

Supplementary Material

Hybrid material based on an amorphous-carbon matrix and ZnO/Zn for the solar photocatalytic degradation of basic blue 41

Silvana Lanfredi^{1,*}, Marcos A. L. Nobre², Po S. Poon³, Juan Matos^{3,4,*}

¹Department of Chemistry and Biochemistry, São Paulo State University (Unesp), School of Technology and Sciences, Laboratory of Composites and Ceramics Functional, Presidente Prudente, Brazil.

²Department of Physics, São Paulo State University (Unesp), School of Technology and Sciences, Presidente Prudente, Brazil.

³Technological Development Unit (UDT), University of Concepcion, Concepcion, Chile.

⁴Millennium Nuclei on Catalytic Processes towards Sustainable Chemistry (CSC), Chile.

*Corresponding authors. Emails: jmatoslale@gmail.com (J. Matos); silvana.lanfredi@unesp.br (S. Lanfredi)

Table S1. Summary of kinetics model for the analysis of the kinetic data of BB41 adsorption.

Kinetic model	Equation	Reference
Pseudo-first-order	$\log(\text{BB41}_{\text{ads-eq}} - \text{BB41}_{\text{ads-t}}) = \log(\text{BB41}_{\text{ads-eq}}) - (k_1/2.303) t$	81
Pseudo-second-order	$(1/\text{BB41}_{\text{ads-eq}} - \text{BB41}_{\text{ads-t}}) = (1/\text{BB41}_{\text{ads-eq}}) + k_2 t$	82
Intraparticle diffusion	$\text{BB41}_{\text{ads-t}} = C + k_p t^{1/2}$	83,84

The pseudo-first-order model showed in Eq. (1) where k_1 is the pseudo-first-order rate constant (min^{-1}) for the adsorption. $\text{BB41}_{\text{ads-t}}$ is the amount of BB41 adsorbed (in μmol) at time t (min) and $\text{BB41}_{\text{ads-eq}}$ is the amount adsorbed at equilibrium (in μmol).

$$d\text{BB41}_{\text{ads}}/dt = k_1(\text{BB41}_{\text{ads-eq}} - \text{BB41}_{\text{ads-t}}) \quad (1)$$

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

$$\log(\text{BB41}_{\text{ads-eq}} - \text{BB41}_{\text{ads-t}}) = \log(\text{BB41}_{\text{ads-eq}}) - (k_1/2.303) t \quad (2)$$

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

$$d\text{BB41}_{\text{ads}}/dt = k_2(\text{BB41}_{\text{ads-eq}} - \text{BB41}_{\text{ads-t}})^2 \quad (3)$$

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

$$(1/\text{BB41}_{\text{ads-eq}} - \text{BB41}_{\text{ads-t}}) = (1/\text{BB41}_{\text{ads-eq}}) + k_2 \cdot t \quad (4)$$

The influence of the intraparticle diffusion phenomena upon the adsorption capacity of BB41 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 $\text{BB41}_{\text{ads-t}} = f(t^{1/2})$, expressed by the Eq. (5), where k_p is the IPD rate constant ($\mu\text{mol min}^{-0.5}$), and C is a constant (μmol) attributed to the extension of the boundary layer thickness.

$$\text{BB41}_{\text{ads-t}} = C + k_p t^{1/2} \quad (5)$$

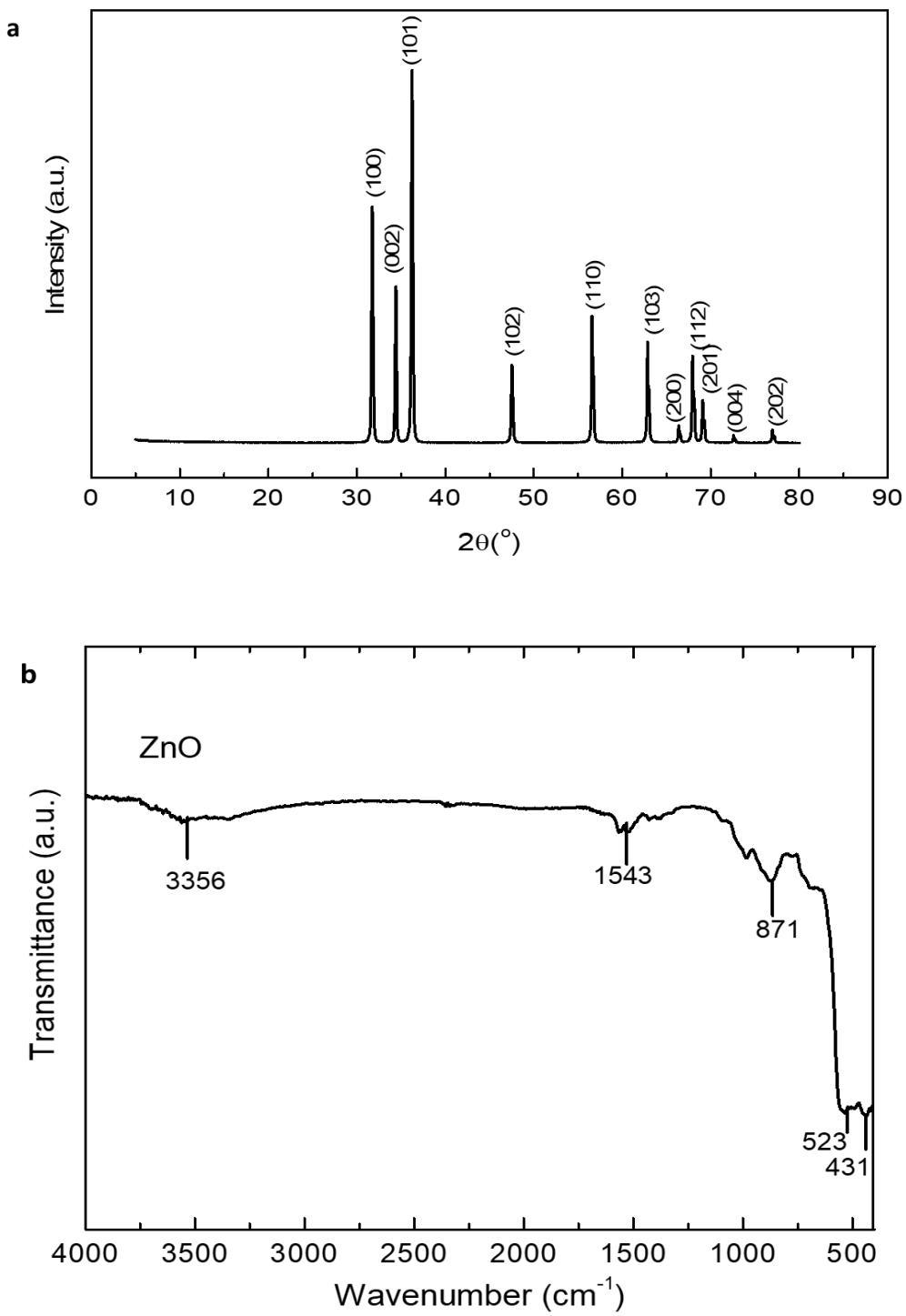


Figure S1. Characterization of commercial ZnO. (a): XRD pattern. (b): FTIR spectra.

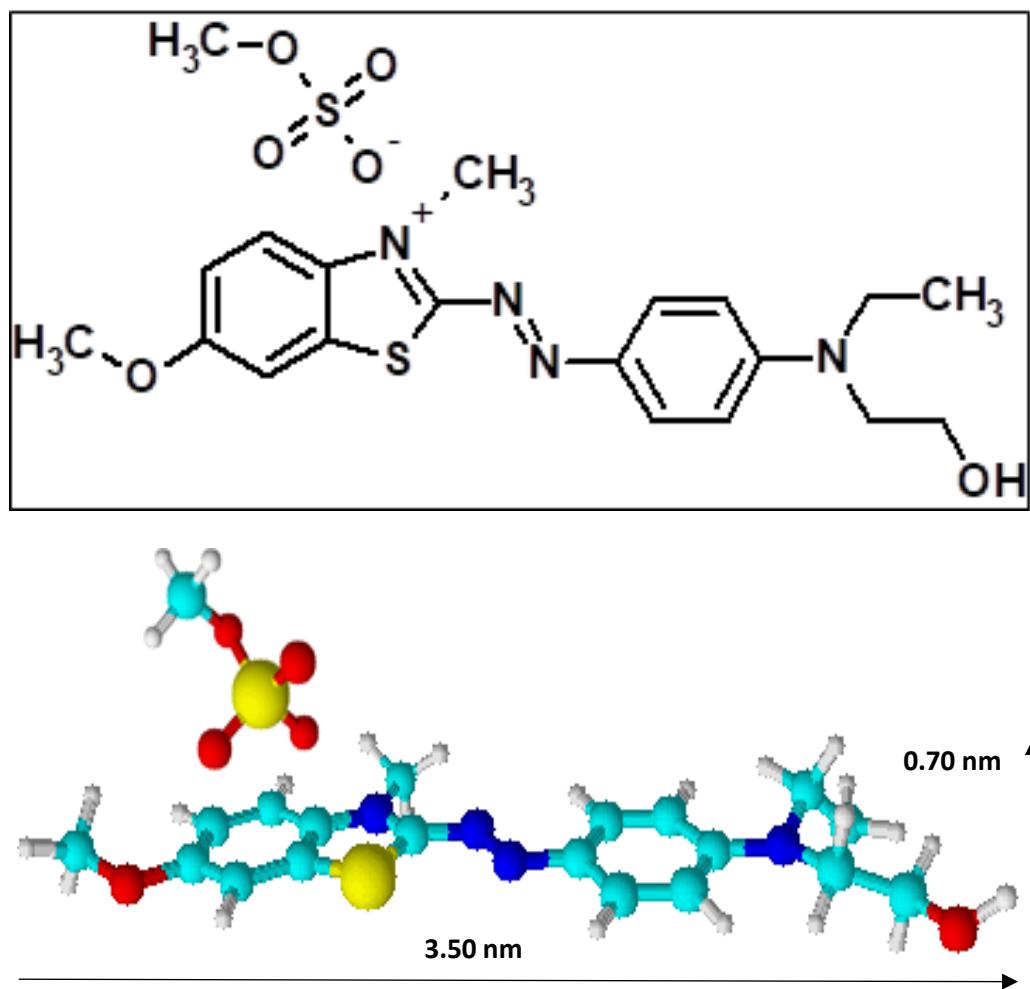


Figure S2. Molecular structure of basic blue 41.

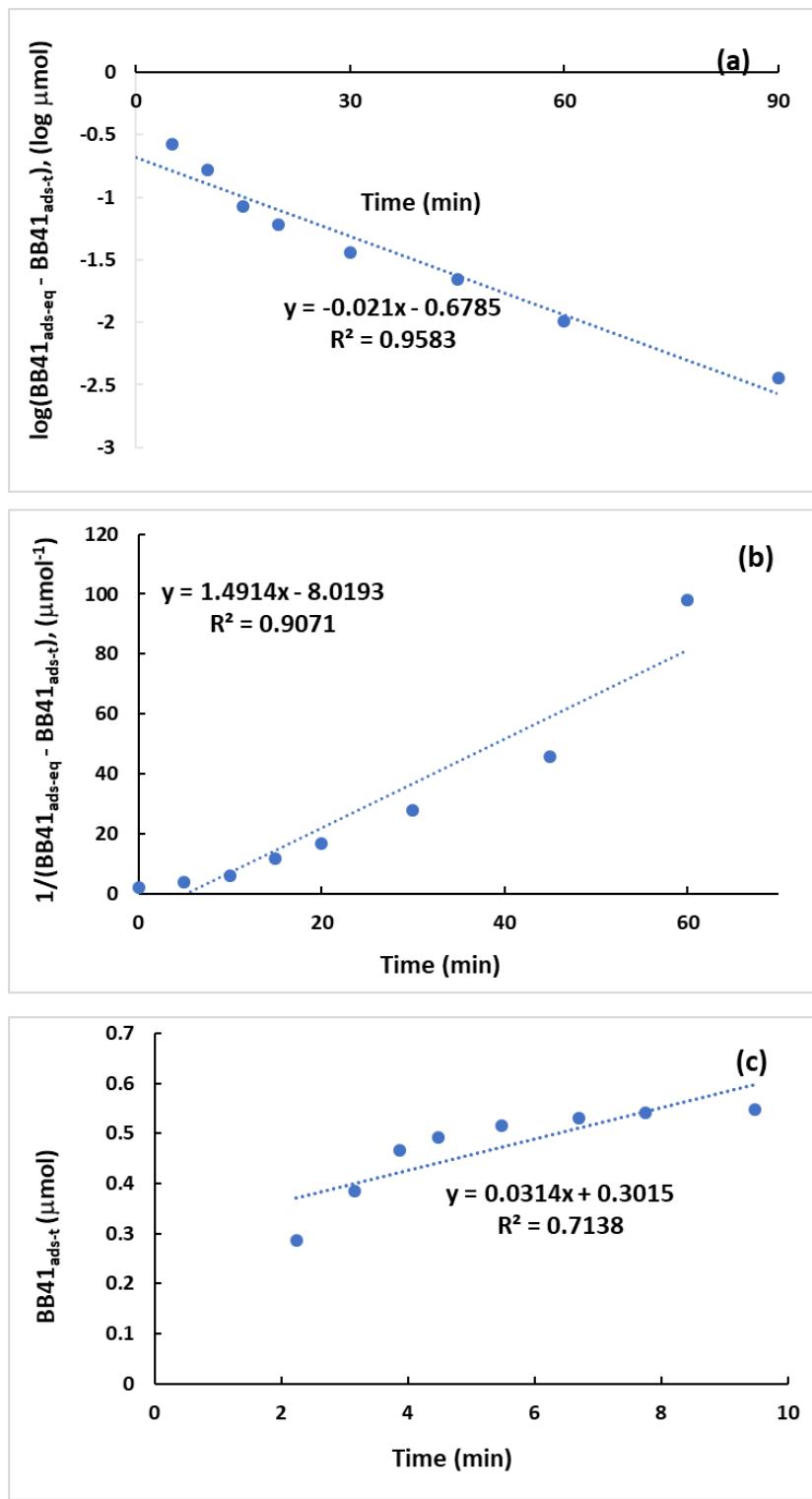


Figure S3. Kinetic treatment of the data of BB41 adsorption on C-amorphous. (a): Pseudo-first order. (b): Pseudo-second order. (c): IPD model.

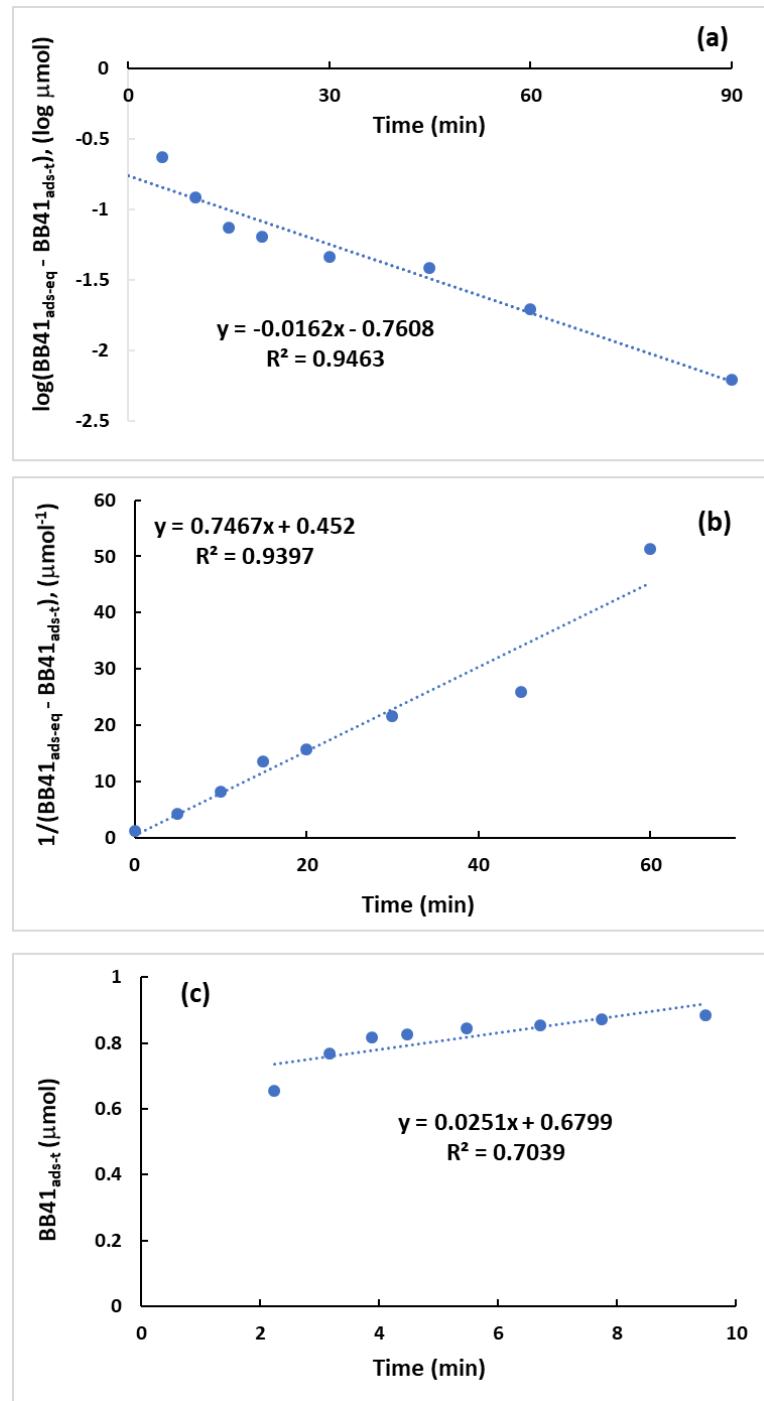


Figure S4. Kinetic treatment of the data of BB41 adsorption on C/Zn. (a): Pseudo-first order. (b): Pseudo-second order. (c): IPD model.

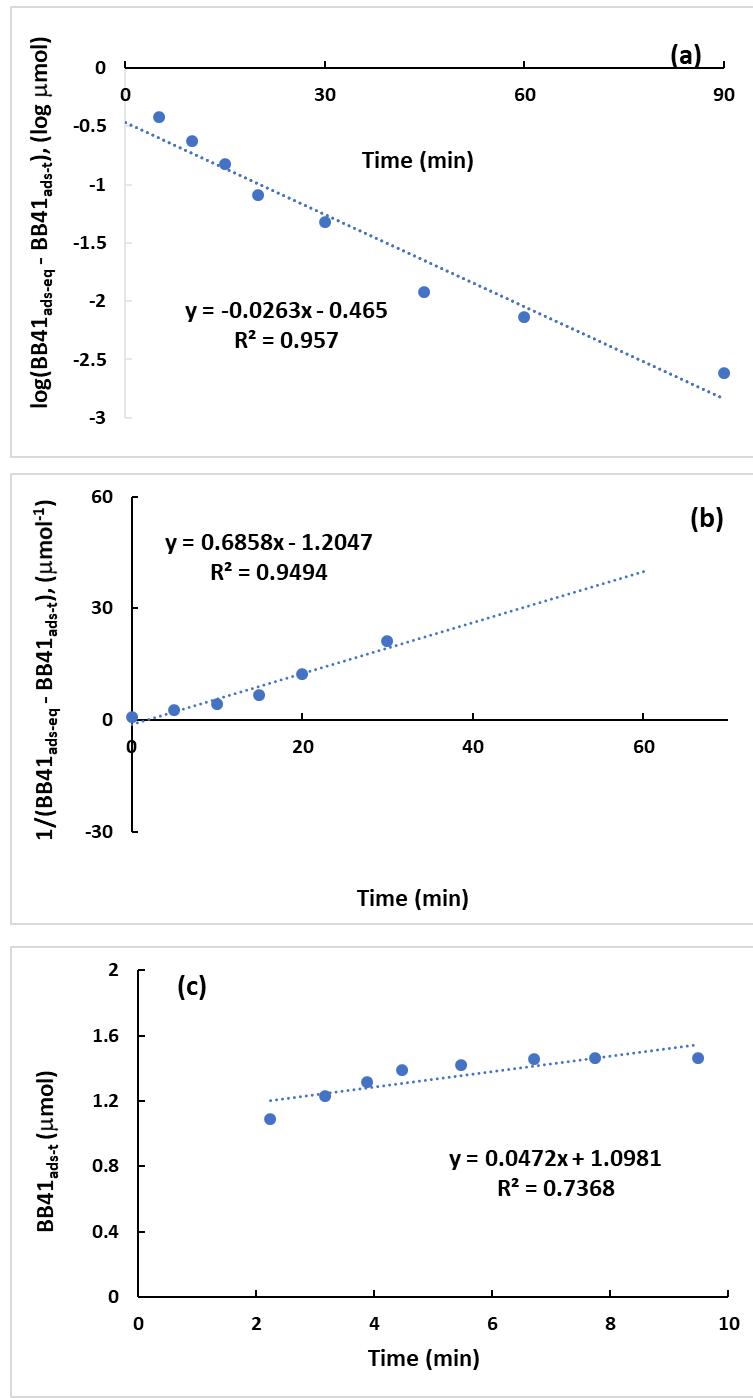


Figure S5. Kinetic treatment of the data of BB41 adsorption on C/ZnO/Zn. (a): Pseudo-first order. (b): Pseudo-second order. (c): IPD model.

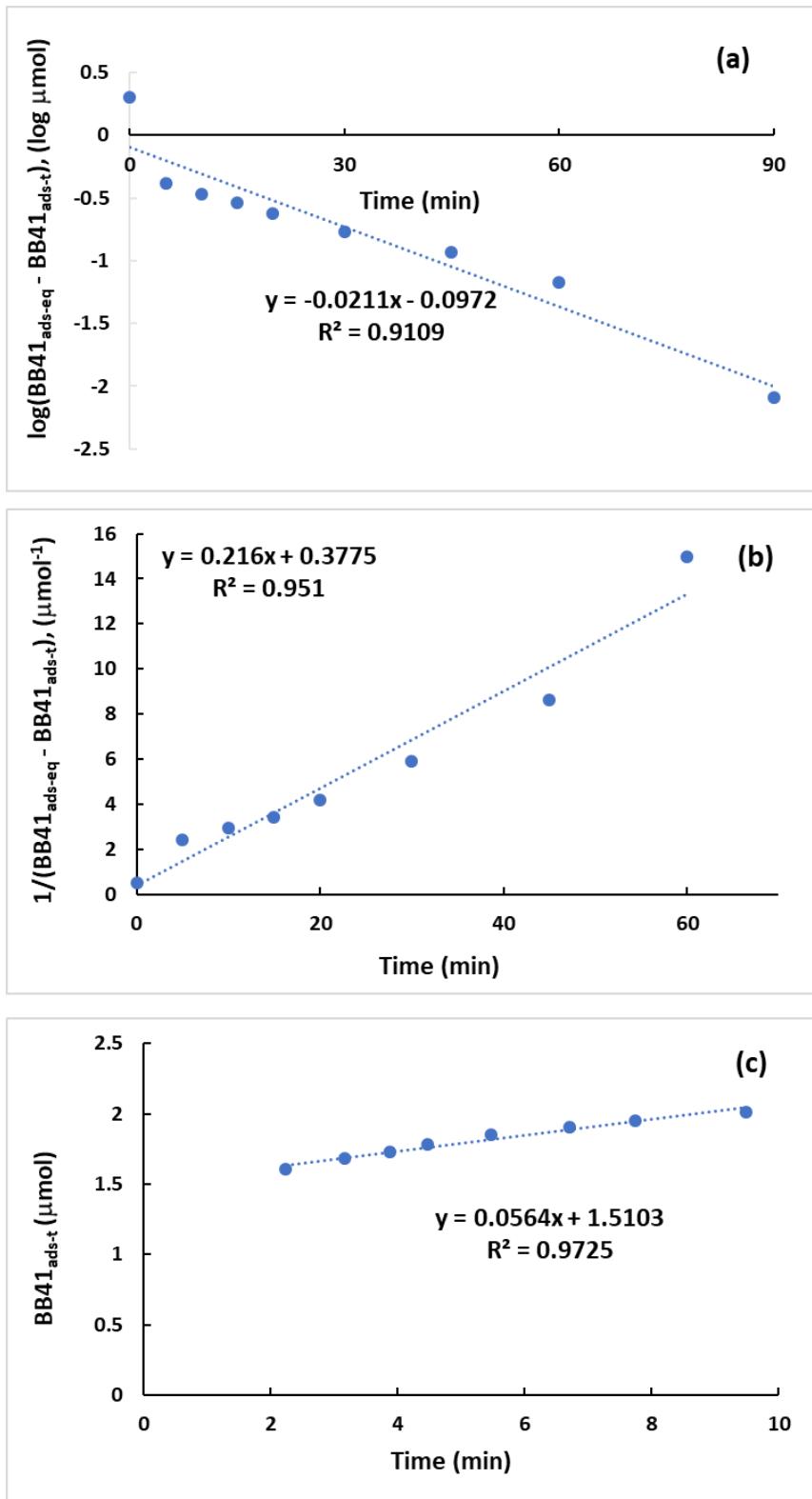


Figure S6. Kinetic treatment of the data of BB41 adsorption on ZnO. (a): Pseudo-first order. (b): Pseudo-second order. (c): IPD model.