

## Supplementary File

### Purification of drinking water from dissolved Bisphenol-A (BPA) using zinc oxide nanoparticles

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**Table S1:** Summarizes the parameters of the three well-known isotherm models employed in this study: Langmuir, Freundlich, and Temkin.

| Isotherm models | Linear form                                                                 | Nonlinear form                               | Parameter                                                                                                                                                                                                                                       | Reference                                           |
|-----------------|-----------------------------------------------------------------------------|----------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------|
| Freundlich      | $\log q_e = \frac{1}{n} \log C_e + \log K_f$                                | $q_e = K_f C_e^{\frac{1}{n}}$                | $q_e$ adsorption capacity at equilibrium (mg/g)<br>$C_e$ final concentration at equilibrium (mg/l)<br>$K_f$ and $n$ Freundlich constants: $K_f$ (L/g)                                                                                           | (El-Nahas, Safaa et al., 2020; Koduru et al., 2016) |
| Langmuir        | $\frac{1}{q_e} = \frac{1}{K_L q_{\max}} + \frac{1}{C_e} \frac{1}{q_{\max}}$ | $q_e = \frac{q_{\max} K_L C_e}{1 + K_L C_e}$ | $q_{\max}$ Langmuir maximum capacity of adsorption (mg/g)<br>$K_L$ Langmuir constant (L/mg)                                                                                                                                                     |                                                     |
| Temkin          | $q_e = B \ln A - B \ln C_e$                                                 | $q_e = B(\ln A C_e)$<br>$B = R_T/b$          | $A$ is the equilibrium binding constant (L/mg)<br>$R$ is the universal gas constant ( $J \cdot mol^{-1} \cdot K^{-1}$ ),<br>$T$ is temperature K<br>$b$ is the heat of adsorption<br>$B$ is a constant related to the heat of sorption (J/mol.) |                                                     |

**Table S2 :** Langmuir dimensionless equilibrium parameter for BPA adsorption onto ZnO NPs at  $25 \pm 2$  °C.

| Initial Concentration (mg/L) | $R_L$ values |
|------------------------------|--------------|
| 1.0425                       | 0.339        |
| 1.9123                       | 0.218        |
| 2.9241                       | 0.154        |
| 4.0283                       | 0.117        |
| 5.0462                       | 0.096        |

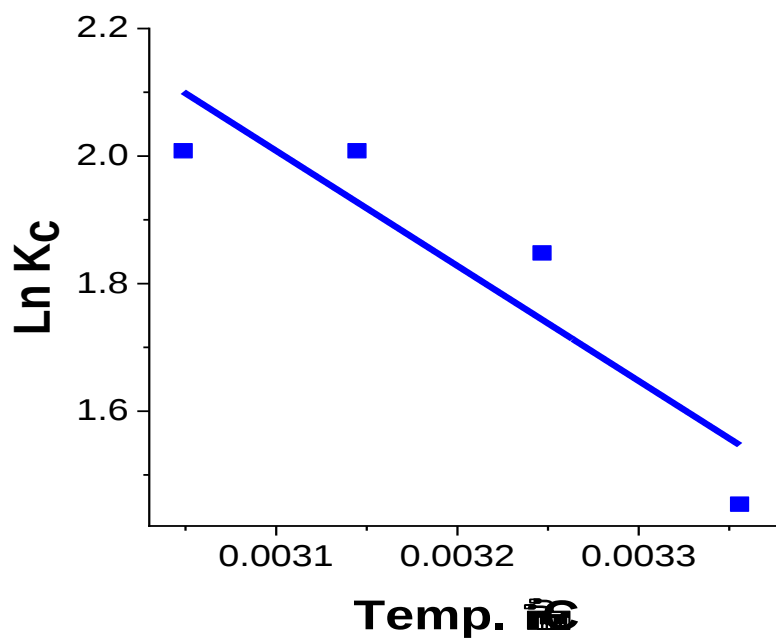
**Table S3: Kinetic models used in this work**

| Kinetic models          | Equation                                                | Parameter                                                                                                                                                                                            | Reference                                                    |
|-------------------------|---------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------|
| Pseudo-first order      | $\log(q_e - q_t) = \log q_e - \frac{K_1}{2.303} t$      | $q_e$ is the amounts of sorbate at the equilibrium (mg. g <sup>-1</sup> ).<br>$q_t$ is the amounts of sorbate at time (t) (mg. g <sup>-1</sup> )<br>$K_1$ (min <sup>-1</sup> ) is the rate constant. | (El-Nahas, Safaa et al., 2020; El-Nahas, Safaa et al., 2018) |
| Pseudo-second order     | $\frac{t}{q_t} = \frac{1}{K_2 q_e^2} + \frac{1}{q_e} t$ | $K_2$ (g/mg. min.) is the rate consistent.                                                                                                                                                           |                                                              |
| Intraparticle diffusion | $q_t = k_{ad} t^{0.5} + C$                              | $K_{ad}$ is the intraparticle diffusion rate constant (mg. g <sup>-1</sup> .min <sup>0.5</sup> )<br>$C$ is related to the thickness of boundary layer.                                               |                                                              |

**Table S4 :** Thermodynamic parameters.

| Thermodynamic parameters                                                    | Equation                                                         | Reference                                                  |
|-----------------------------------------------------------------------------|------------------------------------------------------------------|------------------------------------------------------------|
| Free energy<br>$\Delta G^\circ$ (kJ/mol)                                    | $\Delta G^\circ = RT \ln K_c$<br>$K_c = C_{ad}/C_e$              | (Davoud Balarak, June 2019 ; El-Nahas, Safaa et al., 2020) |
| Van't Hoff equation                                                         | $\ln K_c = \frac{\Delta H^\circ}{R} - \frac{\Delta S^\circ}{RT}$ |                                                            |
| Enthalpy ( $\Delta H^\circ$ kJ/mol)<br>Entropy ( $\Delta S^\circ$ kJ/mol K) | $\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$              |                                                            |

- Where  $K_c$  is the thermodynamic equilibrium constant for BPA adsorption onto ZnO NPs,  $C_s$  is the equilibrium BPA concentration adsorbed on ZnO NPs at (mg/L) and  $C_e$  is the equilibrium BPA concentration in solution (mg/L).



**Figure S1:** Plot of  $\ln(K_c)$  versus  $1/T$  for BPA removal by ZnO NPs at  $25 \pm 2^\circ\text{C}$ .