

Synthesis and Characterization of Green ZnO@polynaniline/Bentonite Tripartite Structure (G.Zn@PN/BE) as Adsorbent for As (V) Ions: Integration, Steric, and Energetic Properties

Mohamed Abdel Salam ¹, Mohamed Mokhtar ¹, Soha M. Albukhari ¹, Doaa F. Baamer ¹, Leonardo Palmisano ², Mariusz Jaremko ³ and Mostafa R. Abukhadra ^{4,5,*}

¹ Department of Chemistry, Faculty of Science, King Abdulaziz University, P.O. Box 80200, Jeddah 21589, Saudi Arabia; mabdelsalam@kau.edu.sa (M.A.S.); mmoustafa@kau.edu.sa (M.M.); salbukhari@kau.edu.sa (S.M.A.); dfbaamer@kau.edu.sa (D.F.B.)

² Schiavello-Grillone Photocatalysis Group, Dipartimento di Ingegneria, Università degli Studi di Palermo, Viale delle Scienze (Ed. 6), 90128 Palermo, Italy; leonardo.palmisano@unipa.it

³ Smart-Health Initiative (SHI), Red Sea Research Center (RSRC), Biological and Environmental Science and Engineering (BESE) Division, King Abdullah University of Science and Technology (KAUST), P.O. Box 4700, Thuwal 23955-6900, Saudi Arabia; mariusz.jaremko@kaust.edu.sa

⁴ Geology Department, Faculty of Science, Beni-Suef University, Beni-Suef City 62511, Egypt

⁵ Materials Technologies and Their Applications Lab, Geology Department, Faculty of Science, Beni-Suef University, Beni-Suef City 62111, Egypt

* Correspondence: abukhadra89@science.bsu.edu.eg

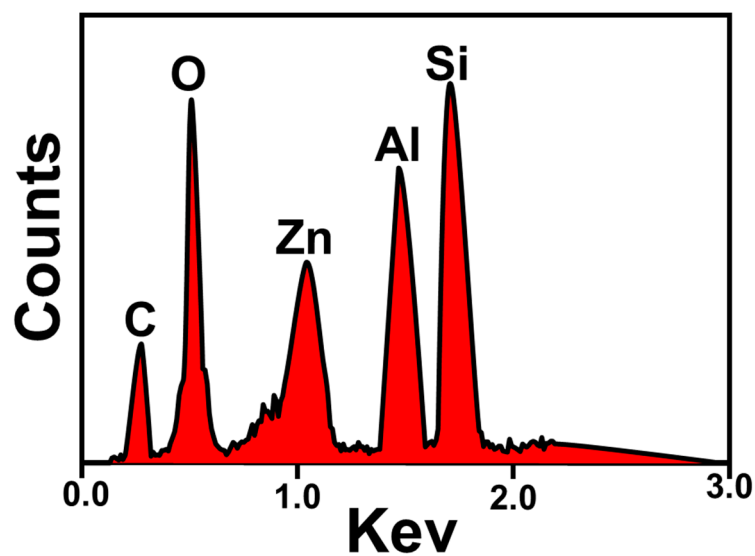


Figure S1. EDX spectrum of the synthetic G.Zn@PN/BE green composite.

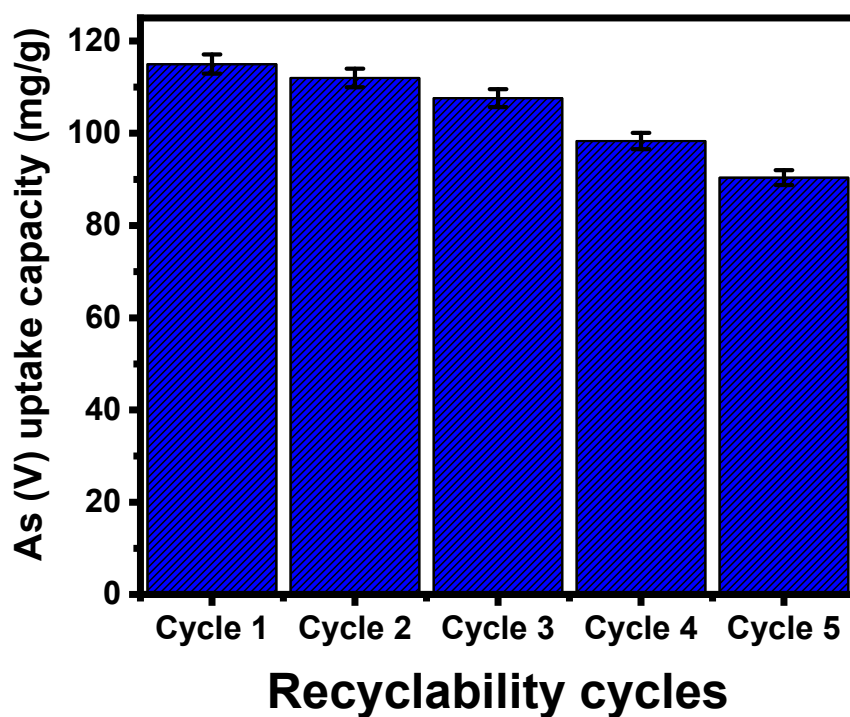


Figure S2. Recyclability of G.Zn@PN/BE during the retention of As (V) ions from water.

Table S1. Nonlinear equations of kinetic, classic isotherm, and advanced isotherm models.

Kinetic models		
Model	Equation	Parameters
Pseudo-first-order	$Q_t = Q_e (1 - e^{-k_1 t})$	Q_t (mg/g) is the adsorbed ions at time (t), and K_1 is the rate constant of the first-order adsorption (1/min)
Pseudo-second-order	$Q_t = \frac{Q_e^2 k_2 t}{1 + Q_e k_2 t}$	Q_e is the quantity of adsorbed ions after equilibration (mg/g), and K_2 is the model rate constant (g/mg min).
Classic Isotherm models		
Model	Equation	Parameters
Langmuir	$Q_e = \frac{Q_{max} b C_e}{(1 + b C_e)}$	C_e is the rest ions concentrations (mg/L), Q_{max} is the theoretical maximum adsorption capacity (mg/g), and b is the Langmuir constant (L/mg)
Freundlich	$Q_e = K_f C_e^{1/n}$	K_f (mg/g) is the constant of the Freundlich model related to the adsorption capacity and n is the constant of the Freundlich model related to the adsorption intensities
Dubinin–Radushkevich	$Q_e = Q_m e^{-\beta \varepsilon^2}$	β (mol ² /KJ ²) is the D-R constant, ε (KJ ² /mol ²) is the polanyiil potential, and Q_m is the adsorption capacity (mg/g)
Advanced isotherm models		
Model	Equation	Parameters
Monolayer model with one energy site (Model 1)	$Q = n N_o = \frac{n N_M}{1 + (\frac{C1}{C})^n} = \frac{Q_o}{1 + (\frac{C1}{C})^n}$	Q is the adsorbed quantities in mg/g n is the number of adsorbed ions per site
Monolayer model with two energy sites (Model 2)	$Q = \frac{n_1 N_{1M}}{1 + (\frac{C_1}{C})^{n_1}} + \frac{n_2 N_{2M}}{1 + (\frac{C_2}{C})^{n_2}}$	N_m is the density of the effective receptor sites (mg/g) Q_o is the adsorption capacity at the saturation state in mg/g
Double layer model with one energy site (Model 3)	$Q = Q_o \frac{(\frac{C}{C1/2})^n + 2(\frac{C}{C1/2})^{2n}}{1 + (\frac{C}{C1/2})^n + (\frac{C}{C1/2})^{2n}}$	$C1/2$ is the concentration of the ions at half saturation stage in mg/L
Double layer model with two energy sites (Model 3)	$Q = Q_o \frac{(\frac{C}{C1})^n + 2(\frac{C}{C2})^{2n}}{1 + (\frac{C}{C1})^n + (\frac{C}{C2})^{2n}}$	$C1$ and $C2$ are the concentrations of the ions at the half saturation stage for the first active sites and the second active sites, respectively $n1$ and $n2$ are the adsorbed ions per site for the first active sites and the second active sites, respectively