Supplementary Information (SI) for RSC Advances.

Supporting Information

1,2,4-Oxadiazolyl Phenoxyacetic Acid-Modified Algae-Derived Biochar for Efficient o-Nitrophenol Removal: Adsorption Performance and Mechanistic Insights

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Table S1. Equations of the applied adsorption isotherm models

Model	Equation
Langmuir	$\frac{C_e}{q_e} = \frac{1}{K_L\, q_{max}} + \frac{C_e}{q_{max}}$ (1)
Freundlich	$\ln q_e = \ln K_f + \frac{1}{n} \ln C_e$ (2)
Temkin	$q_e = B\, lnK_T + B \ln C_e$ (3)
DR	$Ln\, q_e = Ln\, q_s - K_{DR}\varepsilon^2$, $\varepsilon = RT\, Ln\left(1 + \frac{1}{C_e}\right)$ (4, 5)

Where, q_e and C_e are the adsorption capacity and the concentration of the un-adsorbed *o*-NP at equilibrium, respectively. q_{max} and K_L are the monolayer adsorption capacity and Langmuir constant, respectively. n and K_f are Freundlich constants. K_T is the equilibrium binding constant and $B = \frac{RT}{b}$, b is Temkin constant related to heat of adsorption. R is the gas constant (8.314 J/mol.k) and T is the absolute temperature. Q_s is the saturation capacity, ε is the Polanyi potential and K_{DR} is a constant related to the mean free energy of adsorption per mole of the adsorbate.

Table S2. Equations of the applied adsorption kinetic models

Kinetic Model	Equation	
Pseudo−First order	$\ln{(q_e - q_t)} = \ln{q_e} - (\frac{k_1}{2.303})t$	(6)
Pseudo−Second order	${}^{t}/_{q_t} = {}^{1}/_{k_2 q_e^2} + {}^{1}/_{q_e}(t)$	(7)
Elovich model	$q_t = \frac{1}{\beta} ln\,(\alpha\beta) + \frac{1}{\beta} \ln{(t)}$	(8)

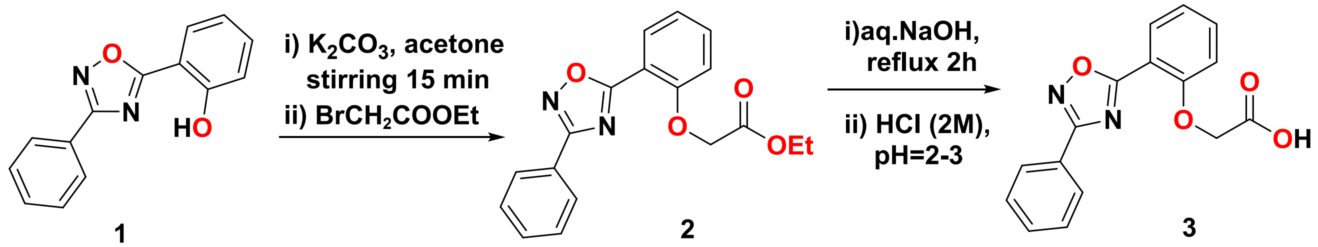
Where, q_t and q_e are amounts of adsorbed *o*-NP at time t and equilibrium, respectively. k_1 and k_2 are the rate constants of Pseudo first order and Pseudo second order, respectively. α and β are Elovich coefficients that represent the initial adsorption rate and the desorption coefficient, respectively, also related to the extent of surface coverage and activation energy for chemisorption.

Text S1. The used materials in the fabrication of POPA@A-BC$_{0.5}$ composite.

Materials and equipment

Chemicals were purchased and used without further purification; NMR spectra were measured using a JEOLJNM ECA 500. All chemical shifts (δ) are stated in units of (ppm) and presented using TMS as the standard reference point. Melting points were recorded using Thermo Scientific, Model NO: 1002D,220-240v; 200 W; 50/60 Hz and are uncorrected. Reaction time was monitored by TLC on Merck silica gel aluminum cards (0.2 mm thickness) with a fluorescent indicator at 254 nm. Visualization of the TLC during monitoring of the reaction was done by UV VILBERLOURMAT 4w-365 nm or 254 nm tube.

Text S2. The synthesis of POPA



Ethyl 2-(2-(3-phenyl-1,2,4-oxadiazol-5-yl)phenoxy)acetate 2

A mixture of 2-(3-phenyl-1,2,4-oxadiazol-5-yl)phenol **1** (1.0 g, 4.20 mmol) and anhydrous potassium carbonate (2.0 g, 14.49 mmol) in dry acetone (20 mL) was stirred 15 minutes, followed by addition of ethyl bromoacetate (1.05 g, 6.30 mmol). The reaction mixture was refluxed for 3 hours, then allowed to cool, and poured onto crushed ice (100 mL). The crude residue was filtered off and recrystallized with absolute ethanol to give **2** as colorless crystals; yield (91 %); m.p= 105 - 108 ºC; IR ν_{max}/cm^{-1}:, 3072, 2984, 1740 (C=O),1595 (**C=N**); ^1H NMR (500 MHz, DMSO-d6) δH: 8.06 (s, 3H, Ar-H), 7.62 – 7.56 (m, 4H, Ar-H), 7.18 (d, 2H, J = 8.0 Hz, Ar-H), 5.00 (s, 2H, ArOCH2), 4.15 – 4.10 (m, 2H, CH_3CH_2O), 1.19 – 1.14 (m, 3H, CH_3CH_2O); ^{13}C NMR (125 MHz, DMSO-d6) δC: 175.3 (O-C=N), 168.8 (O-C=O), 168.1 (N-C=N), 157.1, 135.1, 132.1, 131.9, 129.8, 127.6, 126.8, 122.2, 114.5, 113.3 (Ar-C), 65.8 (O-CH_2-CO), 61.3 (CH_3CH_2O), 14.4 (CH_3)

2-(2-(3-Phenyl-1,2,4-oxadiazol-5-yl)phenoxy)acetic acid 3

Ethyl ester (**2**) was subjected to base hydrolysis by refluxing with 1 M sodium hydroxide (NaOH) in a round-bottom flask at 60-70°C for 2-4 hours. The reaction progress was monitored by thin-layer chromatography (TLC). After cooling, the mixture was acidified with 1 M hydrochloric acid (HCl) to pH < 2 to convert the carboxylate anion to the carboxylic acid. The carboxylic acid was extracted into ethyl acetate, washed with water, dried over sodium sulfate, and filtered. The solvent was removed under reduced pressure using a rotary evaporator, and the crude product was purified by column chromatography and crystallized from THF to give **3** as off white solid (76 % yield); m.p = 171-173 °C; $R_F = 0.30$ (Ethyl acetate: n-hexane: Methanol, 1: 2: 0.5); IR (KBr) $\nu_{max}/(cm^{-1})$: 3477 (**OH**), 1748 (**C=O**), 1601 (**C=N**). ^1H NMR (500 MHz, DMSO-d_6) δ_H: 13.19 (bs, 1 H, O**H**), 8.06 (d, 3H, J = 7.5 Hz, Ar-**H**), 7.63-7.56 (m, 4H, Ar-**H**), 7.17-7.16 (m, 2H, Ar-**H**), 4.91 (s, 2H, O-C**H₂**). ^{13}C NMR (125 MHz, DMSO-d_6) δ_C: 175.5, 170.3, 168.1, 157.3, 135.1, 132.1, 131.9, 129.8, 127.6, 126.8, 122.0, 114.3, 113.2, 65.7