Comparative performance and eco-toxicity assessment of $Y_2(CO_3)_3$), ZnO/TiO_2, and Fe_3O_4 nanoparticles for arsenic removal from water

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Supplementary Information

1. Supplementary information for sub-chapter 2.3.

The kinetic curves were fitted according to nonlinear forms of pseudo-first, pseudo-second-order, Elovich, and Bangham models described in equations 1, 2, 3, and 4, respectively:

$$Q_t = Q_e\left(1 - exp^{\left(-k_1 t\right)}\right) \quad (1)$$

$$Q_t = \frac{Q_e^2 k_2 t}{1 + Q_e K_2 t} \quad (2)$$

$$Q_t = \frac{\ln \alpha\beta}{\beta} + \frac{1}{\beta}\ln t \quad (3)$$

$$Q_t = kt^{\upsilon} \quad (4)$$

where Q_e and Q_t (mg/g) are the capacities for arsenic adsorption at equilibrium and at a correspondent time, respectively. K_1 (min^{-1}) is the pseudo-first-order adsorption rate constant, K_2 (g/mg min) is the pseudo-second-order adsorption rate constant, α is the initial adsorption rate (mg/g min), and β is the desorption constant (g/mg), k (mg/g) and υ (min^{-1}) are constants.

The isotherm curves were fitted to the following models: Langmuir, Freundlich, Temkin, and Dubinin-Radushkevich, which are defined by the equations 5 to 9, respectively:

$$q_e = \frac{Q_{max} b C_e}{1 + bC_e} \quad (5)$$

$$q_e = K_F C_e^{1/n} \quad (6)$$

$$q_e = \frac{RT}{b_T}\ln\left(K_T C_e\right) \quad (7)$$

$$q_e = Q_S exp^{\left(-B_D \varepsilon^2\right)} \quad (8)$$

$$\varepsilon = RT\ln\left(1 + \frac{1}{C_e}\right) \quad (9)$$

where q_e (mg/g) is the As adsorption capacity at a given equilibrium concentration, C_e (mg/L) is the arsenic equilibrium concentration, q_{max} (mg/g) is the maximum adsorption capacity, K_L (L/mg) is the adsorption rate for Langmuir isotherm model, K_F ($L^{1/n}$ $mg^{(1-1/n)}$ g^{-1}) is the adsorption capacity of the adsorbent for Freundlich isotherm model, and *1/n* is a measure of the adsorption intensity, b (J/mol) is Temkin constant, K_T (L/g) Temkin isotherm constant, Q_S (mg/g) is the maximum adsorption capacity, B_D (mol^2/kJ^2) is

Dubinin-Radushkevich constant, ε (kJ/mol) is the adsorption potential, R (8.314 J/mol K) is the universal gas constant, T (K) is the temperature, k and υ are constants. Regarding $1/n$ value, the closer its value to 0, the more heterogeneous is the surface of the nanocomposite membrane.

2. Supplementary information for sub-chapter 2.4.

Table S1. pH of the nanosuspensions measured at the beginning and after 48h of exposure.

		pH	
Treatments	**Concentrations (mg/L)**	**Initial**	**48 h**
Control	0	8.29	8.07
Fe_3O_4	50	8.20	7.81
	100	8.11	7.80
	250	7.77	7.84
	500	7.45	7.99
	1000	7.18	7.64
	2000	6.78	7.49
ZnO/TiO_2	0.1	8.09	7.63
	1	8.12	7.71
	5	8.12	7.69
	10	8.09	7.74
	25	8.03	7.84
	50	7.93	7.96
$Y_2(CO_3)_3$	0.005	8.02	7.74
	0.05	8.10	7.79
	0.1	8.11	7.77
	0.5	8.12	7.83
	1	8.11	7.86
	1.5	8.10	7.88

3. Supplementary information for sub-chapter 3.2.2.

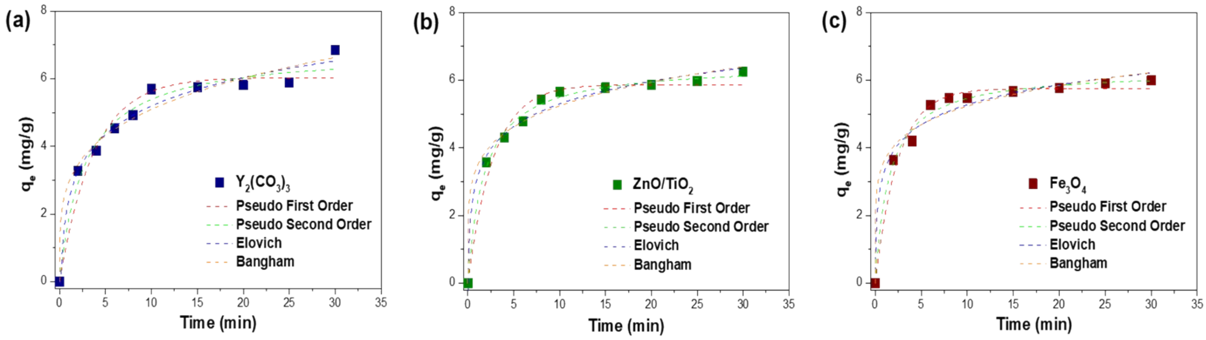

Figure S1. Adsorption kinetics of **(a)** $Y_2(CO_3)_3$, **(b)** ZnO/TiO_2, and **(c)** Fe_3O_4, for As (V) removal ([As] = 100 µg/L; contact time: 30 min; pH = 7).

4. Supplementary information for sub-chapter 3.2.3.

Table S2. Effect of As (V) concentration on efficiency (E) and adsorption capacity (Q_e) of active materials.

[As] (mg/L)	$Y_2(CO_3)_3$		ZnO/TiO_2		Fe_3O_4	
	E (%)	Q_e (mg/g)	E (%)	Q_e (mg/g)	E (%)	Q_e (mg/g)
0.1	99.6	0.10	99.9	0.10	99.8	0.10
0.25	98.9	0.25	98.7	0.25	98.1	0.25
0.5	98.7	0.49	99.4	0.50	98.9	0.49
0.75	98.9	0.74	99.3	0.74	98.5	0.74
1	98.9	0.99	99.4	0.99	98.8	0.99
2	97.9	1.96	98.6	1.97	98.1	1.96
5	97.5	4.88	98.0	4.90	97.9	4.89
10	97.2	9.72	97.9	9.79	97.6	9.76
15	81.1	12.2	84.8	12.7	83.5	12.5
20	68.3	13.7	70.4	14.1	69.7	13.9

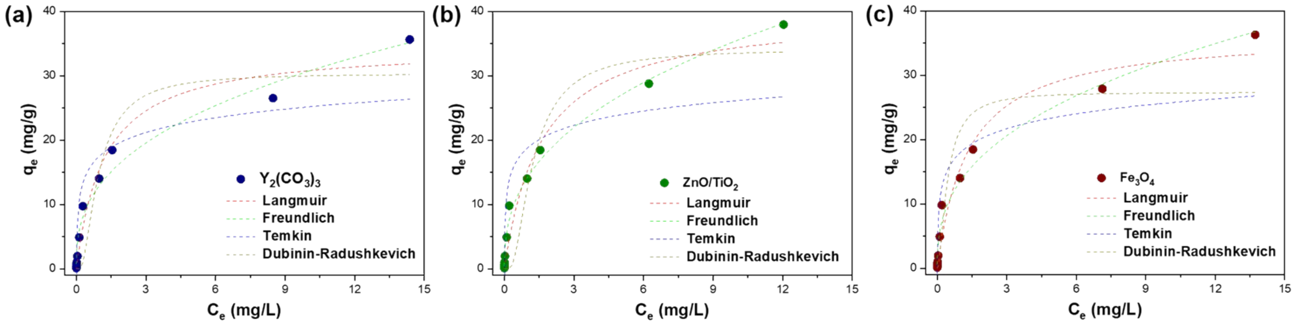

Figure S2. Adsorption isotherm models simulation for **(a)** $Y_2(CO_3)_3$, **(b)** ZnO/TiO_2, and **(c)** Fe_3O_4, for As (V) removal (contact time: 30 min; pH = 7).

5. Supplementary information for sub-chapter 3.3.

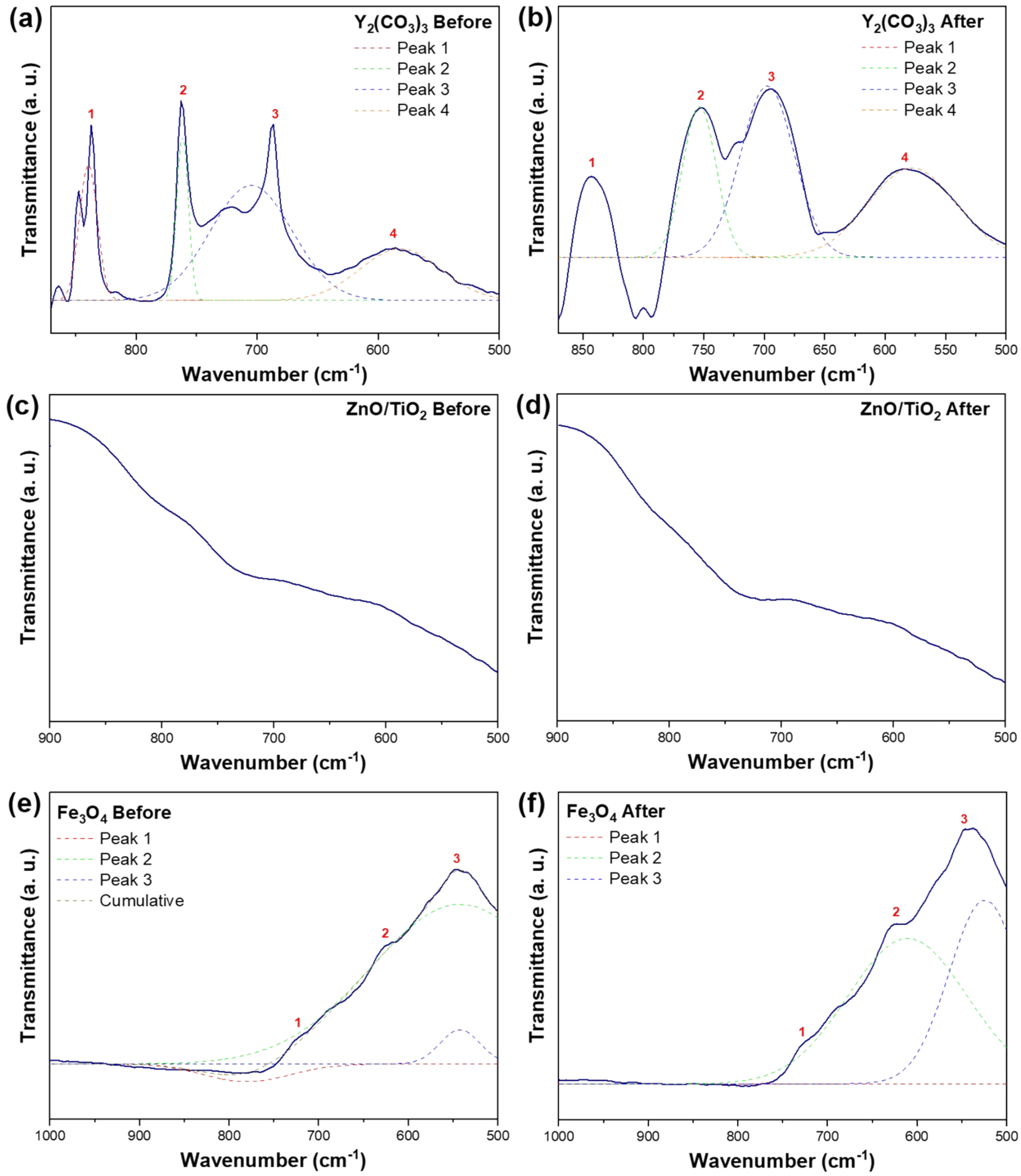

Figure S3. Deconvolution and peak fitting of FTIR spectra before and after As(V) adsorption by **(a - b)** $Y_2(CO_3)_3$, **(c - d)** ZnO/TiO_2, and **(e - f)** Fe_3O_4.