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Electronic supporting information

Origin of the exceptional selectivity of NaA zeolite for the radioactive isotope $^{90}\text{Sr}^{2+}$

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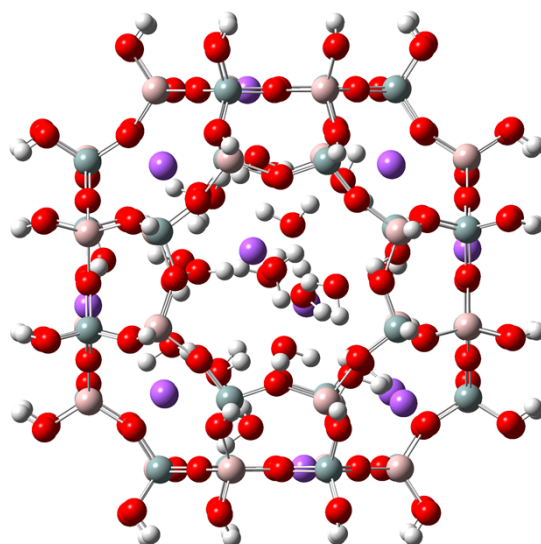


Fig. S1. The structure of the simulation model with the formal formula of $[\text{Na}_{14}\text{Al}_{24}\text{Si}_{24}\text{O}_{72}(\text{OH})_{48}\cdot 20\text{H}_2\text{O}]^{10-}$.

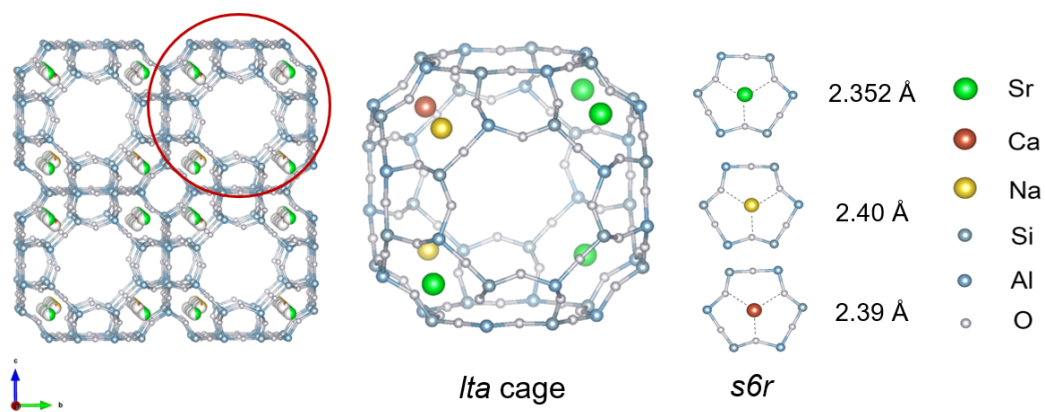


Fig. S2. The crystallographic structure of NaA-Sr-2. All Na^+ , Sr^{2+} , and Ca^{2+} cations locate in the single 6-rings (*s6r*) of the *lta* cage (highlighted in red circle).

Table S1. Adsorption data of NaA toward $^{90}\text{Sr}^{2+}$

Solid/Liquid Ratio (g/mL)	Initial activity concentration (Bq/L)	Equilibrium Activity concentration (Bq/L)	^a Average (Bq/L)	^b Standard Deviation	Removal Efficiency (%)	Average (%)	Standard Deviation	Distribution Coefficient (L/g)	Average (L/g)	Standard Deviation
1/20	400	0.51	0.63	0.12	99.87	99.84	0.0300	15.67	13.07	2.51
		0.75			99.81			10.65		
		0.62			99.85			12.88		
1/100	400	0.75	0.83	0.08	99.81	99.79	0.0200	53.23	48.20	4.73
		0.84			99.79			47.52		
		0.91			99.77			43.86		
1/500	400	1.32	1.38	0.06	99.67	99.65	0.0150	151.02	144.26	6.36
		1.44			99.64			138.39		
		1.39			99.65			143.38		
1/1000	400	1.43	1.56	0.12	99.64	99.61	0.0303	278.72	256.47	20.44
		1.58			99.61			252.16		
		1.67			99.58			238.52		
1/2000	400	1.86	1.89	0.06	99.54	99.53	0.0076	428.11	421.57	13.39
		1.85			99.54			430.43		
		1.96			99.51			406.16		
1/5000	400	40.35	41.52	1.16	89.91	89.62	0.2889	44.57	43.19	1.34
		42.66			89.34			41.88		
		41.55			89.61			43.13		

a: Average:
$$\bar{x} = \frac{\sum_{i=1}^n x_i}{n}$$

Standard Deviation: $S = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n - 1}}$

b:

Table S2. Crystallographic details of Rietveld refinements.

Sample	NaA-Sr-1	NaA-Sr-2	NaA
Space group	<i>Fm-3c</i>	<i>Fm-3c</i>	<i>Fm-3c</i>
a(Å)	24.6803(3)	24.6797(12)	24.5970(4)
V(Å ³)	15033.1(6)	15032(2)	14881.5(6)
R _p	0.03982	0.05238	0.02863
R _{wp}	0.05851	0.07557	0.04300
R _{exp}	0.01321	0.01311	0.01743
R _{bragg}	0.03307	0.03754	0.03150
GOF	4.43	5.76	2.47
Reflections	516	516	512
Parameters	52	52	49
Restraints	6	6	6
CCDC number	2163932	2163933	2163931

Table S3 Hydrated ions form energy of $\text{Na}^+(\text{H}_2\text{O})_6$ and $\text{Sr}^{2+}(\text{H}_2\text{O})_6$

Reaction	ΔE (eV)
$\text{Na}^+ + 6 \text{H}_2\text{O} \rightarrow \text{Na}^+(\text{H}_2\text{O})_6$	-7.31
$\text{Sr}^{2+} + 6 \text{H}_2\text{O} \rightarrow \text{Sr}^{2+}(\text{H}_2\text{O})_6$	-4.04

Table S4 Adsorption data of NaA toward Sr²⁺ at different time

Contact Time (min)	Initial concentration (ppm)	Equilibrium concentration (ppm)	Average (ppm)	Standard Deviation	Removal Efficiency (%)	Average (%)	Standard Deviation
0.25	100	12.384	12.133	3.734	87.616	87.867	0.190
		12.089			87.911		
		11.926			88.074		
0.5	100	10.756	10.774	0.026	89.244	89.226	0.022
		10.804			89.196		
		10.762			89.239		
1	100	4.894	4.888	0.005	95.106	95.112	0.004
		4.885			95.115		
		4.885			95.115		
2	100	0.089	0.091	0.002	99.911	99.909	0.002
		0.093			99.907		
		0.090			99.910		
3	100	0.068	0.062	0.011	99.932	99.938	0.009
		0.069			99.931		
		0.049			99.951		
4	100	0.058	0.057	0.001	99.943	99.943	0.000
		0.057			99.944		
		0.057			99.944		
5	100	0.044	0.047	0.012	99.957	99.953	0.010
		0.037			99.963		
		0.061			99.939		
6	100	0.035	0.035	0.001	99.965	99.965	0.001
		0.037			99.963		
		0.035			99.965		
7	100	0.041	0.042	0.010	99.960	99.958	0.008
		0.052			99.948		
		0.033			99.967		
8	100	0.028	0.038	0.014	99.973	99.962	0.012
		0.054			99.946		
		0.032			99.968		
9	100	0.030	0.046	0.014	99.970	99.954	0.012
		0.049			99.952		
		0.059			99.941		
10	100	0.040	0.038	0.009	99.960	99.962	0.008
		0.046			99.954		
		0.028			99.972		

Table S5 Adsorption data of NaA toward Sr²⁺ at different initial concentration

Initial concentration (ppm)	Equilibrium concentration (ppm)	Average (ppm)	Standard Deviation	Adsorption capacity (mg/g)	Average (mg/g)	Standard Deviation
50	0.0376	0.0241	0.0135	61.153	61.170	0.017
	0.0241					
	0.0106					
100	0.0303	0.0379	0.0123	122.362	122.353	0.015
	0.0314					
	0.0521					
150	0.0893	0.0796	0.0085	183.489	183.501	0.010
	0.0732					
	0.0764					
200	3.5094	3.4933	0.0155	240.503	240.522	0.019
	3.4920					
	3.4785					
250	40.237	41.9388	1.4901	256.747	254.665	1.824
	42.567					
	43.012					
300	76.053	76.3467	0.5086	274.109	273.749	0.623
	76.934					
	76.053					
350	115.817	116.8080	0.9548	286.638	285.425	1.169
	116.885					
	117.722					
400	164.152	163.5083	1.1149	288.676	289.463	1.365
	164.152					
	162.221					

Table S6 Adsorption data of NaA toward Sr²⁺ at different pH values

Initial pH	Initial concentration (ppm)	Equilibrium concentration (ppm)	Average (ppm)	Standard Deviation	Removal Efficiency (%)	Average (%)	Standard Deviation
3	100	43.01	43.240	0.7038	57.32	56.683	0.678
		42.68			55.97		
		44.03			56.76		
4	100	0.037	0.036	0.0010	99.965	99.964	0.095
		0.035			99.964		
		0.036			99.964		
5	100	0.027	0.035	0.0072	99.959	99.962	0.716
		0.041			99.963		
		0.038			99.965		
6	100	0.031	0.040	0.0077	99.954	99.957	0.770
		0.046			99.958		
		0.043			99.960		
7	100	0.073	0.049	0.0255	99.978	99.959	0.255
		0.022			99.949		
		0.051			99.951		
8	100	0.021	0.035	0.0118	99.961	99.961	1.178
		0.039			99.957		
		0.043			99.965		
9	100	0.069	0.045	0.0201	99.964	99.962	0.201
		0.036			99.969		
		0.032			99.955		
10	100	0.044	0.041	0.0056	99.956	99.960	0.561
		0.044			99.966		
		0.034			99.959		
11	100	0.031	0.035	0.0111	99.974	99.964	1.112
		0.026			99.953		
		0.047			99.965		
12	100	0.030	0.046	0.0144	99.952	99.949	0.014
		0.048			99.941		
		0.059			99.954		

Table S7 Adsorption data of NaA toward Sr²⁺ at different adsorbent dosages

Solid/Liquid Ratio (g/mL)	Initial concentration (ppm)	Equilibrium concentration (ppm)	Average (ppm)	Standard Deviation	Removal Efficiency (%)	Average (%)	Standard Deviation	Adsorption capacity (mg/g)	Average (mg/g)	Standard Deviation
1/100	100	0.043	0.038	0.009	99.9566	99.962	0.009	12.235	12.235	0.001
		0.044			99.9562			12.235		
		0.028			99.9719			12.236		
1/200	100	0.042	0.035	0.006	99.9581	99.965	0.006	24.470	24.471	0.001
		0.030			99.9696			24.472		
		0.034			99.9665			24.472		
1/500	100	0.028	0.036	0.008	99.9722	99.964	0.008	61.182	61.177	0.005
		0.038			99.9621			61.176		
		0.044			99.9563			61.173		
1/1000	100	0.040	0.038	0.009	99.9599	99.962	0.009	122.350	122.352	0.011
		0.046			99.9538			122.342		
		0.028			99.9722			122.365		
1/2000	100	1.342	1.337	0.004	98.6581	98.663	0.004	241.513	241.526	0.011
		1.335			98.6651			241.530		
		1.334			98.6664			241.533		