

Supplementary information to:

Repurposing waste plastic into a sustainable adsorbent for removing aromatic dye: Experimental, optimization and theoretical modeling

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1. Techniques used for characterization

To determine which functional groups are included in synthesized activated carbon that has been produced, using a JASCO FT/IR-6100 spectrometer, Fourier Transform Infrared Spectroscopy (FTIR) was used with KBr pellets in the 4000–400 cm⁻¹ range. Nitrogen adsorption–desorption techniques were applied to characterize specific surface area and porosity, using equipment manufactured by Quantachrome. The crystallinity and structural ordering of the activated carbon was analyzed through XRD (X-ray diffraction) that was performed with a Siemens D-500 diffractometer with $\lambda = 1.54 \text{ \AA}$, Cu K α radiation. Morphological and surface features of synthesized activated carbon were examined by means of field emission scanning electron microscopy (FESEM) with a JEM-2100F instrument operating at 200 kV. Additionally, (XPS) X-ray photoelectron spectroscopy was carried out to analyze the surface elemental structure as well as binding energies of the activated carbon.

2. Batch experiments of adsorption

Batch adsorption experiments were conducted using capped bottles at ambient temperature to evaluate the influence of various parameters on the adsorption process, as well as to study the kinetics, isotherms, and thermodynamic behavior of BG dye removal. In each experiment, a known volume of BG dye solution was prepared and adjusted to the desired pH using appropriate concentrations. A known amount of activated carbon was then incorporated into the solution, and the mixtures were shaken in a thermostatic shaker at 250 rpm for 120 minutes. After reaching equilibrium, the suspensions were centrifuged, while the concentration of dye remaining in the solution was quantified by means of UV–

Vis spectroscopy at a wavelength of 625 nm, representing concentration at equilibrium (C_e). Every experiment was conducted in triplicate to guarantee reproducibility. The impact of essential parameters as contact time (ranging from 0 to 120 minutes), temperature (298–328 K), initial concentration of dye (3–30 ppm), pH from 3 to 11, and adsorbent dosage (20–100 mg) was systematically examined. Capacity of adsorption at a given time (q_t , mg/g) as well as removal percentage of dye (%R) were determined using standard adsorption equations.

$$q_t = \frac{(C_0 - C_e)}{W} \times V \quad (1)$$

$$\%R = \frac{(C_0 - C_e)}{C_0} \times 100 \quad (2)$$

In which V is the volume of BG dye solution (L), w is the amount of adsorbent utilized (g), and C_0 and C_e are the concentrations of BG dye (mg L^{-1}) initially and at equilibrium.

3. Determining the mean pore radius of AC

The mean pore radius (\bar{r}_p) of AC was estimated using the following equation based on BET surface area and total pore volume.

$$\bar{r}_p (\text{\AA}) = (2V_p \times 10^4) / S_{\text{BET}}$$

where V_p is the total pore volume (ml g^{-1}), S_{BET} is the BET surface area ($\text{m}^2 \text{ g}^{-1}$), the factor 10^4 is used for unit conversion to obtain the pore radius in angstrom (\AA).

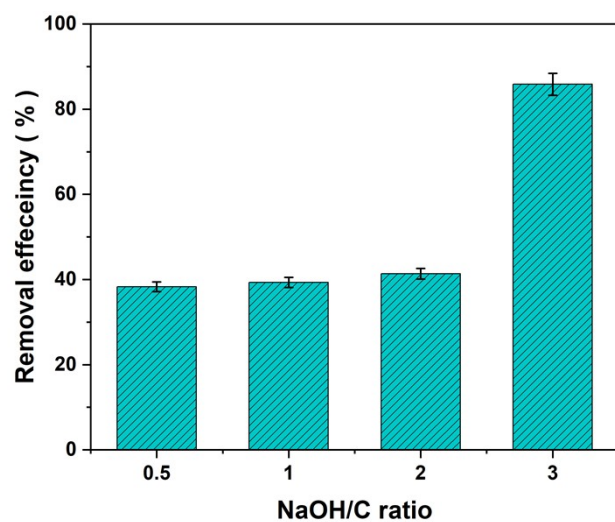


Figure S1. Effect of NaOH/C ratio on the performance of activated carbon toward adsorption of BG dye

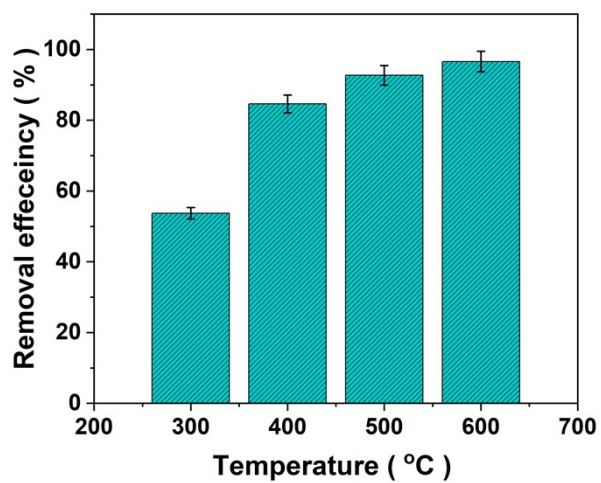


Figure S2. Effect of burning temperature on the performance of activated carbon toward adsorption of BG dye

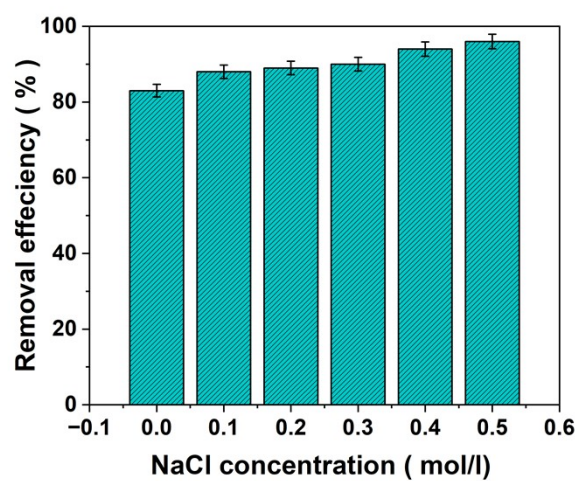


Figure S3: Effect of ionic strength on the adsorption of BG onto activated carbon