

Supporting Information

Elaborately Design of Polymeric Nanocomposite with Mg(II)-buffering Nanochannels for Highly Efficient and Selective Heavy Metal Removal from Water: Case Study for Cu(II)

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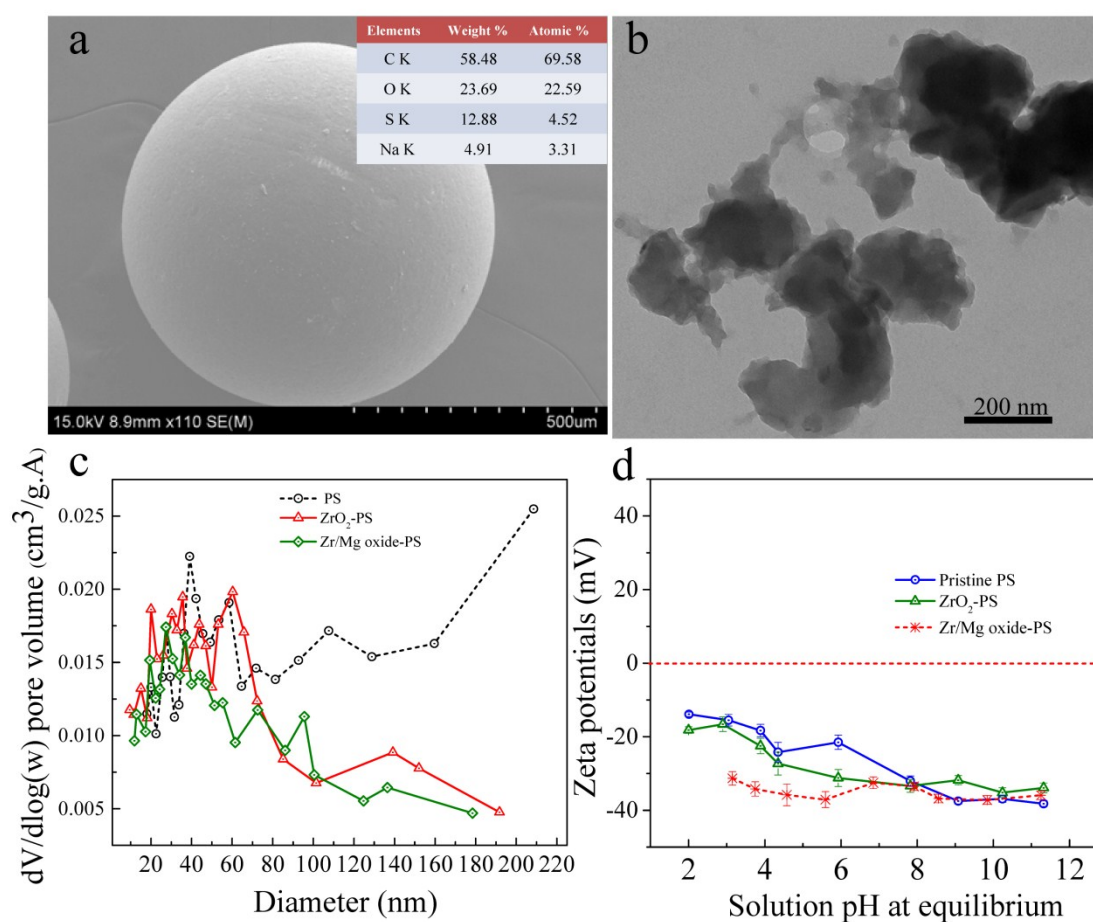


Figure S1 a) the SEM morphology of matrix PS and the corresponding element composition; b) TEM image of matrix PS; c) the pore distributions of pristine PS, hybrid ZrO₂-PS and Zr/Mg oxide-PS; d) zeta potential analysis of pristine PS, hybrid ZrO₂-PS and Zr/Mg oxide-PS.

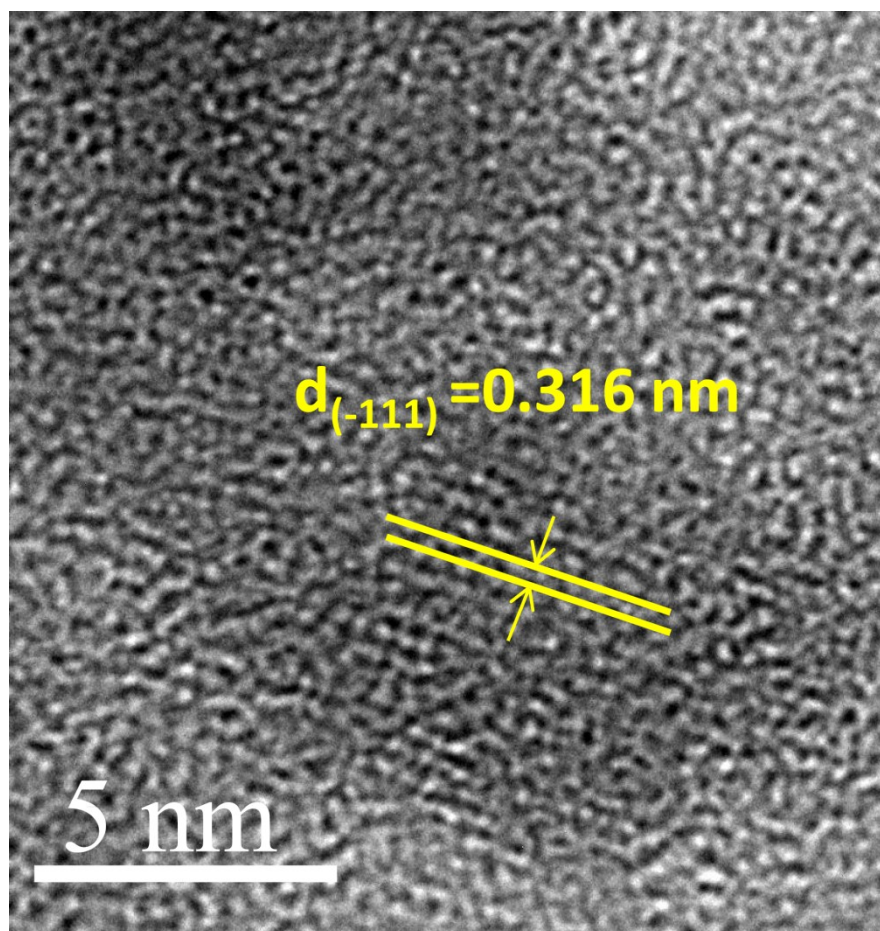


Figure S2 HR-TEM image of ZrO₂-PS

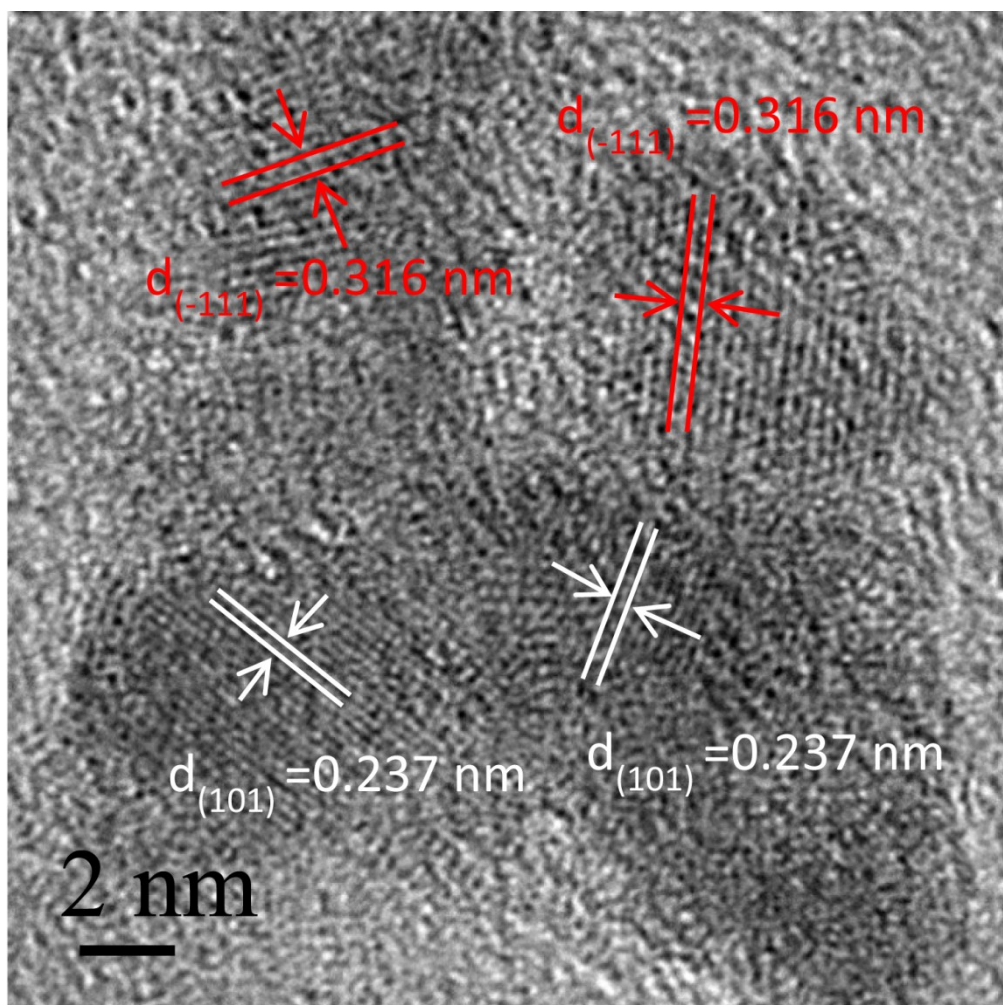


Figure S3 HRTEM image of the Zr/Mg oxide-PS

Figure S4 The XRD pattern of the prepared Zr/Mg oxide-PS

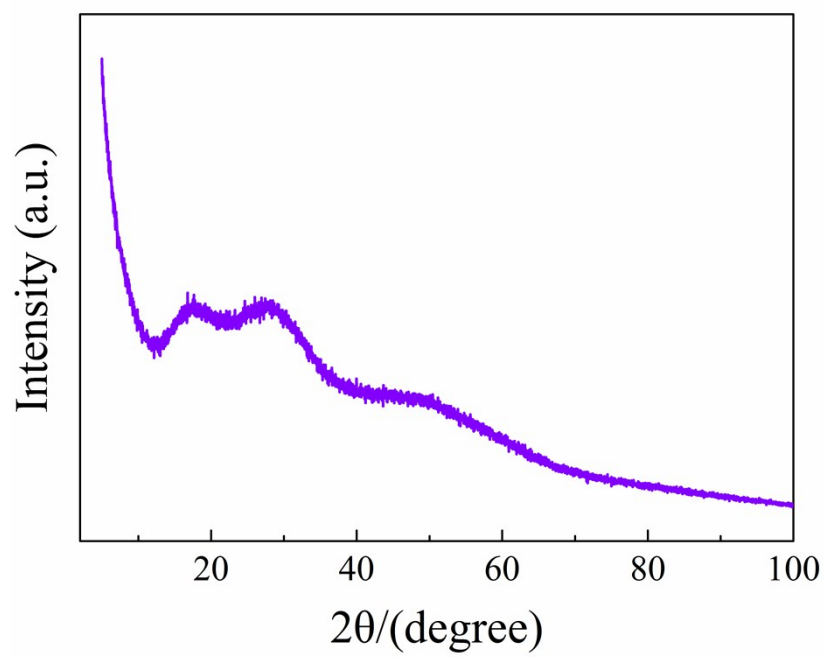
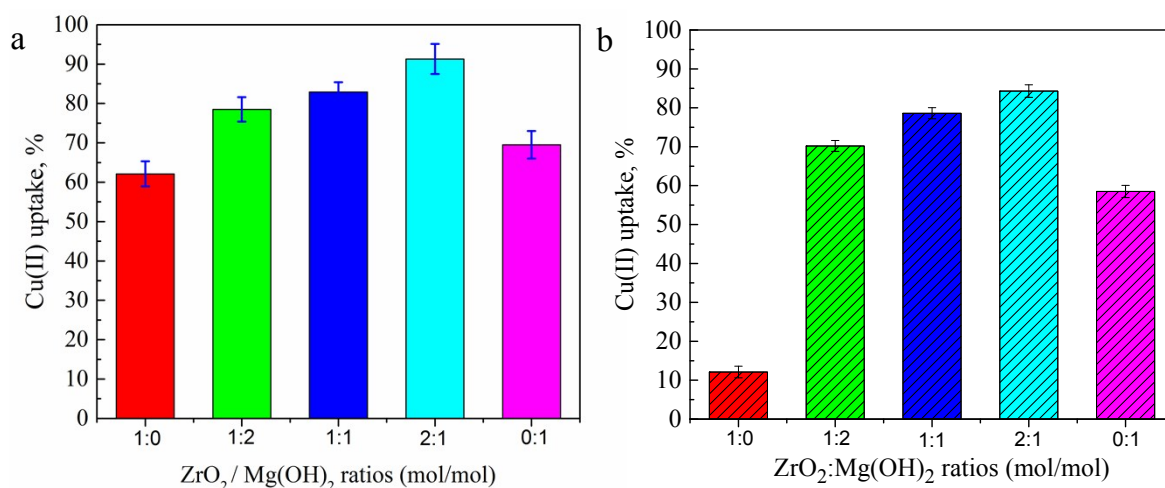


Figure S5 ZrO_2 / $\text{Mg}(\text{OH})_2$ ratios effects on Cu adsorption at different solution environment a)

neutral condition (adsorbent: 0.5g/L, initial Cu 40 mg/L for 10 h sorption equilibrium reaction, pH =5.2-5.5); b) acidic condition (adsorbent: 0.5g/L, initial Cu 40 mg/L for 10 h sorption equilibrium reaction, pH =3.2-3.6, $\text{Ca}(\text{II})=200$ mg/L).



Note: the point of pure $\text{Mg}(\text{OH})_2$ with alkaline pH (pH = 8.5-9.2) due to the strong hydrolysis

Table S1 The effects of common cations on the distribution coefficient K_d of Cu(II) uptake onto the three sorbents

Competing cations(M)	Materials	K_d (mL/g) at different initial competing anions M/Cu(II)(mol/mol)				
		0	8	16	32	64
Ca(II)	Zr/Mg oxide-PS	3.55×10^5	8139	6473	5488	4858
	ZrO ₂ -PS	2.48×10^5	251	271	254	325
	D001	5.83×10^6	568	123	80.5	70.1
Mg(II)	Zr/Mg oxide-PS	3.55×10^5	9490	3952	1864	1381
	ZrO ₂ -PS	2.48×10^5	917	755	306	325
	D001	5.83×10^6	1553	841	59.2	6.61
Na(I)	Zr/Mg oxide-PS	3.55×10^5	2.46×10^5	2.25×10^5	1.85×10^5	2.71×10^4
	ZrO ₂ -PS	2.48×10^5	2.94×10^5	47600	42962	8333
	D001	5.83×10^6	5.83×10^6	1.22×10^5	30000	8412

Table S2 The Parameters of kinetics model for the adsorption of Cu(II) on the host D001 and the hybrid Zr/Mg oxide-PS materials

Materials	Pseudo-first-order model			Pseudo-second-order model			Intraparticle-diffusion model	
	$Q_{ecal}(\text{mg/g})$	$k (/(\text{min}))$	R^2	$Q_{ecal}(\text{mg/g})$	$k \times 10^{-4}(\text{mg/min})$	R^2	$k_p (\text{mg}/(\text{g min}^{1/2}))$	R^2
D001	58.7	0.0163	0.996	75.4	2.05	0.985	5.44	0.995
Zr/Mg oxide-PS	74.5	0.0136	0.994	98.8	1.19	0.988	7.01	0.991

Table S3. Parameters of isotherm model for the adsorption of Cu(II) on the hybrid Zr/Mg oxide-PS at different temperatures at acidic conditions (pH=3.2-3.8).

Temperature (K)	Langmuir model			Freudlich model		
	$Q_{mcal}(\text{mg/g})$	$K_L(\text{Lm/mol})$	R^2	K_F	$1/n$	R^2
288	88.5	4.83	0.856	57.6	0.155	0.948
308	78.1	4.54	0.818	48.5	0.142	0.994
328	77.3	2.75	0.781	44.9	1.24	0.991

Table S4. Sorbent comparison in reported literature for Cu(II) adsorption

Adsorbents	Adsorption capacity(mg/g)	Optimal pH	Reference
γ -alumina nanoparticles	31.30	5.0	s1
imprinting adsorbent	33.33	5.0	s2
xanthate-modified magnetic chitosan	34.5	--	s3
Nanostructured titanium(IV) oxide	52.6	5.0	s4
EGDE-CS-NZVI beads	67.2	6.62	s5
Graphene oxide–CdS	137.17	6.0	s6
CS/PAA-MCM	174.0	5.5	s7
Conjugate nanomaterials	183.81	5.5	s8
EDTA-mGO	301.2	5.1	s9
Zr/Mg oxide-PS	88.5	3.5-5.5	This study

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