

# Electronic Supplementary Material

## Insight into the adsorption behaviour and mechanism of trace impurities from H<sub>2</sub>O<sub>2</sub> solution on functionalized zirconia by tuning the structure of amino groups

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**Table S1** Contents of metallic ions in the H<sub>2</sub>O<sub>2</sub> solution before adsorption

Metallic ions	Content /( $\times 10^{-3}$ mg·L <sup>-1</sup> )	Metallic ions	Content /( $\times 10^{-3}$ mg·L <sup>-1</sup> )
Li	2.74	Rb	3.52
Be	0.02	Sr	7.21
Na	3886	Y	0.03
Mg	101	Zr	1.52
Al	1441	Mo	3.05
K	6963	Ru	0.33
Ca	1744	Cd	0.12
Ti	10.1	Sn	1.38
V	0.20	Sb	0.32
Cr	7.76	Te	0.10
Mn	2.58	Cs	0.30
Fe	16.80	Ce	15.35
Co	0.08	Nd	0.04
Ni	1.07	Sm	0.01
Cu	14.42	Pt	21.2
Zn	44.23	Tl	0.02
Ga	0.60	Pb	2.04
As	2.10	Th	0.05
Se	0.12	U	0.01

**Table S2** Contents of anions and TOC in the H<sub>2</sub>O<sub>2</sub> solution before adsorption

Impurity	Content / (mg·L <sup>-1</sup> )
phosphate	124.36
Cl <sup>-</sup>	8.063
NO <sub>3</sub> <sup>-</sup>	1.639
SO <sub>4</sub> <sup>2-</sup>	1.164
TOC	134.52

**Table S3** Content of impurities in the H<sub>2</sub>O<sub>2</sub> solution after adsorption

Adsorbent	Metallic ions /( $\times 10^{-3}$ mg·L <sup>-1</sup> )						phosphate /(mg·L <sup>-1</sup> )	TOC /(mg·L <sup>-1</sup> )
	Na <sup>+</sup>	K <sup>+</sup>	Ca <sup>2+</sup>	Mg <sup>2+</sup>	Al <sup>3+</sup>	Fe <sup>3+</sup>		
ZrO <sub>2</sub>	3563	6493	977	76	504	8.32	66.85	130.84
ZrO <sub>2</sub> -NH <sub>2</sub>	2727	5584	737	45	222	7.14	64.60	78.19
ZrO <sub>2</sub> -NH	2826	6030	844	72	231	4.64	63.58	87.46
ZrO <sub>2</sub> -N	3290	6336	887	74	358	8.19	60.20	93.91

**Table S4** Fitting results of the adsorption isotherm data

Model	Parameters <sup>a)</sup>	ZrO <sub>2</sub>	ZrO <sub>2</sub> -NH <sub>2</sub>	ZrO <sub>2</sub> -NH	ZrO <sub>2</sub> -N
Langmuir	$q_{m,L}$	1.79	2.85	2.82	3.30
	$K_L$	0.86	3.41	2.07	0.84
Freundlich	$K_F$	0.85	2.11	1.84	1.52
	$n_F$	0.37	0.20	0.26	0.40
Sips	$q_{m,SP}$	1.42	2.70	2.69	2.36
	$K_{SP}$	1.33	4.96	2.50	1.82
	$n_{SP}$	1.97	1.31	1.18	1.24

a):  $q_{m,L}$  is the theoretical maximum adsorption capacity of the Langmuir model, mg/g;  $K_L$  is the Langmuir model coefficient, L/mg;  $K_F$  and  $n_F$  are the Freundlich model coefficient and constant;  $q_{m,SP}$  is the theoretical maximum adsorption capacity of Sips model, mg/g; and  $K_{SP}$  and  $n_{SP}$  are the Sips model coefficient and constant.

**Table S5** Fitting results of the adsorption kinetic data by pseudo-first-order, pseudo-second-order and Elovich models

Model	Parameters <sup>a)</sup>	ZrO <sub>2</sub>	ZrO <sub>2</sub> -NH <sub>2</sub>	ZrO <sub>2</sub> -NH	ZrO <sub>2</sub> -N
Pseudo-first-order	$q_{e,1}$	1.55	2.13	2.10	1.98
	$k_1$	0.276	0.173	0.145	0.155
Pseudo-second-order	$q_{e,2}$	1.70	2.43	2.38	2.30
	$k_2$	0.226	0.087	0.080	0.076
Elovich	a	8.777	3.287	2.326	2.367
	b	4.778	2.873	2.793	2.979

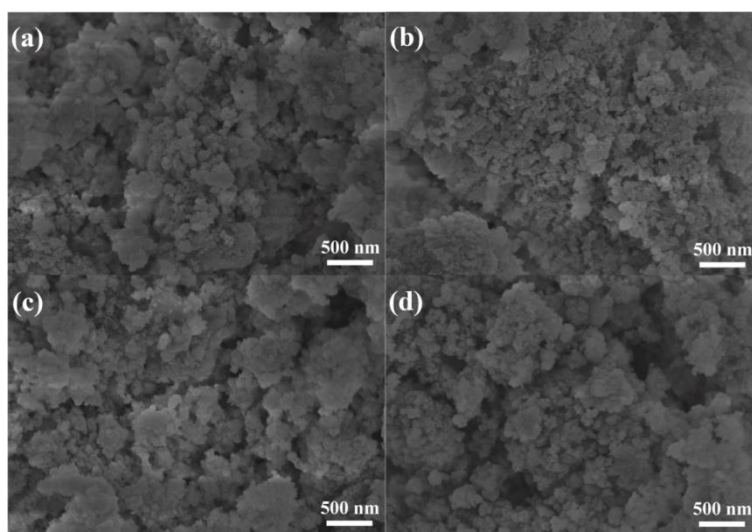
a):  $q_{e,1}$  is the equilibrium adsorption capacity of pseudo-first-order model, mg/g;  $k_1$  is the rate constant

of pseudo-first-order model,  $\text{min}^{-1}$ ;  $q_{e,2}$  is the equilibrium adsorption capacity of pseudo-second-order model,  $\text{mg/g}$ ;  $k_2$  is the rate constant of pseudo-second-order model,  $\text{g}/(\text{mg}\cdot\text{min})$ ;  $a$  is the initial adsorption rate constant,  $\text{mg}/(\text{g}\cdot\text{min})$ ; and  $b$  is the Elovich model constant,  $\text{g}/\text{mg}$ .

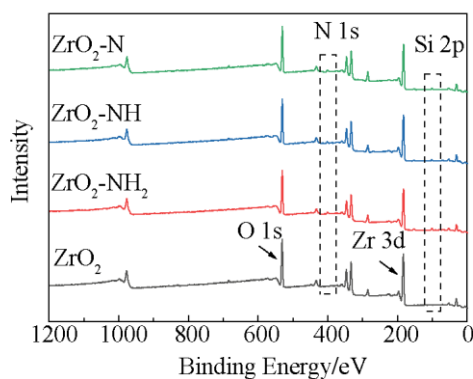
**Table S6** Fitting results of the adsorption kinetic data by Weber–Morris model

Adsorbent	Film diffusion region			Intra particle diffusion region			Surface adsorption region		
	$K^a$	$C^b$	$R^2$	$K^a$	$C^b$	$R^2$	$K^a$	$C^b$	$R^2$
ZrO <sub>2</sub>	0.307	0.380	0.9590	0.183	0.739	0.9976	0.017	1.476	0.9326
ZrO <sub>2</sub> -NH <sub>2</sub>	0.325	0.545	0.9928	0.297	0.617	0.9988	0.062	1.703	0.9396
ZrO <sub>2</sub> -NH	0.332	0.440	0.9999	0.252	0.694	0.9999	0.071	1.554	0.8651
ZrO <sub>2</sub> -N	0.326	0.410	0.9999	0.279	0.533	0.9390	0.065	1.506	0.9867

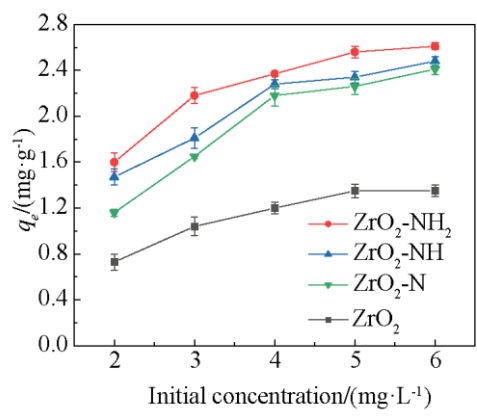
a):  $K$  is the interparticle rate constant (slope of  $q_t-t^{1/2}$  plot),  $\text{mg}/(\text{g}\cdot\text{min}^{1/2})$ ; b):  $C$  is the intercept of  $q_t-t^{1/2}$  plot,  $\text{mg/g}$ .



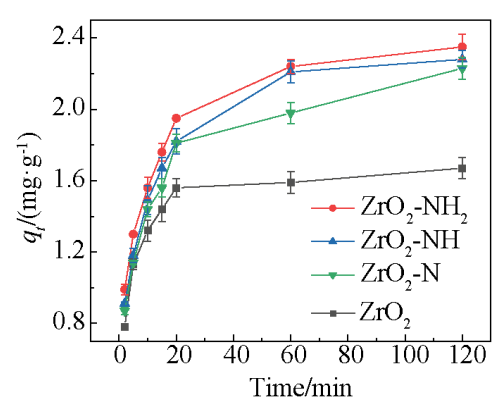
**Fig. S1** SEM images of (a) ZrO<sub>2</sub>, (b) ZrO<sub>2</sub>-NH<sub>2</sub>, (c) ZrO<sub>2</sub>-NH and (d) ZrO<sub>2</sub>-N.



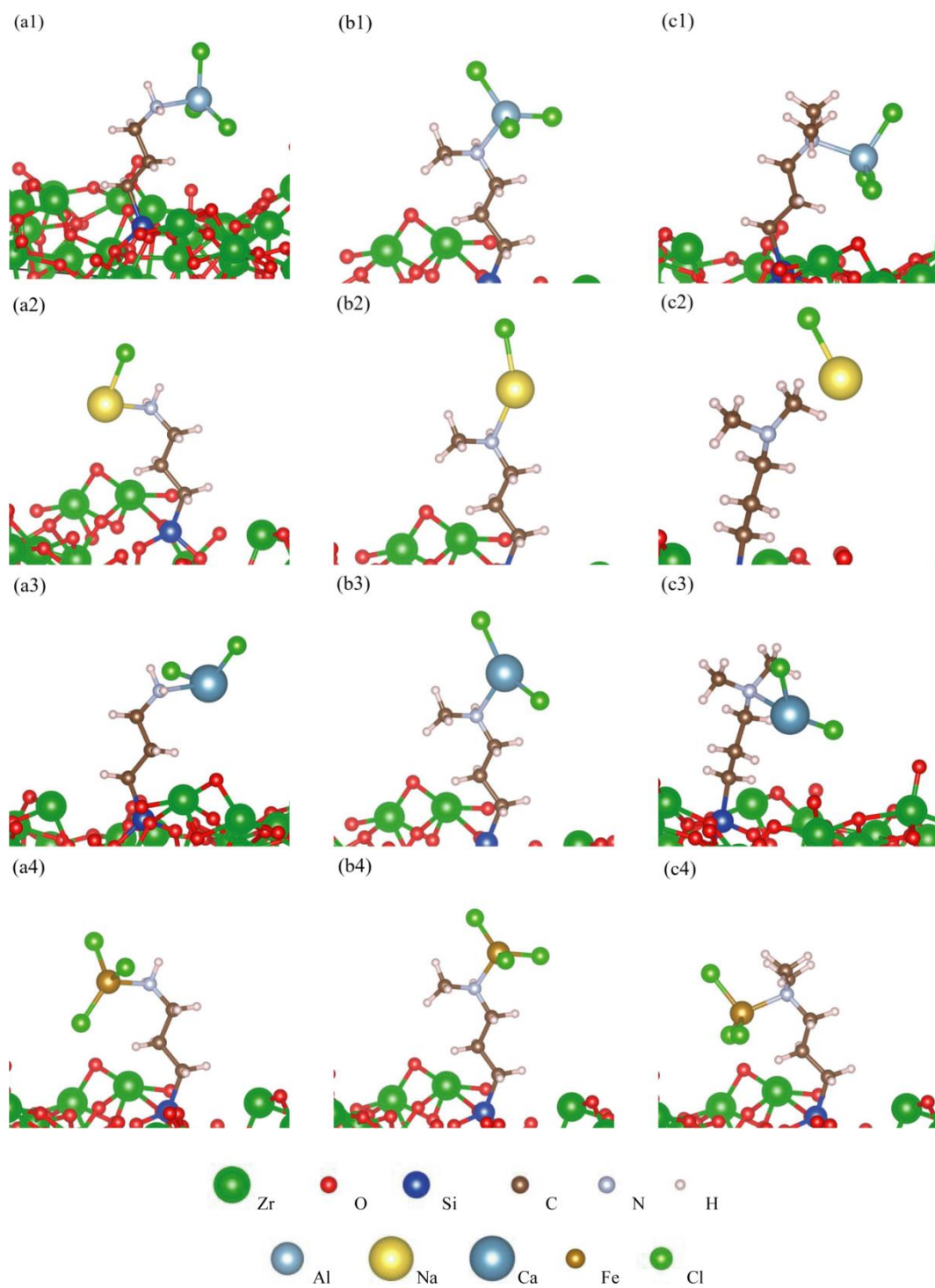
**Fig. S2** XPS spectra of ZrO<sub>2</sub>, ZrO<sub>2</sub>-NH<sub>2</sub>, ZrO<sub>2</sub>-NH and ZrO<sub>2</sub>-N.



**Fig. S3** Effects of the initial concentration on the adsorption removal of Al<sup>3+</sup> at 30 °C (time = 1 h and solution/adsorbent = 20 mL/20 mg).



**Fig. S4** Effects of the contact time on the adsorption removal of Al<sup>3+</sup> at 30 °C and 6 mg/L (solution/adsorbent = 20 mL/20 mg)



**Fig. S5** The optimal configurations of  $\text{AlCl}_3$ ,  $\text{NaCl}$ ,  $\text{CaCl}_2$  and  $\text{FeCl}_3$  adsorbed on  $\text{ZrO}_2\text{-NH}_2$  (a1-a4),  $\text{ZrO}_2\text{-NH}$  (b1-b4) and  $\text{ZrO}_2\text{-N}$  (c1-c4).