Supporting Information

Regulating the particle sizes of NaA molecular sieves toward enhanced heavy metal adsorption

WenLi Cui[a,#], Ke Tang[a,#], Yunqiang Chen[b], Zhou Chen[a], Yihong Lan[b], YuBin Hong[b,*], WeiGuang Lan[a,b,*]

[a] Ms. W.L. Cui, Mr. K. Tang, Dr. Z. Chen, Prof. W.G. Lan

Xiamen University Center for Membrane Application and Advancement, College of Materials, Xiamen University, Xiamen 361005, Fujian, China.

[b] Dr. Y.H. Lan, Mr. Y.Q. Chen, Mr. Y.B. Hong, Prof. W.G. Lan

Suntar Membrane Technology (Xiamen) Co., Ltd., Xiamen 361022, Fujian, China.

# These authors contributed equally to this work.

Corresponding authors: Mr. Y.B. Hong (hongyb@suntar.com); Prof. W.G. Lan (wglan@xmu.edu.cn)

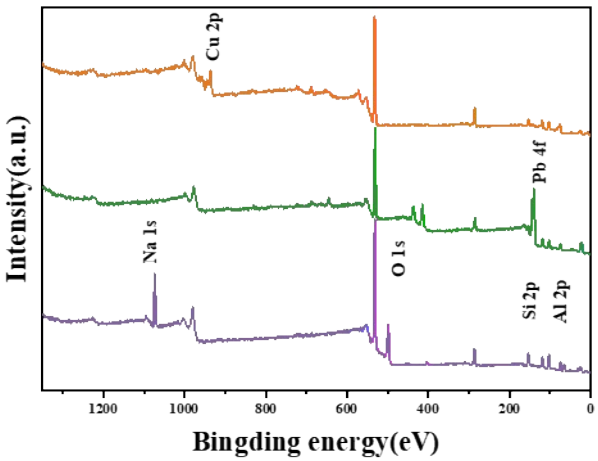

Fig. S1 XPS full spectrum of NaA molecular sieve before and after adsorption.

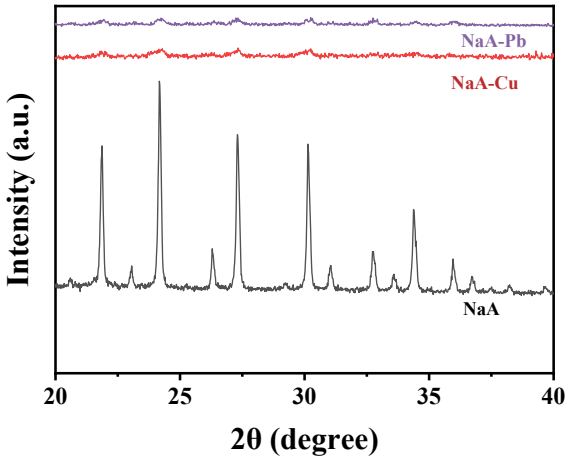

Fig. S2 XRD patterns before and after adsorption of heavy metals ions..

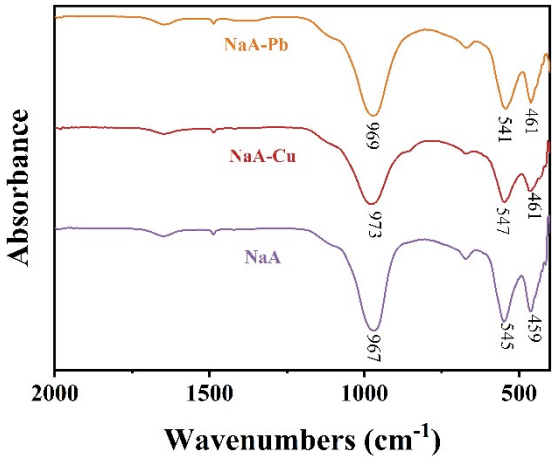

Fig. S3 FTIR spectra before and after adsorption of heavy metals ions

Table S1. NaA molecular sieve synthesis conditions

Number	**Na_2O/Al_2O_3**	**$(TMA)_2O/Al_2O_3$**	**Synthesis time (h)**	**Synthesis temperature (℃)**	**Ageing time (d)**
A1	0.15	6	24	80	1
A2	0.3	6	24	80	1
A3	0.45	6	24	80	1
A4	0.6	6	24	80	1
A5	0.75	6	24	80	1
A6	0.3	4	24	80	1
A7	0.3	8	24	80	1
A8	0.3	10	24	80	1

Table S2. Langmuir adsorption isothermal parameters of Pb(II) on NaA molecular sieves at different temperatures

Heavy metal	**Temperature（℃）**	**q_{max} (mg/g)**	**K_L**	**R^2**
Cu	25	357.1428	0.0223	0.9873
	35	381.6793	0.0239	0.9993
	45	406.50406	0.0241	0.9970
	55	429.1845	0.0270	0.9696
Pb	25	606.0606	0.8638	0.9935
	35	628.9308	1.1276	0.9972
	45	645.1612	1.2109	0.9974
	55	666.6666	1.3513	0.9978

Table S3. Freundlich adsorption isothermal parameters of Pb(II) on NaA molecular sieves at different temperatures

Heavy metal	**Temperature（℃）**	**1/n**	**K_F**	**R^2**
Cu	25	0.5498	0.0212	0.9975
	35	0.5607	0.0226	0.9795
	45	0.5633	0.0240	0.9812
	55	0.5722	0.0260	0.9263
Pb	25	0.1364	0.3601	0.9921
	35	0.13733	0.3810	0.9615
	45	0.1387	0.3932	0.9429
	55	0.1396	0.4087	0.9319

Table S4. Parameters of quasi-primary kinetic modelling of NaA molecular sieve adsorption at different metal ion concentrations

Heavy metal	**Initial concentration (mg/L)**	**$Q_{e, exp}$ (mg/g)**	**$Q_{e, cal}$ (mg/g)**	**K_1**	**R^2**
Pb	25	250			
	50	450	181.8196	0.03591	0.9943
	75	540	195.5079	0.03999	0.9812
	100	600	101.2548	0.03262	0.8817
Cu	25	95	35.2611	0.0255	0.7882
	50	153	42.3213	0.0203	0.9063
	75	193	42.4242	0.0247	0.8180
	100	230	36.8421	0.0263	0.9707

Table S5. Parameters of quasi-secondary kinetic modelling of NaA molecular sieve adsorption at different heavy metal ion concentrations

Heavy metal	**Initial concentration (mg/L)**	**$Q_{e, exp}$ (mg/g)**	**$Q_{e, cal}$ (mg/g)**	**K_1**	**R^2**
Pb	25	250			
	50	450	467.2897	0.00041	0.9995
	75	540	555.5556	0.00045	0.9998
	100	600	609.7561	0.00071	0.9999
Cu	25	95	99.8004	0.0012	0.9981
	50	153	157.9778	0.0014	0.9987
	75	193	195.3125	0.0015	0.9997
	100	230	233.6449	0.0017	0.9999

Table S6. Thermodynamic parameters of Cu and Pb adsorption on NaA molecular sieves

Heavy metal	T (K)	ΔH (kJ/mol)	ΔS (J/mol·K)	ΔG (kJ/mol)
Cu	298	6.8846	32.1798	-2.7112
	308			-3.0142
	318			-3.3495
	328			-3.6765
Pb	298	6.2536	43.4836	-6.7095
	308			-7.1390
	318			-7.5516
	328			-8.0274

Table S7 Changes in heavy metal ion concentration before and after adsorption

	Heavy metal ion concentration before adsorption (mg/L)	Heavy metal ion concentration after adsorption(mg/L)
Cu	100	77
Pb	100	40

We observed a significant reduction in metal ion concentration after the adsorption process, as shown in Table S7. This reduction indicates the effective adsorption capability of NaA molecular sieves. Specific adsorption quantities can be calculated according to Eq. 1 in section 2.3 of the manuscript.

Table S8 Comparison of the performance of NaA molecular sieve and other adsorbents

Absorbent	Adsorbates	Adsorption capacity	Reference
CS-ZIF-8 composite beads	Pb (II) Cu(II)	165.7 mg/g 131.4mg/g	[1]
DTC-AC	Pb (II) Cu(II)	203.36 mg/g 53.13 mg/g	[2]
3DP of zeolite-Y	Cu(II) Pb (II)	7.8 mg/g 8.3 mg/g	[3]
magnetic hollow $MnFe_2O_4$ nanospheres	Pb^{2+}	291.07mg/g	[4]
SBA-15 molecular sieves	Pb^{2+}	131mg/g	[5]
nano-zeolites	Cu(II) Pb (II)	431 mg/g 337.8mg/g	[6]
NaA molecular sieve	Cu(II) Pb (II)	230 mg/g 600 mg/g	This work

Table S9 Specific surface area and pore structure parameters of NaA molecular sieves before and after adsorption of heavy metal ions

Samples	S_{BET} (m^2/g)	V_{BJH} (cm^3/g)	D_{avg} (nm)
NaA molecular sieve	36.9	0.20	21.9
NaA-Pb	21.8	0.15	25.4
NaA-Cu	31.7	0.17	26.8

References:

1. C. Wang, Q. Sun, L. Zhang, T. Su and Y. Yang, *Journal of Environmental Chemical Engineering*, 2022, **10**.
2. H.-Y. Niu, X. Li and J. Li, *New Journal of Chemistry*, 2022, **46**, 5234-5245.
3. A. Khalil, R. Hashaikeh and N. Hilal, *Journal of Water Process Engineering*, 2021, **42**.
4. C. Jin, G. Teng, Y. Gu, H. Cheng, S. Fu, C. Zhang and W. Ma, *New Journal of Chemistry*, 2019, **43**, 5879-5889.
5. V. Hernández-Morales, R. Nava, Y. J. Acosta-Silva, S. A. Macías-Sánchez, J. J. Pérez-Bueno and B. Pawelec, *Microporous and Mesoporous Materials*, 2012, **160**, 133-142.
6. H. Luo, W. W. Law, Y. Wu, W. Zhu and E.-H. Yang, *Microporous and Mesoporous Materials*, 2018, **272**, 8-15.