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Supplementary data

Fig. S1 X-ray photoelectron spectrums of Zr 3d (a), O 1s (b) on Zr-ATP before adsorbing As and Zr 3d(c, e), O 1s(d, f), As 3d(g, h) on Zr-ATP after adsorbing As

Fig. S2 The effect of cations on Zr-ATP adsorption to As(III) and As(V)

Fig. S3 Time-response changes of pH in the overlying waters in As-contaminated sediments

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 sediments after 30-d Zr-ATP/ATP capping("-" represents below the water-sediment interface)

Table S3 Reduction efficiencies of DGT-labile As in the vertical profiles of As-contaminated

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 represents below the water-sediment interface)

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Text S1 Adsorption calculations, kinetics and isotherm models



Fig. S1 X-ray photoelectron spectrums of Zr 3d (a), O 1s (b) on Zr-ATP before adsorbing As and Zr 3d(c, e), O 1s(d, f), As 3d(g, h) on Zr-ATP after adsorbing As



Fig. S2 The effect of cations on Zr-ATP adsorption to As(III) and As(V)



Fig. S3 Time-response changes of pH in the overlying waters in As-contaminated sediments

Adsorbent	Elements	С	0	Mg	Al	Si	Zr
	Weight ratio(%)	31.18	42.92	2.38	6.02	17.50	0
AIP	Atomic ratio(%)	41.72	43.11	1.57	3.59	10.01	0
7. ATD	Weight ratio(%)	28.27	43.73	2.89	7.12	16.10	1.89
Zr-ATP	Atomic ratio(%)	38.14	45.50	2.05	2.20	11.75	0.36

Table S1 Percentages of elements on ATP and Zr-ATP

 Table S2 Reduction efficiencies of dissolved As in the vertical profiles of As-contaminated

 sediments after 30-d Zr-ATP/ATP capping ("-" represents below the water-sediment interface)

Depth	0 1	0 mg/kg		10 mg/kg			20 mg/kg		
layer(mm)	ATP	Zr-ATP		ATP	Zr-ATP		ATP	Zr-ATP	
0 to -20	48.7	54.8		66.1	80.4		42.9	80.0	
-20 to -40	34.5	54.4		24.8	78.1		54.8	78.5	
-40 to -60	43.5	45.6		4.2	34.5		53.1	70.5	
-60 to -80	66.9	72.9		12.9	28.8		38.6	56.9	

Table S3 Reduction efficiencies of DGT-labile As in the vertical profiles of As-contaminated

 sediments after 30-d Zr-ATP/ATP capping ("-" represents below the water-sediment interface)

Depth	0 mg/kg		10 mg/kg			20 mg/kg		
layer(mm)	ATP	Zr-ATP		ATP	Zr-ATP		ATP	Zr-ATP
0 to -20	53.7	71.8		48.5	91.8		56.0	95.8
-20 to -40	21.1	38.6		10.0	43.3		35.4	70.1
-40 to -60	12.4	18.8		4.7	34.0		13.6	31.4
-60 to -80	8.3	20.0		5.7	25.3		12.1	29.6

 Table S4 Comparison of passivation materials to As in the sediments("-" represents below the water-sediment interface)

		Dissol	ved As	DGT-la		
Passivation materials	Passivation time(d)	Max passivation depth	Max passivation efficiencies	Max passivation depth	Max passivation efficiencies	References
		(mm)	(%)	(mm)	(%)	
LMB	32	-50.0	31.9	-17.5	44.9	28
Zr-LMB	30	-20.0	58.0	-40.0	34.7	50
ALS	30	-20.0	51.1	-26.0	29.6	53
$Ca(NO_3)_2$	60	-50.0	47.7	-32.5	70.8	28
ATP	30	-80.0	66.9	-20.0	8.3	This study
Zr-ATP	30	-80.0	72.9	-20.0	71.8	This study

Demonsterne		0 mg/kg			10 mg/kg	5		20 mg/kg		
Parameters	CK	ATP	Zr-ATP	CK	ATP	Zr-ATP	CK	ATP	Zr-ATP	
R	0.217	0.219	0.327	0.142	0.334	0.355	0.276	0.282	0.375	
$K_{\rm d}({\rm cm}^3~{\rm g}^{-1})$	9352	9486	9623	1819	5147	6917	3458	3551	4150	
$T_{\rm c}({\rm s})$	2924	2866	897	7852	838	712	1381	1305	593	
$K_{-1}(10^{-4} \text{ s}^{-1})$	1.74	1.75	2.64	1.19	4.20	3.59	4.13	4.22	5.44	
$K_1(10^{-4} \text{ s}^{-1})$	1.67	1.74	8.50	0.0828	7.74	10.46	3.11	3.44	11.43	

Table S5 Parameters modeled by DIFS for As in As-contaminated sediments with different treatments

Table S6 Sequential extraction procedures for Arsenic fractions in sediments based on Wenzel's method

Steps	As fractions	Extractants	Conditions	
1	Non-specifically adsorbed As(F1)	0.05 M (NH ₄) ₂ SO ₄	25 °C, shaking for 4 h	
2	Specifically adsorbed As(F2)	0.05 M NH ₄ H ₂ PO ₄	25 °C, shaking for 16 h	
3	Amorphous and poorly-crystalline Fe-Al hydrous oxide bound As(F3)	0.2 M Ammonium oxalate (pH=3)	25 °C, shaking for 4 h	
4	Well-crystallized Fe-Al hydrous oxide bound As(F4)	0.2 M Ammonium oxalate+0.1 M Ascorbic acid (pH=3)	96 °C, shaking for 30 min	
5	Residual As(F5)	Aqua regia	Determination after digestion	

Text S1 Adsorption calculations, kinetics and isotherm models

The adsorption efficiency (E) of Zr-ATP to As(III)/As(V) was calculated using the Eq. (1):

$$E = \frac{(C_0 - C_e)}{C_0} \times 100\%$$
(1)

The adsorption amounts $({}^{q}_{t})$ and $({}^{q}_{e})$ of Zr-ATP to As(III)/As(V) were calculated using the Eq. (2) and Eq. (3):

$$q_{t} = \frac{(C_{0} - C_{t})V}{m}$$
(2)
$$(C_{0} - C_{e})V$$

$$q_e = \frac{1}{m} \tag{3}$$

where *E* is adsorption efficiency in the equilibrium solution; $t(\min)$ is the contact time; q_t and $q_e(\mu g/g)$ are adsorption amount at *t* min and adsorption capacity in equilibrium solutions, respectively; C_0 , C_t and $C_e(\mu g/L)$ are concentrations of As at the initial time, *t* min and equilibrium, respectively; V(L) is the volume of As solution and m(g) is the mass of adsorbent.

PFO model is represented by Eq. (4).

$$\ln\left(q_e - q_t\right) = \ln q_e - k_1 t \tag{4}$$

PSO model is represented by Eq. (5).

$$\frac{t}{q_t} = \frac{1}{k_2 \cdot q_e^2} + \frac{t}{q_e}$$
(5)

Langmuir model is represented by Eq. (6).

$$\frac{c_e}{q_e} = \frac{c_e}{q_m} + \frac{1}{K_L \cdot q_m} \tag{6}$$

Freundlich model is represented by Eq. (7).

$$lnq_e = lnK_F + \frac{1}{n}lnc_e \tag{7}$$

Where $q_m (mg/g)$ is theoretical adsorption capacities; $k_1(min^{-1})$ and $k_2(g/(mg min))$ are the equilibrium rate constants of the corresponding kinetic models; $K_L (L/mg)$ is the equilibrium coefficient; $K_F (mg^{1-1/n} \cdot L^{1/n}/g)$ is the Freundlich isotherm constant; 1/n is the heterogeneity factor.