

Novel Application of $\text{MnO}_2\text{--H}_2\text{O}_2$ System for Highly Efficient Arsenic Adsorption and Oxidation

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Supporting Information:

- S1. Simulation for kinetic curves
- S2. Simulation of isotherm
- S3. Simulation of thermodynamics
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S1. Simulation for kinetic curves

The expressions of pseudo-first-order model and the pseudo-second-order model are described as Eqs. (S1) and (S2), shown as follows:

$$q_t = q_e \left(1 - e^{-k_1 t} \right) \quad (\text{S1})$$

$$q_t = \frac{q_e^2 k_2 t}{1 + q_e k_2 t} \quad (\text{S2})$$

where q_e (mg/g) is the equilibrium adsorption capacity; q_t (mg/g) is the adsorption capacities (mg/g) at time t (h); k_1 (h^{-1}) and k_2 ($\text{g/mg}\cdot\text{h}$) are the related adsorption rate constants.

Table S1. Parameters for the simulation of adsorption kinetics

Model	Parameter	Value
Pseudo-first-order model	R^2	0.975
	k_1 (min^{-1})	0.0840
	q_e ($\text{mg}\cdot\text{g}^{-1}$)	1.682
Pseudo-second-order model	R^2	0.999
	k_2 ($\text{min}\cdot\text{g}\cdot\text{mg}^{-1}$)	0.125
	q_e ($\text{mg}\cdot\text{g}^{-1}$)	3.610

S2. Simulation of isotherm

The isotherms described Langmuir and Freundlich models can be described by Eq.S3 and Eq.S4 as follows:

$$q_e = \frac{q_{\max} K_L C_e}{1 + K_L C_e} \quad (\text{S3})$$

$$q_e = K_F C_e^n \quad (\text{S4})$$

where q_e (mg/g) is and represent the amount of equilibrium adsorption capacity; q_{\max} (mg/g) is the maximum adsorption capacity; K_L (L/mg) is the Langmuir constant related to the affinity of binding sites; C_e (mg/L) is the equilibrium solution concentration; K_F is an indicator of the adsorption capacity; n is the heterogeneity factor which has a lower value for more heterogeneous surfaces.

Table S2. Parameters for the simulation of isotherms

Langmuir model				Freundlich model		
Concentration	K_L	q_{\max}	R^2	K_F (mg ¹⁻	n	R^2
(mg/L)	(L/mg)	(mg/g)		^{1/n} ·L ^{1/n} ·g ⁻¹)		
5	0.0001	39.752	0.986	42.202	0.816	0.994
25	0.0629	22.33	0.987	21.748	0.491	0.995

S3. Simulation of thermodynamics

The thermodynamic parameters including the changes in standard free energy (ΔG^0 , kJ/mol), enthalpy (ΔH^0 , kJ/mol) and entropy (ΔS^0 , J* mol^{-1} * K^{-1}) can be calculated by the following equations:

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \quad (\text{S5})$$

$$\Delta G^0 = -RT \ln K^0 \quad (\text{S6})$$

$$\ln K^0 = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{R} \times \frac{1}{T} \quad (\text{S7})$$

Where R (8.314 J/mol K) is the gas constant; T (K) is the absolute temperature; K^0 is the standard thermodynamic equilibrium constant defined by q_e/C_e (C_e is the amount of As in solution at equilibrium). Values of ΔH^0 and ΔS^0 can be obtained from the relationship between $\ln K^0$ and $1/T$. the simulation curves is shown in Fig. S1

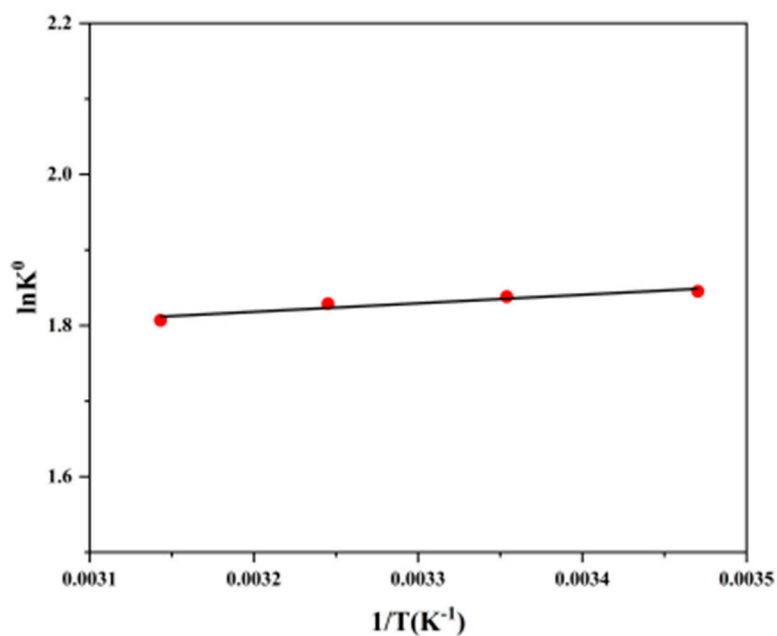


Fig. S1. Relationship between $\ln K^0$ and $1/T$

S4. Detailed histogram of regeneration and reuse of MnO₂ particles

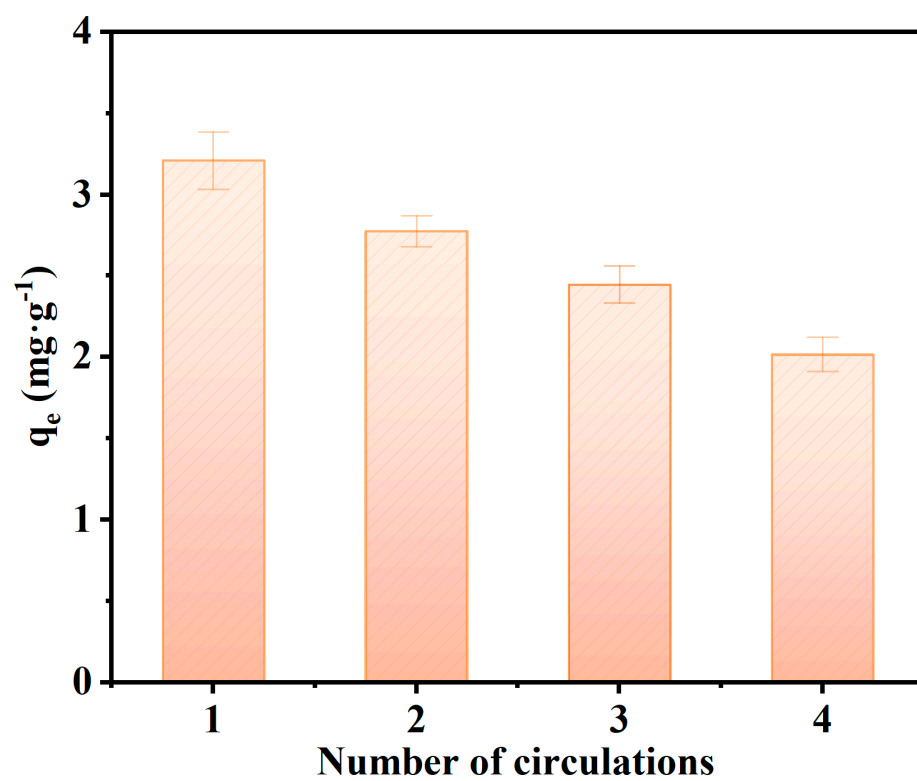
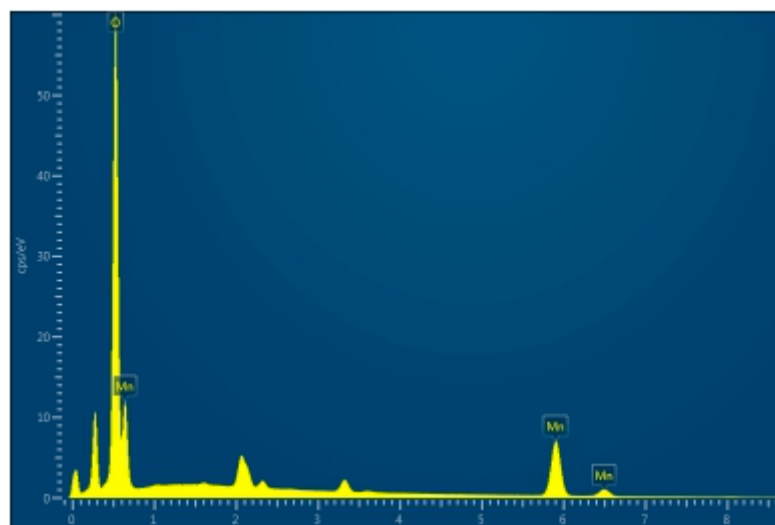
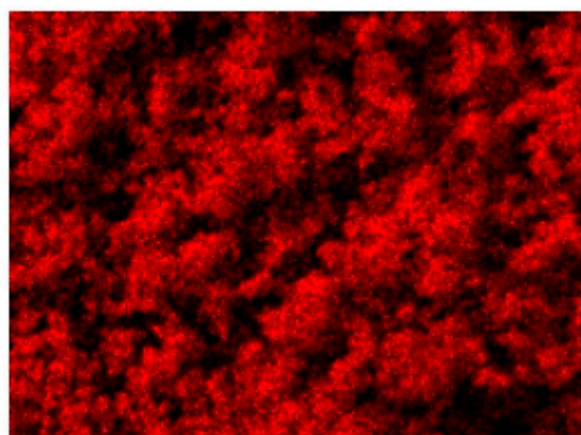


Fig. S2. Evolution of q_e for the consecutive adsorption and regeneration

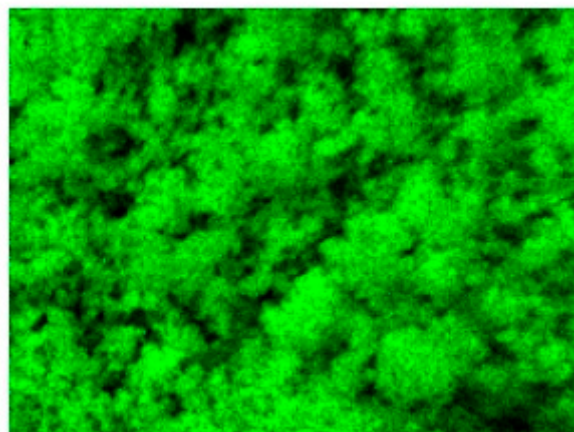
S5. SEM-EDS of synthesized MnO_2



Mn $L\alpha_{1,2}$



O $K\alpha_1$



S6. Characteristics of ground water and river water

Parameter	Ground water	River water
pH	7.41	6.80
DO (mg/L)	2.68	5.34
TOC (mg/L)	8.3	4.56
Ca ²⁺ (mg/L)	102.2	20.35
Mg ²⁺ (mg/L)	21.6	5.47
Cl ⁻ (mg/L)	55.8	8.66
Fe (mg/L)	0.47	0.52
Initial As (μg/L)	105	1.78
Added As(III) (μg/L)	0	100