

Supporting Information Cover Sheet

Influence of the Surface Structure of Graphene Oxide on the Adsorption of Aromatic Organic Compounds from Water

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Text S1 The procedure of Boehm titration of GO ^{R1}.

Boehm titration method ^{R1} has been carried out to determine the amount surface oxygen-containing groups on GO.

Before the titration, GO underwent pretreatments to protonate all the neutralizable groups. Sufficient amount of GO sample was dispersed and equilibrated with excess 0.1 mol dm⁻³ HCl for 2 days, then thoroughly washed with deionized water to remove HCl, and vacuum dried in 333 K for 48 hours. Three protonated GO samples, each 0.2 g, was mixed with 100 cm³ of 0.02 mol dm⁻³ NaOH, 50 cm³ of 0.01 mol dm⁻³ Na₂CO₃ and 50 cm³ of 0.01 mol dm⁻³ NaHCO₃, respectively. The mixtures were shaken for 24 hours and then centrifuged at 10000 rpm for 10 min, followed by filtration using 0.22 micron filters to remove the GOs. 15 cm³ of the filtrate was mixed with 15 cm³ 0.02 mol dm⁻³ HCl and the excess acid was titrated with 0.01 mol dm⁻³ NaOH, using a pH meter as reference. Surface acidity was calculated based on the assumption that NaHCO₃ neutralizes carboxyl groups only, Na₂CO₃ neutralizes carboxyl and lactonic groups, and NaOH neutralizes all acidic groups including carboxyl, lactonic, and phenolic groups. Blank experiments without GO were also carried out for all experimental conditions.

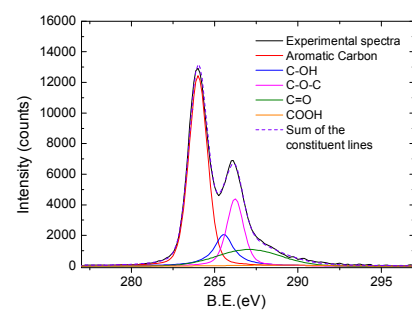
Text S2 The procedure of surface area determination by methylene blue titration^{R2}.

This method is based on the principle and methods proposed by Pedro Montes-Navajas et al^{R2}. In the experiment, about 3 mg of GO sample was carefully weighted and fully dispersed in 100 cm³ of deionized water. The mixture was titrated using 50 mg dm⁻³ methylene blue solution. The terminal was set at the point when clear gree-blue aggregates formed and the supernatant was colorless. Then the surface area of the GO samples was calculated according to the following equation,

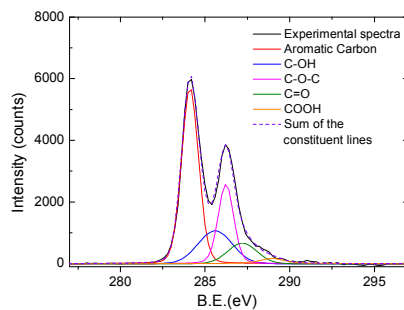
$$A = \frac{CV}{m} \times A_{MB} \quad (S1)$$

Where A (m² g⁻¹) is the surface area of a GO sample; C (mg dm⁻³) is the concentration of the methylene blue solution; V (cm³) is the volume of the methylene blue solution; m (mg) is the mass of the GO sample, and A_{MB} (m² mg⁻¹) is the cover area of 1 mg of methylene blue molecules which is 2.54 m² mg⁻¹.

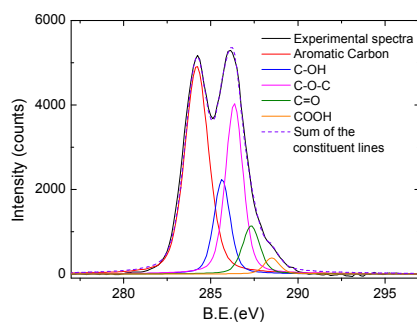
For lowly-oxidized GO samples, the titration results not directly available as the terminal point is very difficult to determine. It was roughly deduced by the methylene blue uptake of the GO sample with the terminal uptake of a GO sample with a known surface area.



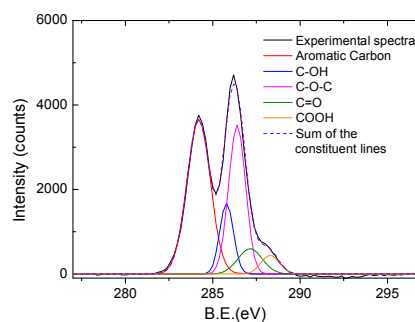
(a)



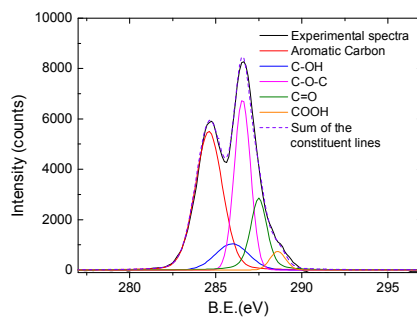
(b)



(c)



(d)



(e)

Fig. S1 Line shape analysis for the C1s XPS spectra of GO1 (a), GO2 (b), GO3 (c), GO4 (d), and GO5 (e). The dashed line in each figure indicates the composite curve of the constituent lines shown by thin solid lines.

Reference

- (R1) Boehm, H. P. Some Aspects of the Surface Chemistry of Carbon Blacks and Other Carbons. *Carbon* **1994**, 32(5), 759-769.
- (R2) Montes-Navajas, P.; Asenjo, N. G.; Santamaría, R.; Menéndez, R.; Corma, A.; García, H. Surface Area Measurement of Graphene Oxide in Aqueous Solutions. *Langmuir* **2013**, 29(44), 13443-13448.