**Supporting Information**

**Self-Nitrogen doped carbons aerogel derived from waste cigarette butts (cellulose acetate) for the adsorption of BPA: Kinetics and adsorption mechanisms**

**1. Characterization**

The Fourier transform-infrared spectroscopy (FT-IR) of NDC was used to characterize the functional groups and recorded on Bruker Tensor 27 spectrophotometer in the range of 4000–400 cm−1 with KBr pellet technique. The thermogravimetric (TG) analysis was investigated on a SDT Q 600 (TA instrument) at heating rate of 10 °C/min. X-Ray diffraction (XRD) analysis of the NDC  was performed using a PANalyticalX'pert Pro MPD diffractometer equipped with a Cu Kα radiation source. Raman spectrum were recorded on a RENISHAW instrument using an Ar laser source of 488 nm. The surface properties of nanocomposite was explored via Brunauer-Emmett-Teller (BET) surface area analyzer using adsorption instrument (Quantachrome Instruments v4.0,USA). The zeta potential of NDs in ultrapure water was measured by a zeta potential analyzer (Zetasizer, Malvern Instruments, Worcestershire, UK, model Nano ZS). Surface morphology was analyzed using scanning electron microscopy (SEM) (JEOL, model JSM 6060). The detail of NDCsurface and interaction was determined using HRTEM (JEM 2010, JEOL, Japan). The surface chemical states of the adsorbents were analyzed using X-ray photoelectron spectroscopy (XPS) performed on on a PHI QuanteraSXM photoelectron spectrometer with Al Kα radiation. Carbon, oxygen, hydrogen, nitrogen and sulfur contents of biochar were analyzed by an Elemental analyzer (Perkin Elmer) through dry combustion. The initial and residual concentrations of the heavy metal ions were determined on an inductive coupled plasma emission spectrometer (ICPE-9000, Shimadzu). Contact angle data was obtained on a Kruss Drop Shape Analysis System-100 (DSA 100), using a sessile water drop method with 5–10 μL liquid drops.

### 2. Adsorption assay

Batch adsorption techniques were used for the adsorption of BPA from aqueous solution using 150 mL conical flasks. The metals stock solution with an initial concentration of 500 mg/L were prepared further diluted in the concentration of 5, 10, 20, 40, 60, 80, 100, 150 and 200 mg L−1 using deionized water. The pH values of the solutions were adjusted to with HNO3and NaOH solutions. Process variables selected in the present study included solution's pH, temperature, contact time and the concentration of BPA. The adsorption capacity (qe) and removal efficiency (R) were calculated according to Eq. (i), (ii), respectively(He et al., 2018; Huang et al., 2018):

$q\_{e}=\frac{\left(C\_{0}-C\_{e}\right)V}{m}$ (i)

$R(\%)=\frac{\left(C\_{0}-C\_{e}\right)100}{C\_{0}}$ (ii)

Where C0 and Ce are the initial and equilibrium concentrations of BPA (mg/L), respectively; V is volume of solution (L), and m is the mass (g) of NDC. Desorption of BPA form the NDC was carried out using methanol solution and the regenerated NDC adsorbent was further used for next cycle.

**3. Adsorption kinetics**

The kinetic studies of adsorption play an important role in understanding the adsorption dynamics and mechanism through the order of the rate constant. Three commonly used kinetics models-pseudo-first-order, pseudo-second-order and intra-particle diffusion model were applied to interpret the kinetics data(Al-Kahtani et al., 2019; Alhokbany et al., 2019; Naushad et al., 2019a). The nonlinear forms of the models are shown as in eq (3-5).

$q\_{t}=q\_{e}-q\_{e}e^{-k\_{1}t}$ (4)

$q\_{t}=\frac{k\_{2}q\_{e}^{2}t}{1+k\_{2}+q\_{e}t}$ (5)

$q\_{t}=K\_{dif}t^{\frac{1}{2}}+C$ (6)

Where qe (mg/g) was the equilibrium adsorption capacity and qt (mg/g) was the time-dependent amount of BPA adsorbed per unit mass of NDC microspheres. k1 (min−1) and k2 (g·(mg·min)−1) were the equilibrium constant of pseudo-first-order and pseudo-second-order models, respectively. Kdif (mg/gmin−1/2) is the intra-particle diffusion rate constant, while C is the boundary layer thickness.

**4. Adsorption Isotherm:**

Three commonly used adsorption isotherms, namely Langmuir, Freundlich, and Temkin, were used(Naushad et al., 2019b; Sharma et al., 2019a; Sharma et al., 2019b), the nonlinear equation of these isotherm shown as shown in equation (6-8):

$q\_{e}=\frac{K\_{L}q\_{max}C\_{e}}{1+ K\_{L}C\_{e}}$ (6)

$q\_{e}=K\_{f}C\_{e}^{\frac{1}{n}}$ (7)

$q\_{e}=\frac{RT}{b\_{t}}lnK\_{t} . C$ (8)

Where qe mg/g) and Ceq(mg/ L) are the adsorption capacity of NDC and the concentration of the BPA at equilibrium; KL(L/g), Langmuir constant related to the adsorption energy, and qm(mg/g) is Langmuir's maximum adsorption capacity KF(mg/g)/(mg/L)1/n,  n (dimensionless) is the Freundlich constant indicative of the sorption intensity and heterogeneity and Kt(L/g) is the Temkin isotherm constant.

**5 Adsorption thermodynamics**

For better understanding the adsorption of BPA on NDC, three thermodynamic parameters, ΔH, ΔS and ΔG are investigated respectively. The thermodynamic parameters are determined by the Van't Hoff equation as below:

$∆G^{o}=-RTlnK\_{d}$ (7)

$∆∆G^{o}=∆H^{o}-T∆S^{o}$ (8)

Where, R (J/mol K) represents the gas constant (8.314), T (K) is adsorption temperature, and Kd is the distribution coefficient for adsorption. The linear fitting by plotting lnKd against 1/T and the ΔH0 and ΔS0 values were calculated from the slope and the respectively.



Figure SF1: (a) N2 adsorption-desorption isotherms for NDC (b) the pore size distributions of NDC



Figure SF2: (a) adsorption mechanism (b) FTIR spectra of NDC after BPA adsorption (b) XRD of NDC after BPA adsorption (d) XPS of the NDC after BPA adsorption

**Table ST 1:** Thermodynamics parameters for the adsorption of BPA over NDC

|  |  |
| --- | --- |
| **Temperature (K)** | **Thermodynamics Parameters** |
| lnKc | ΔS (kJ/mol/k) | ΔH (kJ/mol) | ΔG (kJ/mol) |
| 298 | 1.875771 | 0.0292 | 4.071 | -4.64 |
| 303 | 1.90756 | - | - | -4.79 |
| 308 | 1.933285 | - | - | -4.94 |
| 313 | 1.961272 | - | - | -5.08 |
| 318 | 1.977903 | - | - | -5.23 |

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