

Supplementary file

Graphene oxide supported highly porous TiO₂ nano leaflets for ultrafast adsorption and photochemical decomposition of 2,4,6-trinitrotoluene from water

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Journal: New Journal of chemistry

1. Synthesis of reduced Graphene Oxide (rGO) Nanosheets:

Graphite oxide (GO) was synthesized using a modified Hummers' process¹ with some modifications. Graphite (G) powder (6 g) was treated with a mixture of 98% concentrated sulphuric acid (130 mL) and 70% concentrated nitric acid (6 mL) in a round bottom flask under continuous magnetic stirring in an ice bath. The temperature of the solution was maintained below 5 °C for 5 hours. Eighteen grams of potassium permanganate (KMnO₄) was added gradually maintaining the temperature of solution. After complete addition of KMnO₄, the solution was continuously stirred for 24 h at room temperature. Then, distilled water (140 mL) was added to the above mixture and the temperature of the solution was maintained below 80 °C. After 15 min, the above mixture was diluted with 450 mL of distilled water and filtered. Two hundred milliliters of 20% HNO₃ was added and heated to 80 °C for 30 min. The resulting suspension was washed and centrifuged at 4000 rpm repeatedly till the pH of the solution reached ~ 7. The product was dried in an

oven at 60 °C for 8 h. The synthesized graphite oxide was exfoliated to reduced graphene oxide nanosheets (rGO) by heat treatment at 300 °C under atmospheric pressure.

2. BET and BJH analysis:

Two stages are involved in the application of the BET method.² First, it is necessary to transform a physisorption isotherm into the ‘BET plot’ and from it derive a value of the BET monolayer capacity, n_m . In the second stage, the BET-area, A_s (BET), is calculated from n_m by adopting an appropriate value of the molecular cross-sectional area, σ . The BET equation in the linear form

(1)

$$\frac{p/p^0}{n(1-p/p^0)} = \frac{1}{n_m C} + \frac{C-1}{n_m C} \left(\frac{p}{p^0} \right) \quad (1)$$

where p is the equilibrium pressure of the adsorbed gas; p^0 is the saturated vapor pressure of the adsorbed gas; V is the actual (multi-layer) adsorption amount of the sample, cm^3/g ; V_m is the single-layer saturated adsorption amount per unit sandstone mass, cm^3/g ; C is the constant reflecting the adsorption heat.

$$A_s = \left(\frac{V_m N a_m}{22400} \right) 10^{-1} \quad (2)$$

The specific surface area is shown in the above (**Equation 2**): where A_s is the multi-point BET-specific surface area, m^2/g ; V_m is as described above; N is Avogadro's constant, 6.022×10^{23} ; a_m is the cross-sectional area of a single nitrogen molecule, the adsorption layer is a hexagonal close-packed structure, the nitrogen molecules are considered spherical, at 77.3 K.

The pore size distribution of the low-temperature nitrogen adsorption method is usually calculated by the BJH method based on the Kelvin equation (**equation 3**).³

$$\ln \frac{p}{p^o} = -2\gamma \frac{v \cos \theta}{r_k RT} \quad (3)$$

where p/p^o is the equilibrium pressure over the saturated vapor pressure of the adsorbed gas; \tilde{v} is the mole volume of the liquid nitrogen; γ is the interfacial tension of the liquid nitrogen.

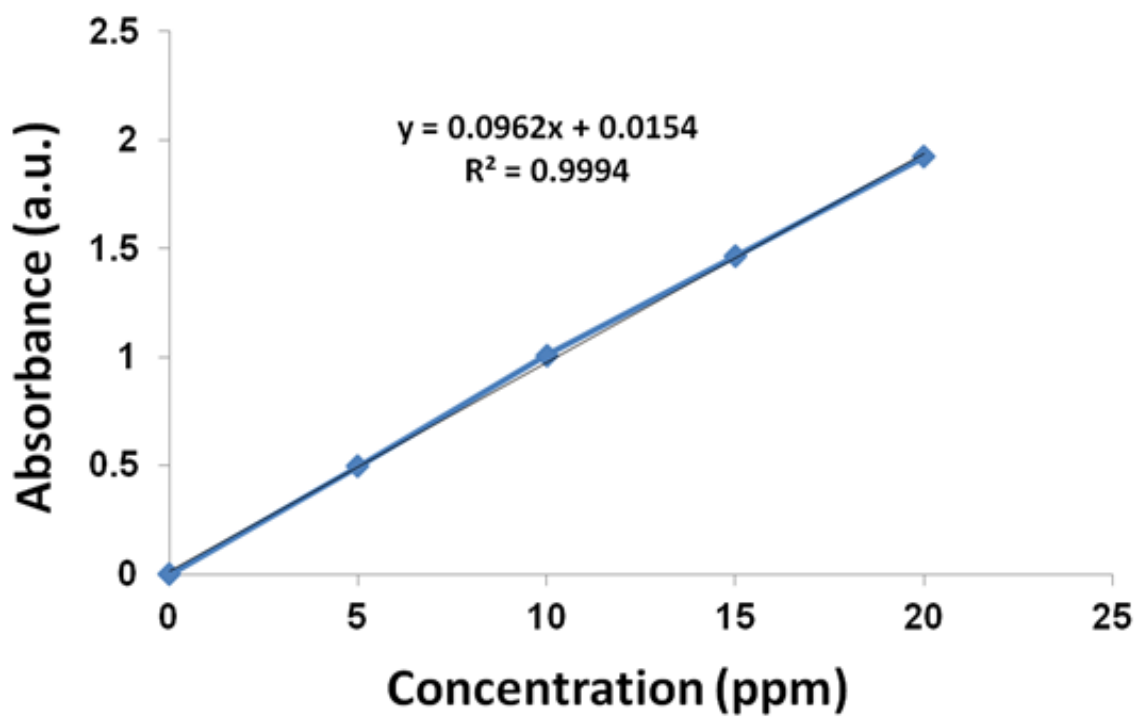


Fig. S1. Calibration curve for 2,4,6-trinitrotoluene.

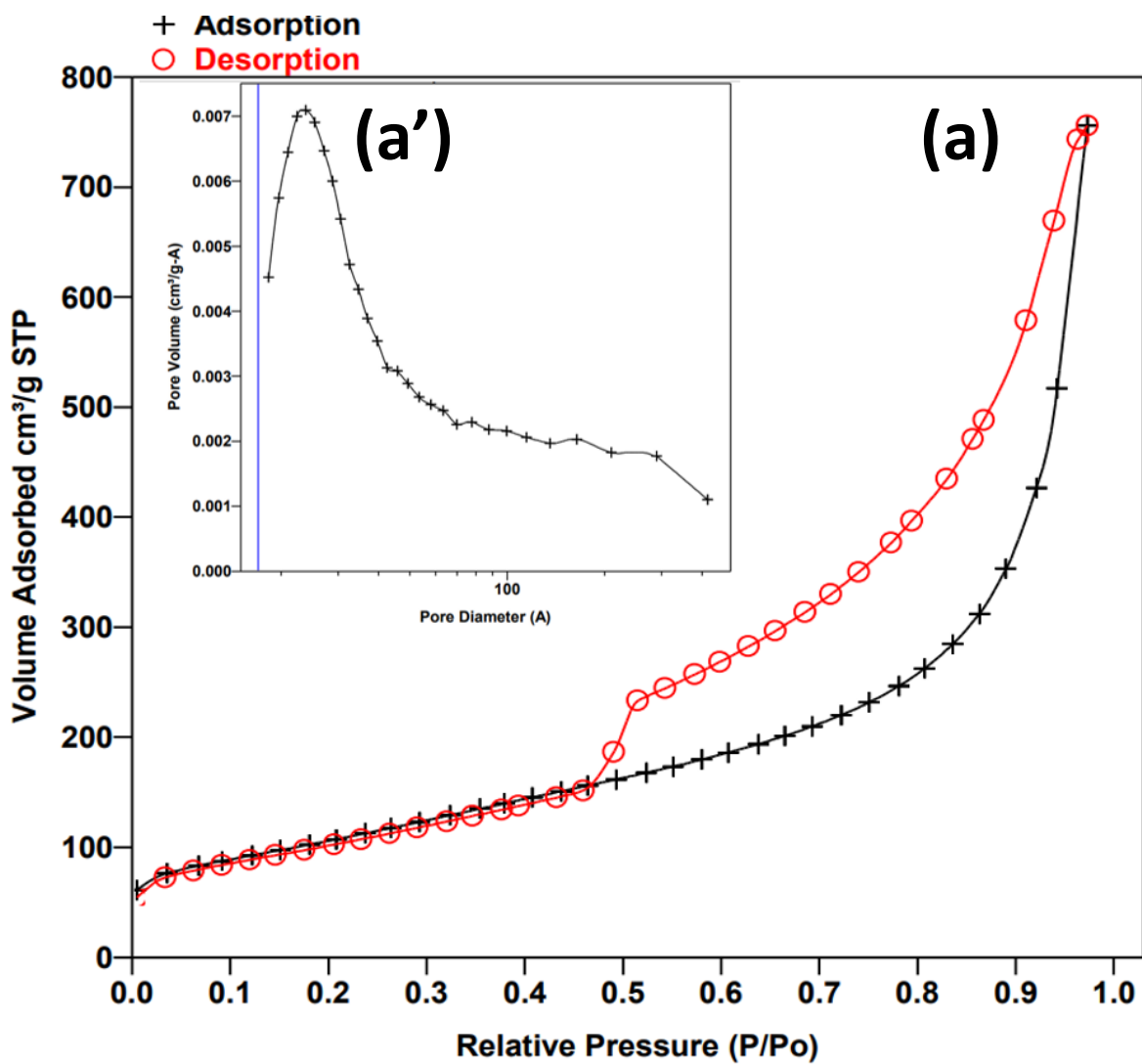


Fig. S2a. (a) BET adsorption isotherm and inset (a') BJH pore distribution curve of rGO

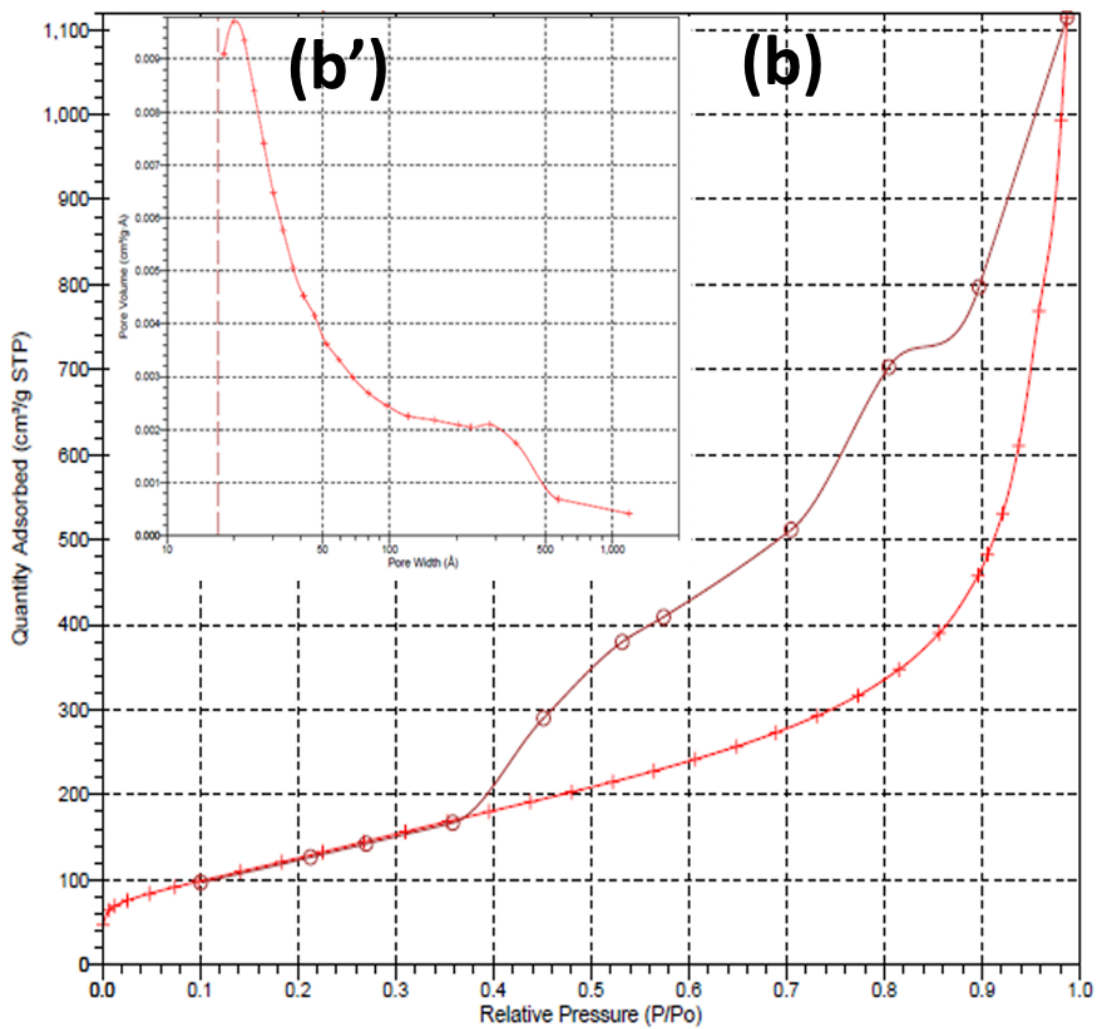


Fig. S2.b. (b) BET adsorption isotherm and inset (b') BJH pore distribution curve of TGO

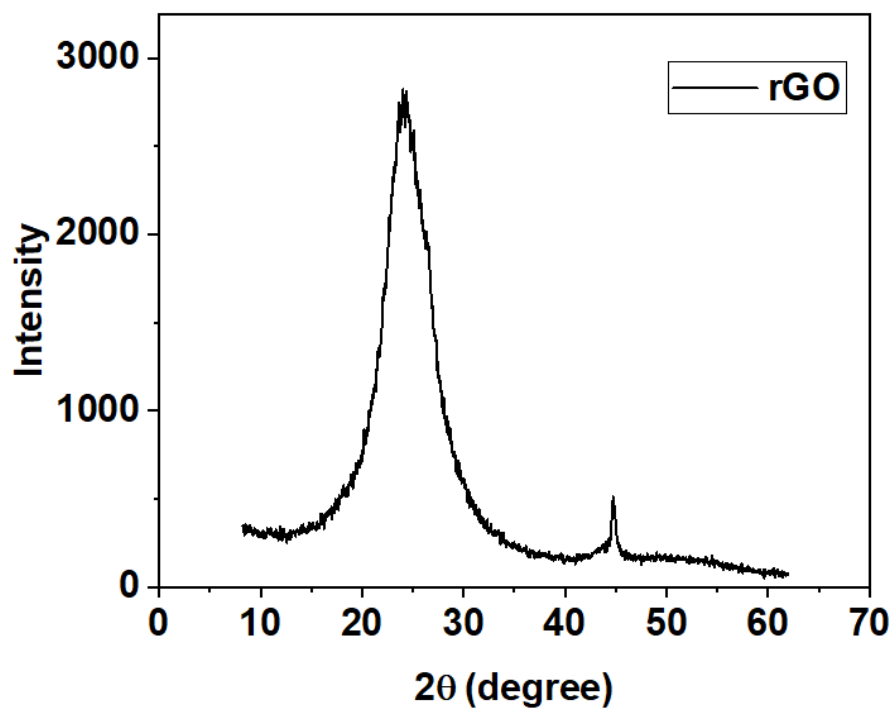


Fig. S3. X-Ray Diffraction of reduced graphene oxide (rGO)

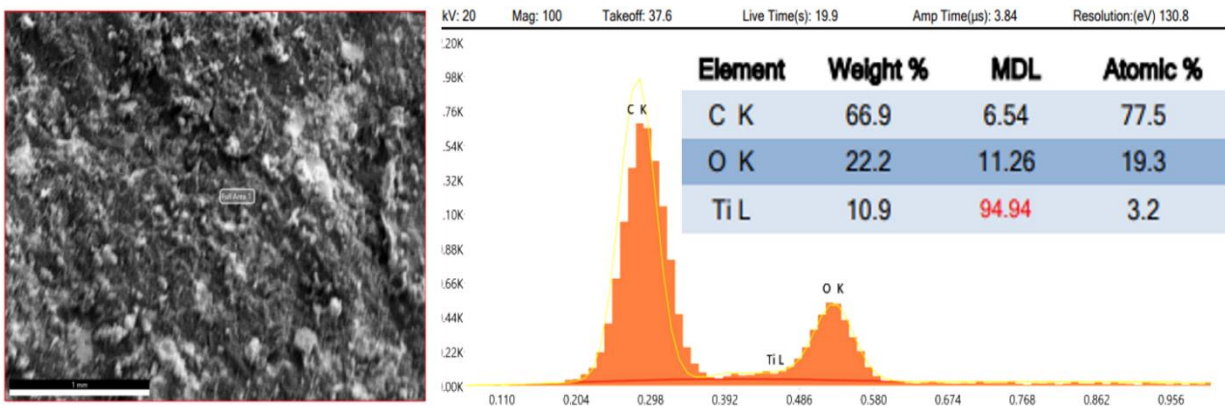


Fig S4. EDAX analysis of TGO

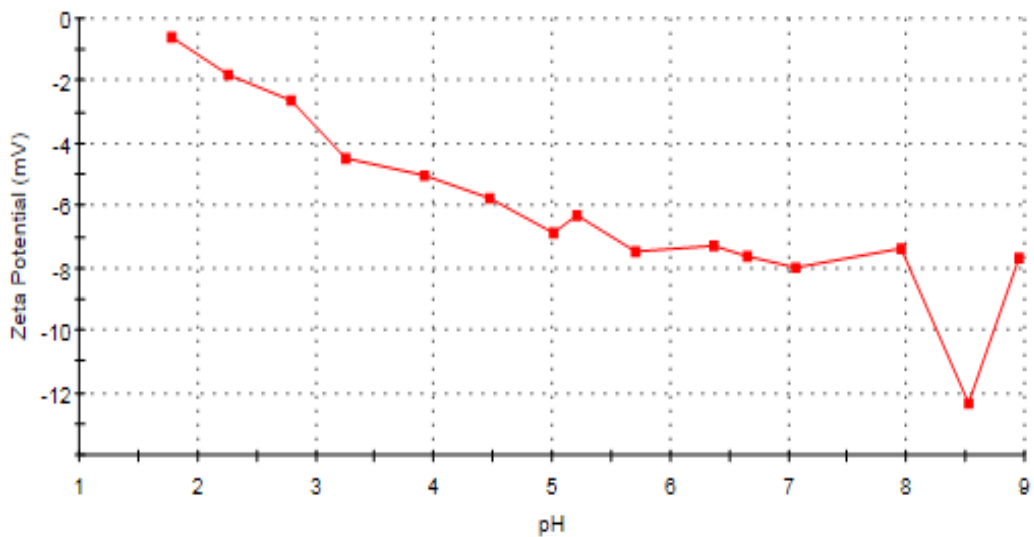


Fig. S5a. Zetapotential plot for reduced graphene oxide (rGO)

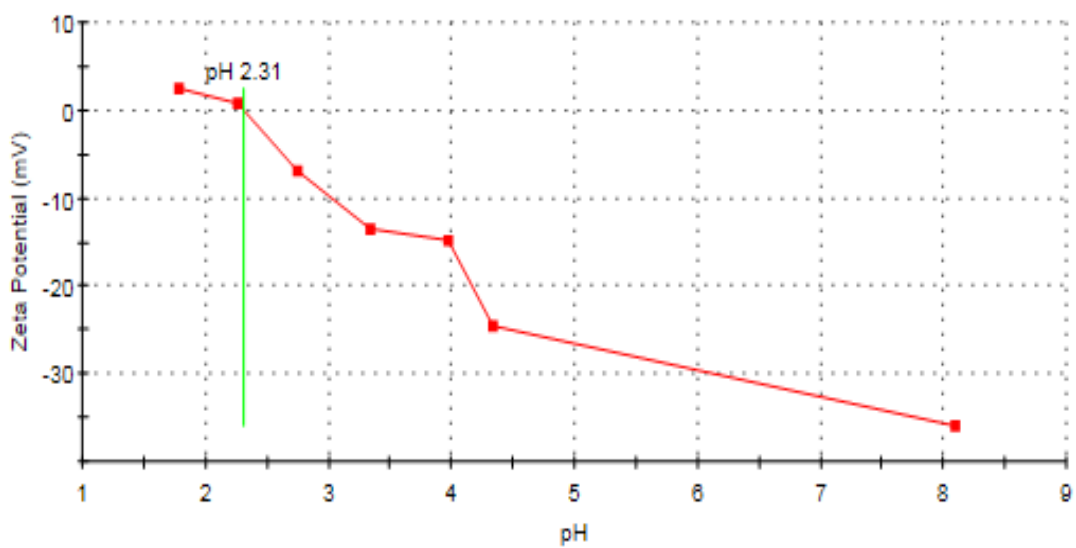


Fig. S5b. Zetapotential plot for TGO

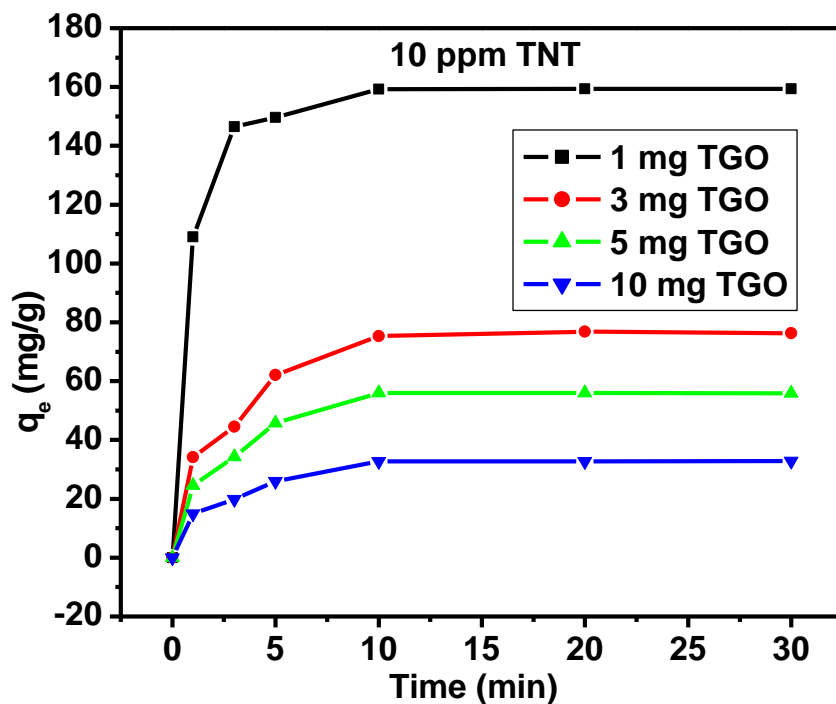


Fig. S6: Effect of doses of composite (TGO) for removal of 2,4,6-Trinitrotoluene (TNT).

References:

- 1 S. Hummers, R. E. Offeman, Preparation of graphitic oxide. *Journal of the American Chemical Society*, 1958, **80**, 1339.
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