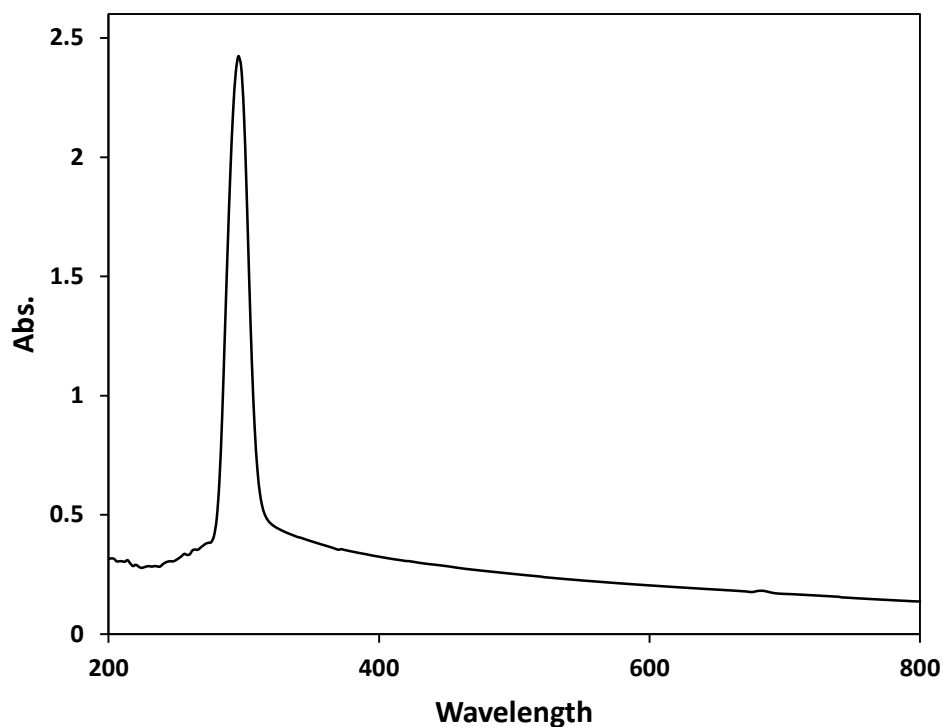

Figure S1 (a). UV-Vis absorption spectrum of the main glycolysis product.

Raman

The generated glycolysis product was analyzed using Raman spectroscopy and the resultant spectrum is presented in Fig. S1(b). The bands appear at 3440 and 1125 cm^{-1} are assigned to the terminal hydroxyl group while that appears at 1719 cm^{-1} is assigned to C=O stretching vibration. The bands appear at 2881, 2931 and 2964 cm^{-1} are assigned to CH stretching vibration of the alkyl group while the band appears at 3095 cm^{-1} is assigned to the aromatic CH stretching. The bands appear at 1612, 1455 and 1382 cm^{-1}, correspond to the aromatic C=C stretching, aromatic C−C stretching and CH$_2$ wagging, respectively. The aromatic C−H in plane bending and C−O stretching vibrations appear at 1127 cm^{-1} while the alkyl C−C stretching appears at 1017 cm^{-1}. The bands appear at 906, 847, 709 and 633 cm^{-1} are assigned to CH$_2$ rocking, C−O stretching vibration, aromatic C−H out of plane bending and aromatic C−C−C in plane bending, respectively.
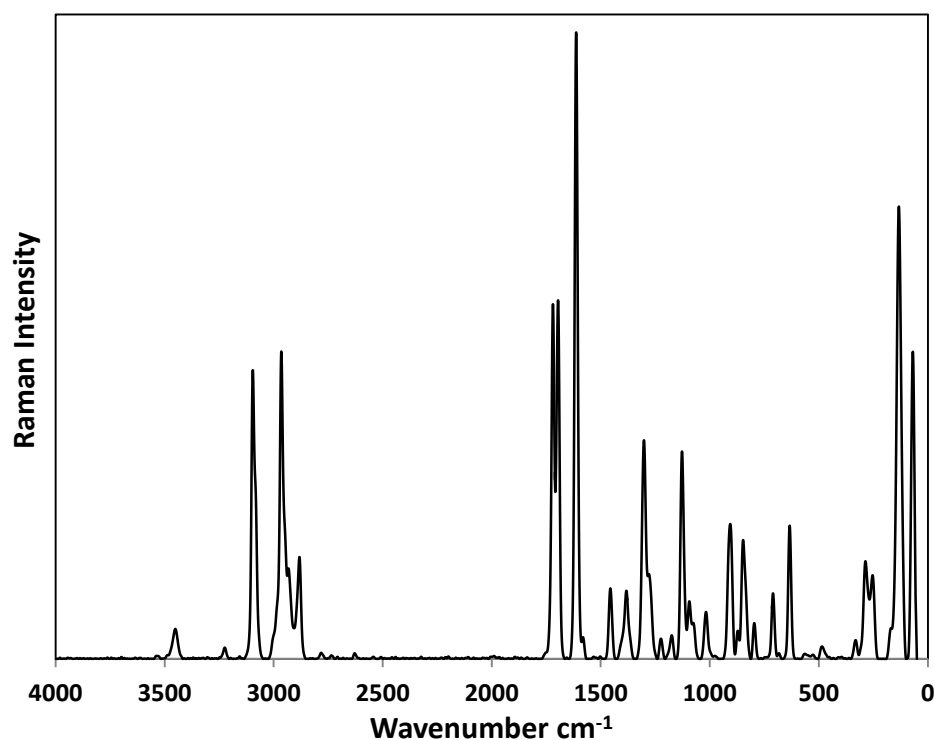

Figure S1 (b). Raman spectrum of the main glycolysis product.

TGA and DSC analyses

To proceed with the identification of the generated glycolysis product, thermal analyses including TGA and DSC analyses were carried out as shown in Fig. S1(c). The presence of an intense peak at 109.16°C in the DSC curve that corresponds to the melting

temperature of the sample indicates that the generated product has the correct melting temperature for BHET. Thus, it can be concluded that the generated glycolysis product is the desired monomer (BHET). The TGA curve of the generated glycolysis product exhibits two weight losses, which resemble those of BHET where its TGA curve possess two weight losses, the first corresponds to its decomposition while the other corresponds to the decomposition of the polymer generated through thermal analysis.[1]
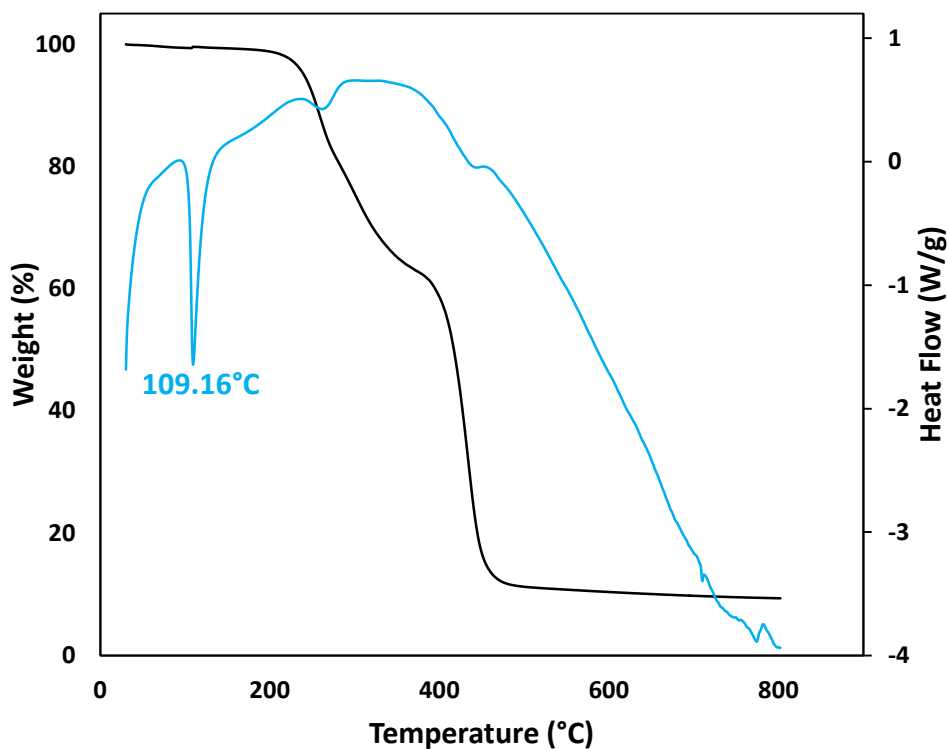

Figure S1 (c). TGA and DSC curves of the main glycolysis product

Mass spectroscopy

The generated glycolysis product was analyzed using EI–MS and the data show that the molecular weight of the glycolysis product resembles that of BHET (254 g mole^{-1}) as shown in Fig. S1(d).
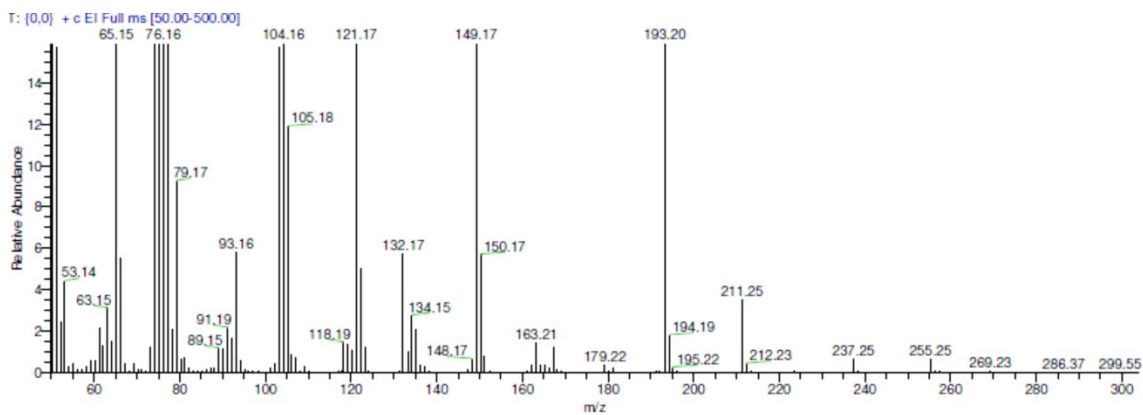
Figure S1 (d). EI-MS spectrum of the main glycolysis product
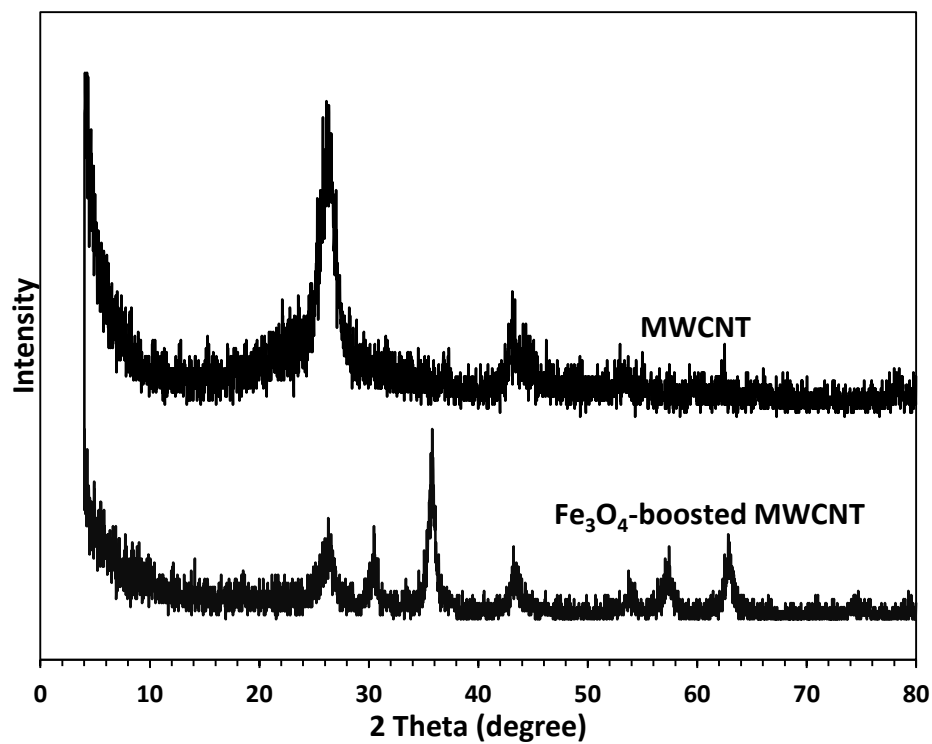
2. Catalyst characterizations

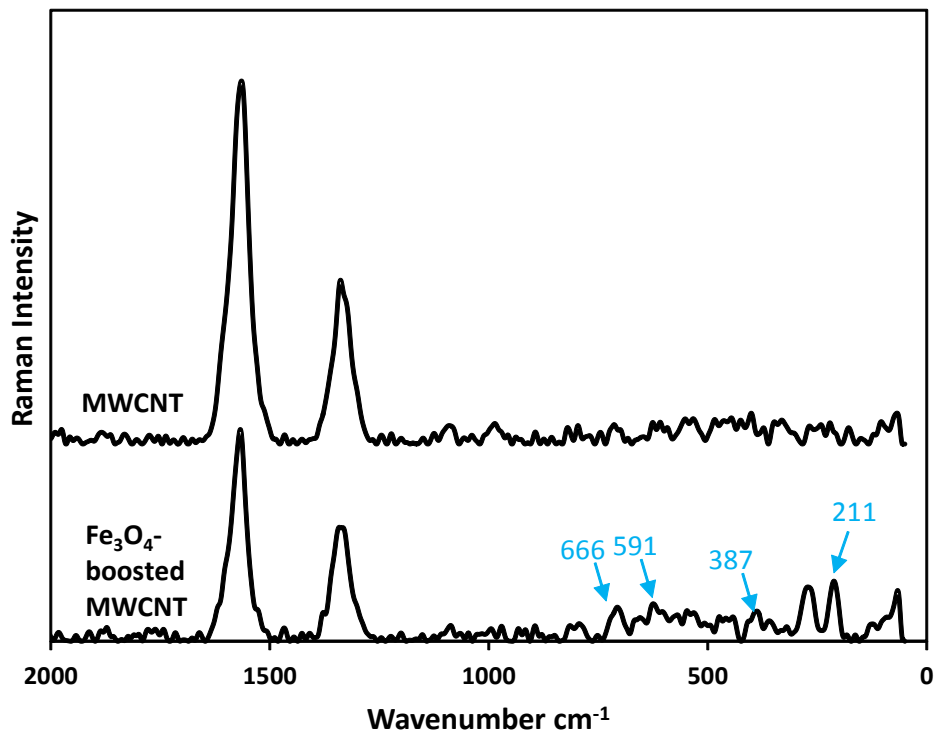Figure S2. XRD patterns of MWCNT and Fe_3O_4-boosted MWCNT.

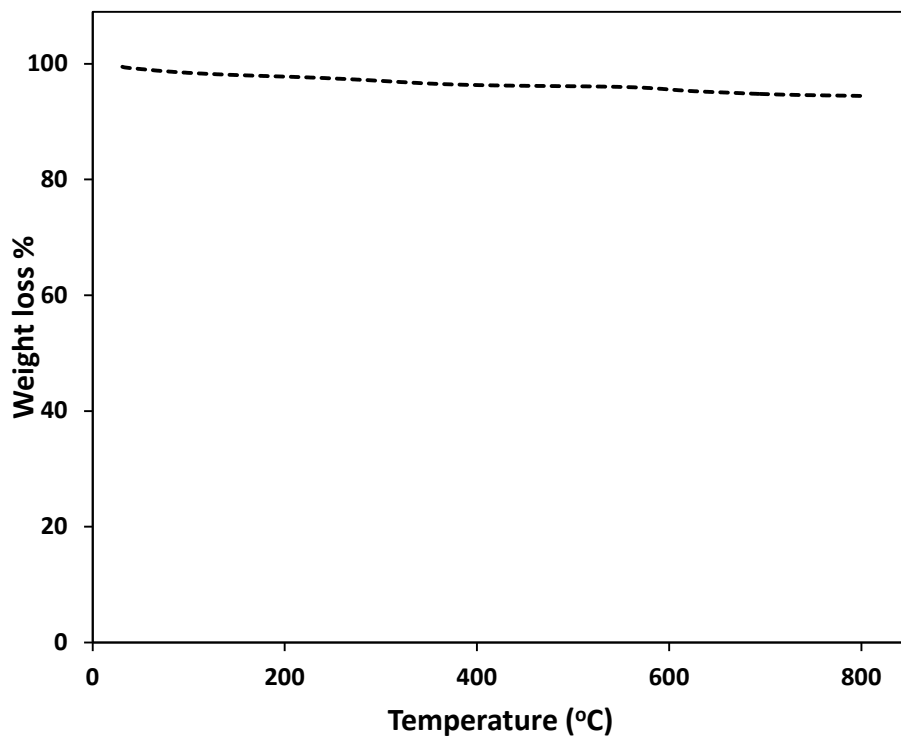Figure S3. Raman spectra of MWCNT and Fe_3O_4-boosted MWCNT.
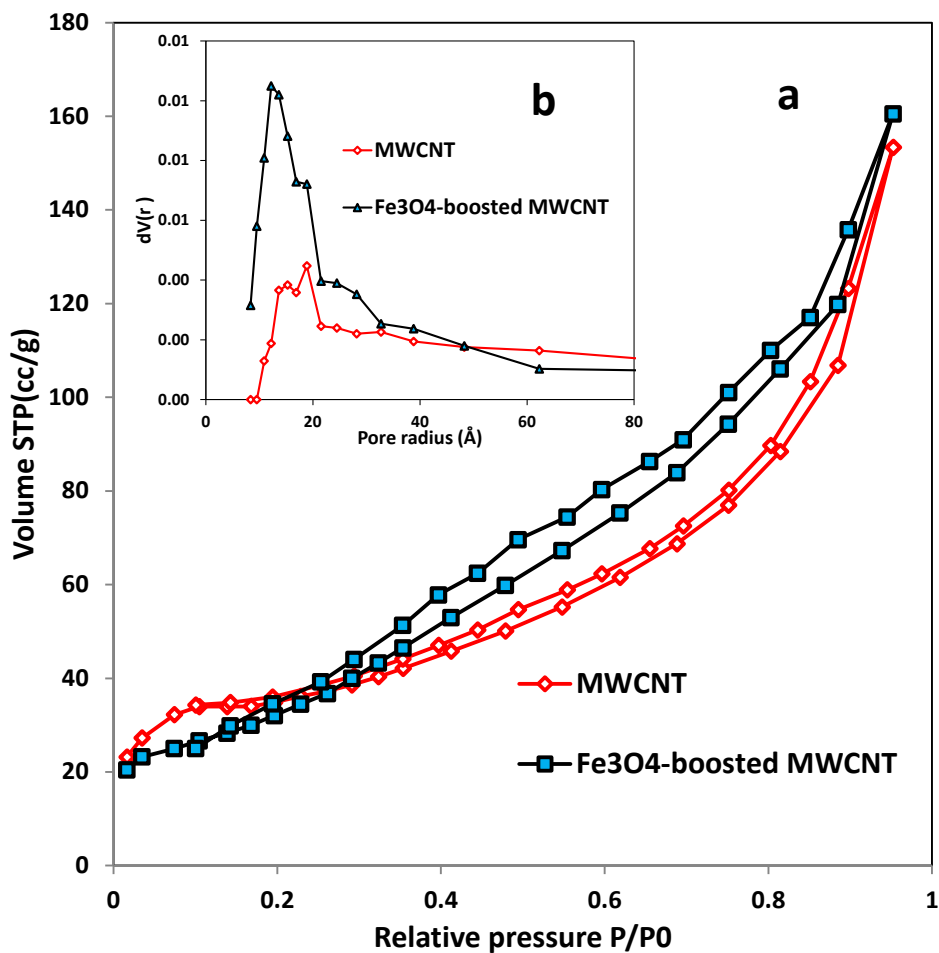

Figure S4. TGA curve of Fe_3O_4-boosted MWCNT.

Figure. S5. (a) N_2 adsorption-desorption isotherms of MWCNT and Fe_3O_4-boosted MWCNT (b) pore size distribution curves of MWCNT and Fe_3O_4-boosted MWCNT.

References

(1) Chen, C. H. Study of glycolysis of poly (ethylene terephthalate) recycled from postconsumer soft-drink bottles. III. Further investigation. J. Appl. Polym. Sci. **2003**, 87, 2004-2010.