Research on Modification of Oxygen-Producing Adsorbents for High-Altitude and Low-Pressure Environments

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Separation coefficient calculation formula

（1）Calculation of the ratio of nitrogen and oxygen adsorption capacity

$$\mathrm{S}=\frac{\Delta q_{\mathrm{N2}}}{\Delta q_{\mathrm{O2}}} \quad \text{（S1）}$$

（2）Langmuir's formula fitting calculations

$$\alpha_{\mathrm{N_2O_2}}=\frac{(x/\mathrm{y})_{\mathrm{N_2}}}{(x/\mathrm{y})_{\mathrm{O_2}}} \quad \text{（S2）}$$

$$\alpha_{\mathrm{N_2O_2}}=\frac{x_{\mathrm{N_2}}/y_{\mathrm{N_2}}}{x_{\mathrm{O_2}}/y_{\mathrm{O_2}}}=\frac{x_{\mathrm{N_2}}/y_{\mathrm{N_2}}}{(1-x_{\mathrm{N_2}})/(1-y_{\mathrm{N_2}})}=\frac{q_{\mathrm{mN2}}\mathrm{b}_{\mathrm{N2}}}{q_{\mathrm{mO2}}\mathrm{b}_{\mathrm{O2}}} \quad \text{（S3）}$$

$$\mathrm{S}=\frac{q_{\mathrm{mN2}}\mathrm{b}_{\mathrm{N2}}}{q_{\mathrm{mO2}}\mathrm{b}_{\mathrm{O2}}} \quad \text{（S4）}$$

（3）IAST calculation method

$$Py_{\mathrm{i}}\phi_{\mathrm{i}}=x_{\mathrm{i}}\gamma_{\mathrm{i}}f_{\mathrm{i}}^{0} \quad \text{（S5）}$$

$$Py_{\mathrm{i}}=f_{\mathrm{i}}^{0}x_{\mathrm{i}} \quad \text{（S6）}$$

$$\phi_{\mathrm{i}}=-RT\int_{0}^{f_{\mathrm{i}}^{0}}N_{\mathrm{i}}^{0}(f_{\mathrm{i}})\mathrm{d}\ln f_{\mathrm{i}} \quad \text{（S7）}$$

$$N=A_{1}\frac{\mathrm{b}_{1}P}{1+\mathrm{b}_{1}P} \quad \text{（S8）}$$

$$Py_{1}=f_{1}^{0}x_{1} \quad \text{（S9）}$$

$$\phi_{1}=\phi_{2} \quad \text{（S10）}$$

$$x_{1}+x_{2}=1 \quad \text{（S11）}$$

$$y_{1}+y_{2}=1 \quad \text{（S12）}$$

$$\mathrm{S}=\left(\frac{x_{1}}{x_{2}}\right)\left(\frac{y_{2}}{y_{1}}\right) \quad \text{（S13）}$$

（4）Calculation of Nitrogen-Oxygen Separation Factor for Oxygen Generating Adsorbents in Process Utilization

$$\mathrm{S}=\frac{\Delta q_{\mathrm{N2}}}{\Delta q_{\mathrm{O2}}}\cdot\frac{q_{m\mathrm{N2}}b_{\mathrm{N2}}}{q_{m\mathrm{O2}}b_{\mathrm{O2}}} \quad \text{（S14）}$$

The total pore volume varies with the pore width

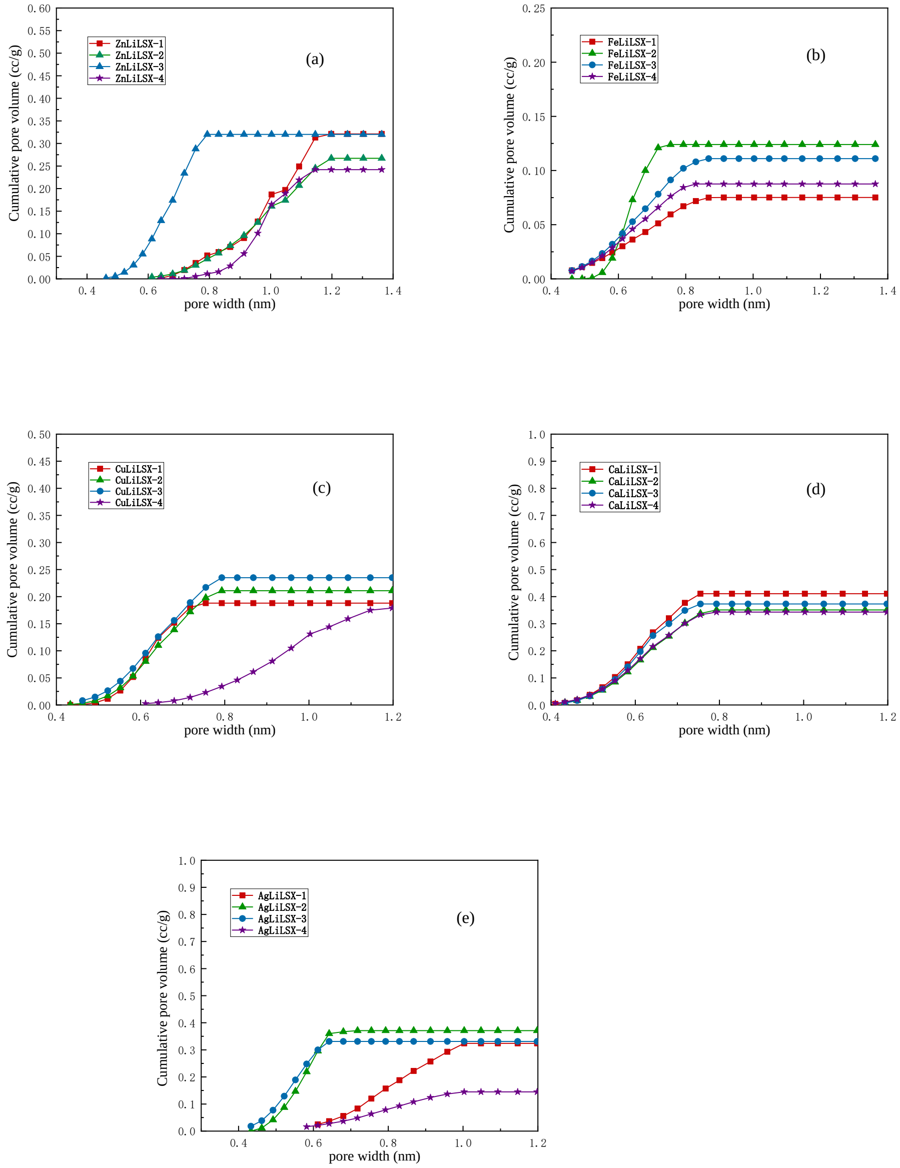

Figure S1. Curve of total pore volume of adsorbent with pore width ((a) Li-LSX, (b) AgLi-LSX, (c) CaLi-LSX, (d) ZnLi-LSX, (e) CuLi-LSX, (f) FeLi-LSX)

adsorption isotherm

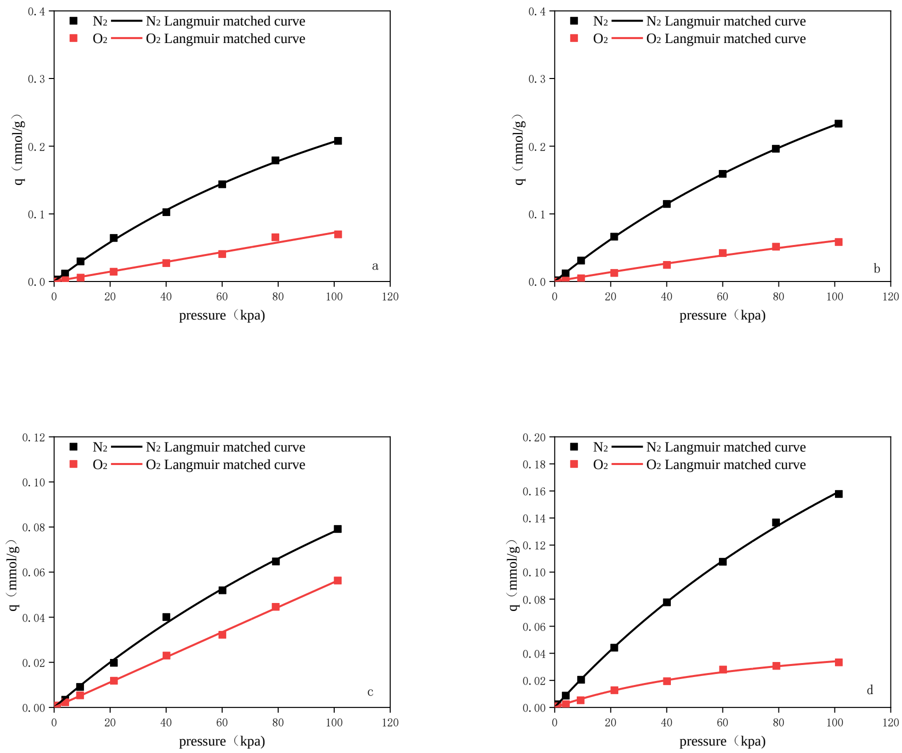

Figure S2. FeLi-LSX adsorption isotherm（a,b,c,d is FeLi-LSX-1, FeLi-LSX-2, FeLi-LSX-3, FeLi-LSX-4）

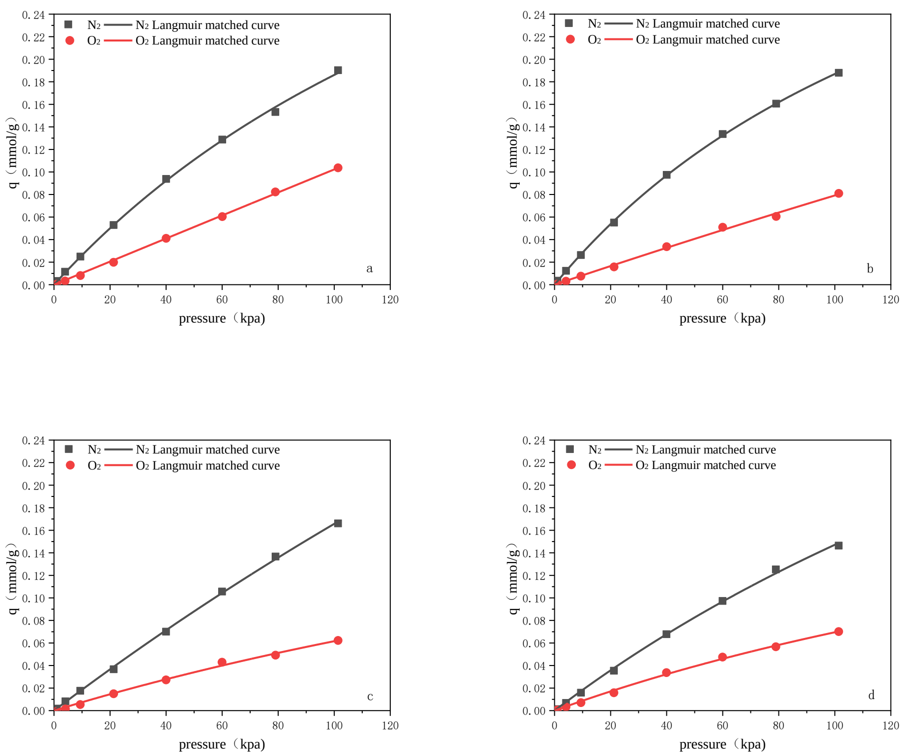

Figure S3. CuLi-LSX adsorption isotherm（a,b,c,d is CuLi-LSX-1, CuLi-LSX-2, CuLi-LSX-3, CuLi-LSX-4）

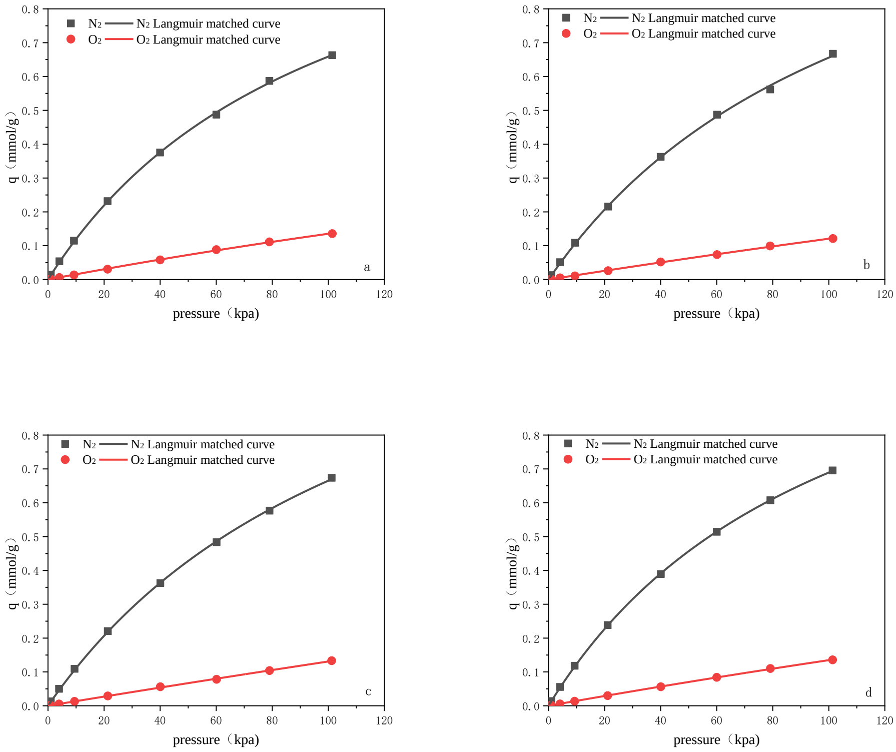

Figure S4. ZnLi-LSX adsorption isotherm（a,b,c,d is ZnLi-LSX-1、ZnLi-LSX-2、ZnLi-LSX-3,ZnLi-LSX-4）

Table S1. Agilent ICPOES730 instrument element test

adsorbent	Sample quality /g	constant volume /ml	Dilution factor	element	instrument reading	unit	Converted content	unit	wt.%
AgLi-LSX-1	0.0542	25	50	Ag	6.8328	mg/L	157582.8	mg/kg	15.7583
AgLi-LSX-2	0.0529	25	50	Ag	6.8354	mg/L	161516.8	mg/kg	16.1517
AgLi-LSX-3	0.0489	25	50	Ag	6.3201	mg/L	161556.0	mg/kg	16.1556
AgLi-LSX-4	0.0554	25	50	Ag	6.7909	mg/L	153223.8	mg/kg	15.3224
AgLi-LSX-1	0.0542	25	50	Al	5.2967	mg/L	122156.1	mg/kg	12.2156
AgLi-LSX-2	0.0529	25	50	Al	5.3390	mg/L	126157.4	mg/kg	12.6157
AgLi-LSX-3	0.0489	25	50	Al	4.9141	mg/L	125615.0	mg/kg	12.5615
AgLi-LSX-4	0.0554	25	50	Al	5.1861	mg/L	117015.3	mg/kg	11.7015
AgLi-LSX-1	0.0542	25	50	Li	1.1146	mg/L	25705.7	mg/kg	2.5706
AgLi-LSX-2	0.0529	25	50	Li	1.0771	mg/L	25452.3	mg/kg	2.5452
AgLi-LSX-3	0.0489	25	50	Li	1.0450	mg/L	26713.4	mg/kg	2.6713
AgLi-LSX-4	0.0554	25	50	Li	1.1048	mg/L	24928.0	mg/kg	2.4928
CaLiLSX-2	0.0569	25	50	Al	6.6735	mg/L	146605.9	mg/kg	14.6606
CaLiLSX-2	0.0569	25	50	Li	1.0472	mg/L	23004.2	mg/kg	2.3004

Table S2. Summary of specific surface area and pore volume

name	S（m^2/g）	V（cm^3/g）
Li-LSX	643	0.356
AgLi-LSX-1	677.403	0.656
AgLi-LSX-2	689.436	0.472
AgLi-LSX-3	662.317	0.478
AgLi-LSX-4	471.219	0.433
CaLi-LSX-1	797.156	0.514
CaLi-LSX-2	845.654	0.633
CaLi-LSX-3	881.097	0.630
CaLi-LSX-4	865.132	0.664
ZnLi-LSX-1	714.209	0.469
ZnLi-LSX-2	935.210	0.809
ZnLi-LSX-3	910.260	0.724
ZnLi-LSX-4	604.862	0.375
CuLi-LSX-1	451.933	0.378
CuLi-LSX-2	513.806	0.528
CuLi-LSX-3	863.182	0.820
CuLi-LSX-4	724.122	0.730
FeLi-LSX-1	706.817	0.973
FeLi-LSX-2	466.071	0.469
FeLi-LSX-3	718.816	0.843
FeLi-LSX-4	699.334	0.923

Table S3. Maximum pore volume per unit pore diameter of different adsorbents between 0.4-0.728nm

name	dV（cm^3/nm/g）	name	dV（cm^3/nm/g）
Li-LSX	1.00	ZnLiLSX-3	1.58
AgLiLSX-1	1.01	ZnLiLSX-4	1.86
AgLiLSX-2	2.56	CuLiLSX-1	1.25
AgLiLSX-3	2.00	CuLiLSX-2	1.00
AgLiLSX-4	0.52	CuLiLSX-3	1.02
CaLiLSX-1	2.04	CuLiLSX-4	0.62
CaLiLSX-2	1.54	FeLiLSX-1	0.25
CaLiLSX-3	1.97	FeLiLSX-2	1.02
CaLiLSX-4	1.52	FeLiLSX-3	0.36
ZnLiLSX-1	1.78	FeLiLSX-4	0.30
ZnLiLSX-2	1.03		

Note：dV represent Maximum pore volume per unit aperture.

Table S4. Nitrogen and oxygen separation performance of adsorbent

name	N_2（ml/g）	O_2（ml/g）	S1	S2	S3	$q_{m_{N_2}}$	$q_{m_{O_2}}$	b_{N_2}	b_{O_2}
Li-LSX	24.68	3.48	7.09	11.58	11.23	2.5694	37.788	0.0074	0.00004
ZnLi-LSX-1	14.85	3.04	4.88	8.37	9.45	1.3224	0.9679	0.0099	0.0016
ZnLi-LSX-2	14.94	2.71	5.51	9.23	9.03	1.4357	1.5555	0.0084	0.0008
ZnLi-LSX-3	15.09	2.98	5.06	8.77	7.64	1.4944	3.1019	0.0080	0.0004
ZnLi-LSX-4	15.58	3.04	5.13	9.21	8.83	1.4045	1.6285	0.0096	0.0009
CuLi-LSX-1	4.26	2.32	1.84	2.67	2.24	0.5813	39.730	0.0047	0.00003
CuLi-LSX-2	4.21	1.81	2.33	3.61	3.12	0.4909	1.4963	0.0062	0.0006
CuLi-LSX-3	3.72	1.39	2.68	2.48	2.99	1.4028	0.3269	0.0013	0.0023
CuLi-LSX-4	3.28	1.57	2.09	2.08	2.40	0.6682	0.2998	0.0028	0.0030
FeLi-LSX-1	5.23	1.31	3.99	4.75	5.61	0.5760	21.084	0.0056	0.00003
FeLi-LSX-2	4.65	1.56	2.98	4.45	3.66	0.7215	0.3733	0.0047	0.0019
FeLi-LSX-3	3.53	0.75	4.71	3.11	11.95	0.2848	13.485	0.0038	0.00004
FeLi-LSX-4	1.77	1.26	1.40	1.93	1.66	0.5010	0.0629	0.0046	0.0118

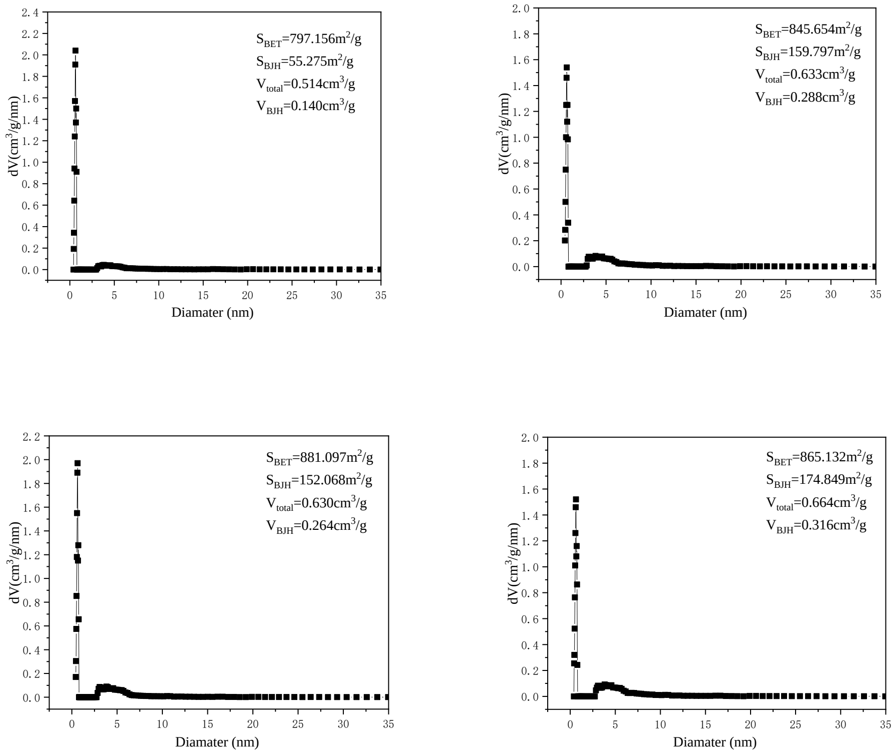

Figure S5. Specific surface area obtained from CaLi-LSX modification (abcd in order of modification 0.5h, 1.0h, 1.5h and 2.0h). [S_{BET} represents the total specific surface area, S_{BJH} represents the mesoporous specific surface area, V_{tatal} represents the total pore volume, and V_{BJH} represents the mesoporous pore volume.]

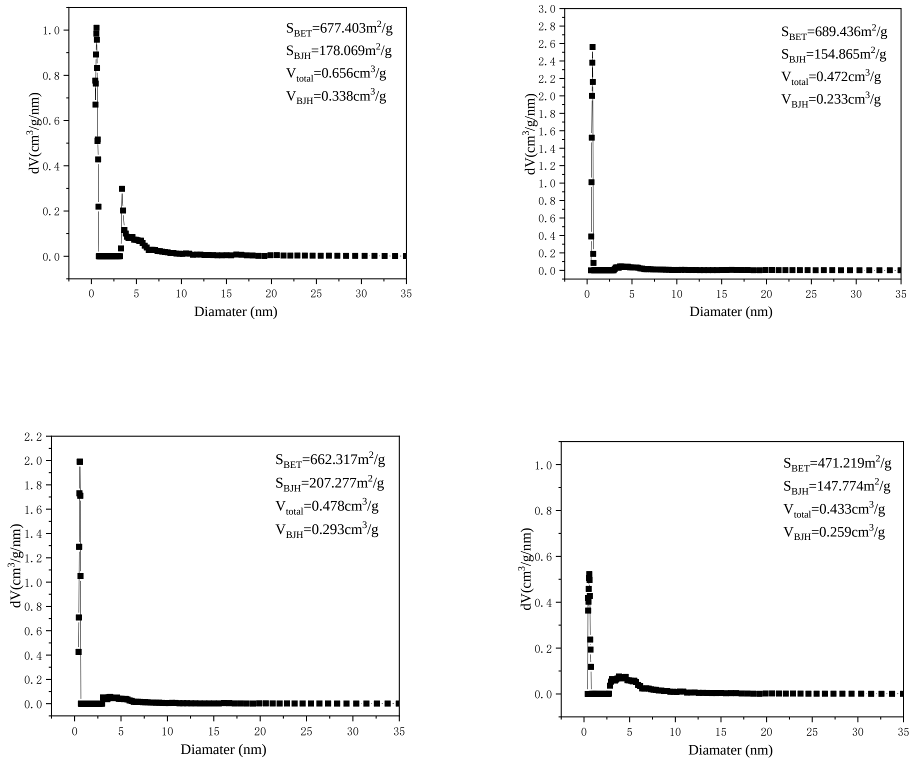

Figure S6. Specific surface area obtained from AgLi-LSX modification (abcd in order of modification 0.5h, 1.0h, 1.5h and 2.0h)

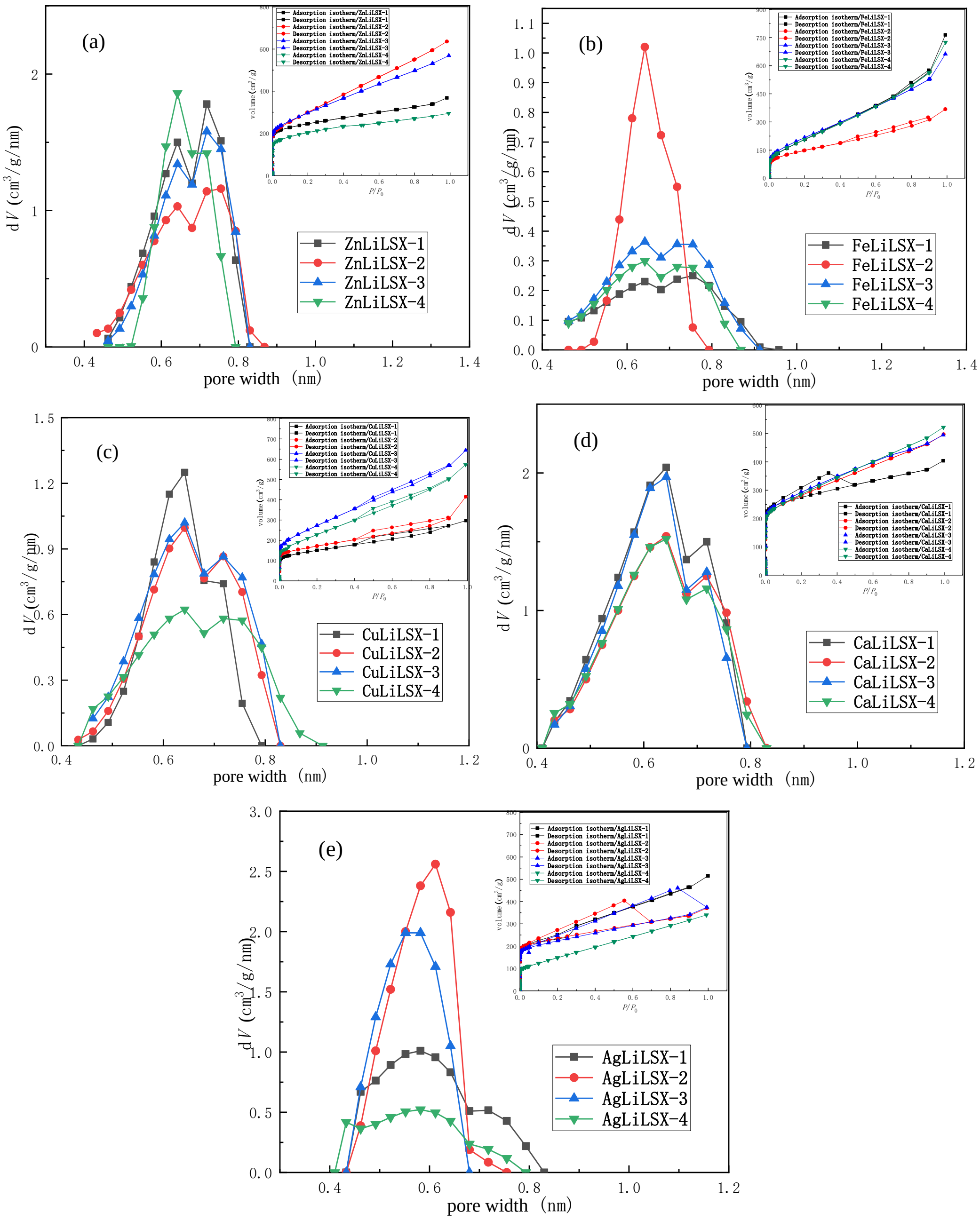

Figure S7. Pore size distribution and Ar adsorption and desorption of modified adsorbents (a for ZnLi-LSX, b for FeLi-LSX, c for CuLi-LSX, d for CaLi-LSX, e for AgLi-LSX)