Supporting Information for

Macrocyclic Ligands Decorated Ordered Mesoporous Silicas with Large-Pore and Short-Channel Characteristics for Effective Separation of Lithium Isotopes: Synthesis, Adsorptive Behavior Study and DFT Modeling

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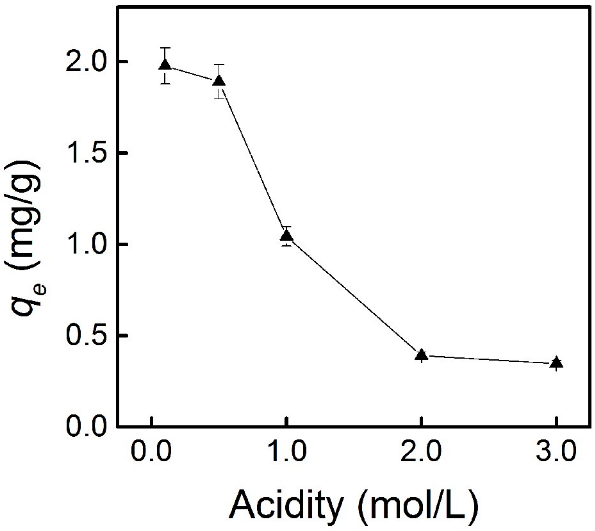

Figure S1. Influence of acidity in aqueous phases on the Li(I) adsorption capacity of SBA-NH-B15C5

Table S1 Kinetic parameters fitted by using different kinetic models.

Pseudo-second-order model [a]			Pseudo-second-order model				Intraparticle diffusion model [b]		
k_1 (min^{-1})	R^2	$q_{t,cal}$ (mg/g)	k_2 (g mg^{-1} min^{-1})	R^2	$q_{t,cal}$ (mg/g)	h (mg g^{-1} min^{-1})	k_3 (mg g^{-1} $min^{1/2}$)	R^2	C (mg/g)
0.039	0.697	0.84	0.096	0.998	2.38	0.54	0.108	0.461	1.29

[a] The pseudo-first-order model is written as $\log(q_e - q_t) = \log(q_e) - \frac{k_1}{2.303}t$, where q_e and q_t (mg/g) are the adsorption capacity of Li(I) at equilibrium and at time t (min), respectively, k_1 (min^{-1}) is the rate constant.

[b] The intraparticle diffusion model is written as $q_t = k_3 t^{1/2} + C$, where k_3 (mg g^{-1} $min^{1/2}$) is the rate constant, q_t (mg/g) is the adsorption capacity of Li(I) at time t (min), and C represents the thickness of the boundary layer.

Table S2. Enthalpy changes ΔH^0, entropy changes ΔS^0 and Gibbs free energy change ΔG^0 of the Li(I) adsorption reaction $\mathrm{Li}^+_{aq} + nL_s + X^-_{aq} = (\mathrm{Li}^+ nL)X^-_s$. L_s represents the SBA-NH-B15C5 OMSs.

Sample	Temperature (K)	ΔH^0 (kJ/mol)	ΔS^0 J/(mol K)	ΔG^0 (kJ/mol)
SBA-NH-B15C5	288.15	-26.2	-89.3	-0.46
	298.15			0.42
	311.15			1.59

Table S3. Comparison of separation factor of lithium isotopes by the SBA-NH-B15C5 and other sorbents reported in the literature.

Sorbents	Experimental conditions	α	Ref.
B15C5 impregnated silica resin	T=35 °C, 0.55 M Li(I) in methanol/HCl (V/V=3/7)	1.013	1
B15C5 bonded phenol resin	T=35 °C, 0.6 M Li(I) in methanol/HCl (V/V=3/7)	1.033	2
Azacrown merrifield resin	T=25 °C, 1000 ppm Li(I) in DI water	1.001	3
N_4O_2 azacrown ion exchanger	T=20 °C, 1000 ppm Li(I) in DI water	1.038	4
N_4S_2 azacrown ion exchanger	T=25 °C, 500 ppm Li(I) in DI water	1.034	5
B15C5 bonded merrifield resin	T=20 °C, 485 ppm Li(I) in DI water	1.026	6
IL17-5SGs & IL17-5IRs	T=25 °C, 20 mM Li(I)	1.048	7
IL15SGs	Room temperature, 20 mM Li(I)	1.046	8
SBA-NH-B15C5	T=15 °C, 2.0 g/L Li(I) in DI water	1.049	This work

Supporting references

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