Supplementary Material

Experimental and theoretical estimations of atrazine´s adsorption on mangosteen peel-derived nanoporous carbons

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Table S1. Kinetics model used for the analysis of ATZ adsorption.

Kinetic model	Equation	Reference
Pseudo-first-order	$\log(q_{eq} - q_t) = \log(q_t) - (k_1/2.303)\ t$	[53,56]
Pseudo-second-order	$(1/q_{eq} - q_t) = (1/q_{eq}) + k_2\ t$	[53,57]
Intraparticle diffusion	$q_t = C + k_p\ t^{1/2}$	[53-55]

The pseudo-first-order model showed in Eq. (1) where k_1 is the pseudo-first-order rate constant (min^{-1}) for the adsorption, q_t is the amount of MB adsorbed (in μmol), at time t (min) and q_{eq} is the amount adsorbed at equilibrium (in μmol).

$$dq_t/dt = k_1(q_{eq} - q_t) \qquad (1)$$

The integration of Eq. (1) at the initial conditions ($q_{at} = 0$ at $t = 0$) yields the Eq. (2):

$$\log(q_{eq} - q_t) = \log(q_{eq}) - (k_1/2.303).t \qquad (2)$$

In addition, a pseudo-second-order equation may be expressed by Eq. (3):

$$dq_t/dt = k_2(q_{eq} - q_t)^2 \qquad (3)$$

Where k_2 is the pseudo-second-order rate constant ($\mu mol^{-1}.min^{-1}$) for the adsorption. Applying the initial conditions, Eq. (3) can be integrated to obtain:

$$(1/q_{eq} - q_t) = (1/q_{eq}) + k_2.t \qquad (4)$$

The influence of the intraparticle diffusion phenomena upon the adsorption capacity of MB was verified keeping in mind that the fractional approach to equilibrium change is done according to a function of $(D_t/r^2)^{1/2}$, where r is the radius of adsorbent particle and D is the effective diffusivity of solute within the particle. Thus, the initial rate according to the intraparticle diffusion model (IPD) is obtained from the liner regression of the curve $q_t = f(t^{1/2})$, expressed by the Eq. (5) where k_p is the IPD rate constant expressed in $\mu mol\ min^{-0.5}$, and C is the IPD capacity constant (μmol) attributed to the extension of the boundary layer thickness.

$$q_t = C + k_p.t^{1/2} \qquad (5)$$

Table S2. Models for the adsorption´s isotherms and mathematical expression involved in the different equilibrium adsorption isotherms.

Model	Equation	Reference
Langmuir	$q_{eq} = q_T.K_L.C_{eq}/(1 + K_L.C_{eq})$ $\theta = q_{eq}/q_T$ = Surface coverage	[62]
Freundlich	$q_{eq} = K_F.C_{eq}^{1/n}$	[63]

q_{eq}: Amount of ATZ adsorbed at equilibrium (μmol); q_T: Maximum capacity for the ATZ adsorption in the monolayer (μmol); C_{eq}: Concentration in equilibrium (μmol·L^{-1}); K_L: adsorption constant according to Langmuir model (L·μmol^{-1}); K_F: adsorption constant according to Freundlich model (L); n: Freundlich´s heterogeneity factor.

Table S3. Atrazine´s selected properties.

Property	Property value
Molecular weight (g mol^{-1})	215.68
Vapour pressure (Pa)	3.8×10^{-5} at 25ºC 4.0×10^{-5} at 20ºC
Melting point (ºC)	175.8
Solubility in water (mg L^{-1})	28 at 20ºC 35 at 25ºC
Density (g cm^{-3})	1.187 at 20ºC
- Ln(pKa)	1.62 at 20ºC, 1.70 at 21ºC
Molecular size	Width: 0.96 nm Depth: 0.84 nm Cross sectional diameter: 0.544 nm^2

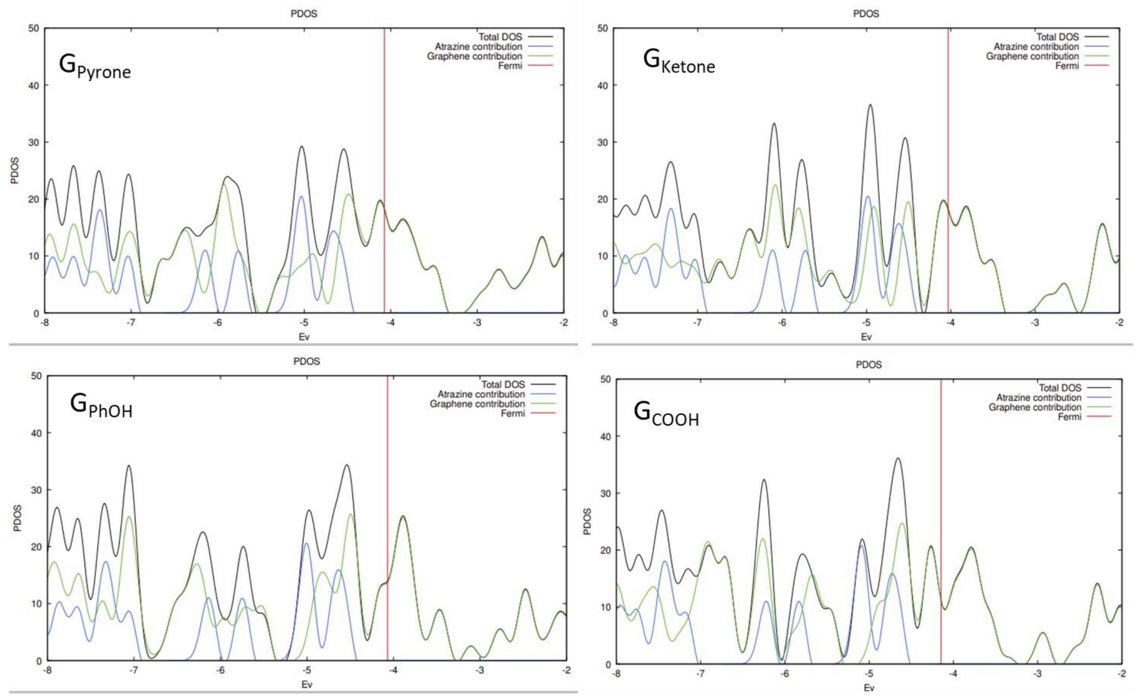

Table S1. DOS (black line) and projected DOS on the oxygen-containing graphene (green line) and atrazine (blue line) with PBE exchange–correlation functional.

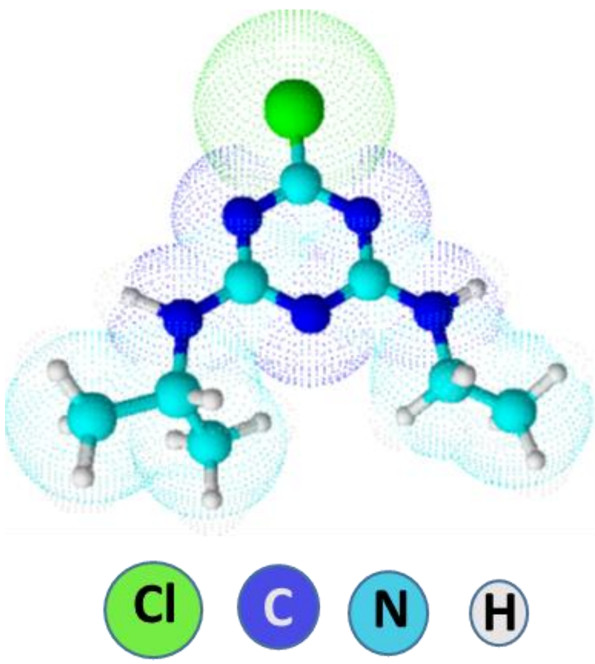

Figure S2. Molecular structure of atrazine ($C_8H_{14}ClN_5$).