Supplementary Information (SI) for Nanoscale.

Mesoporous Silica-Amine Beads from Blast Furnace Slag for CO_2 Capture Applications

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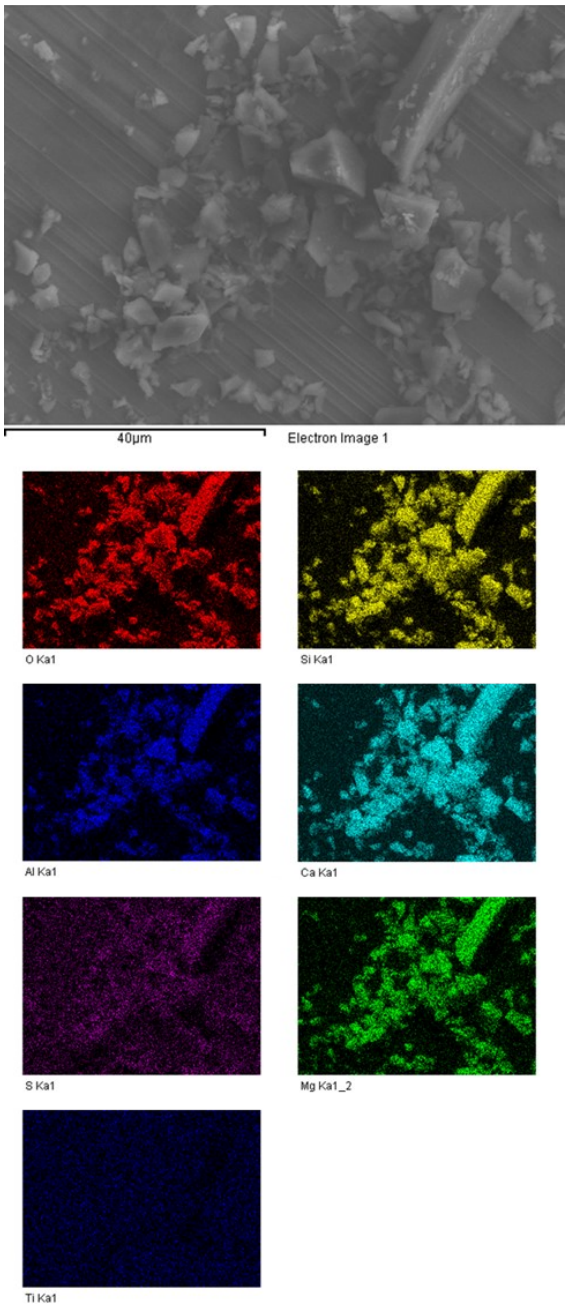

Figure S1. Elemental mapping of original BFS sample.

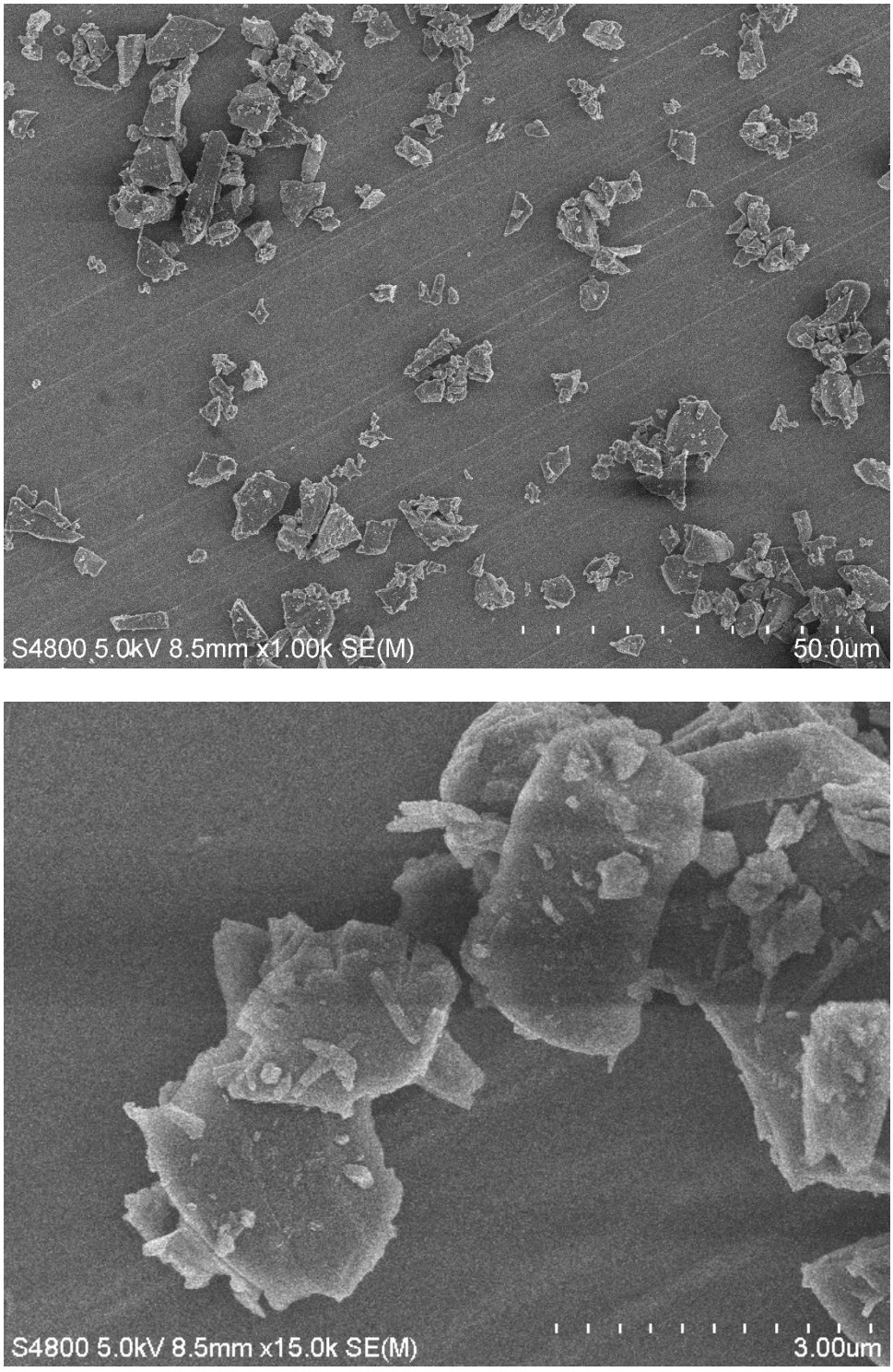

Figure S2. SEM images of BFS.

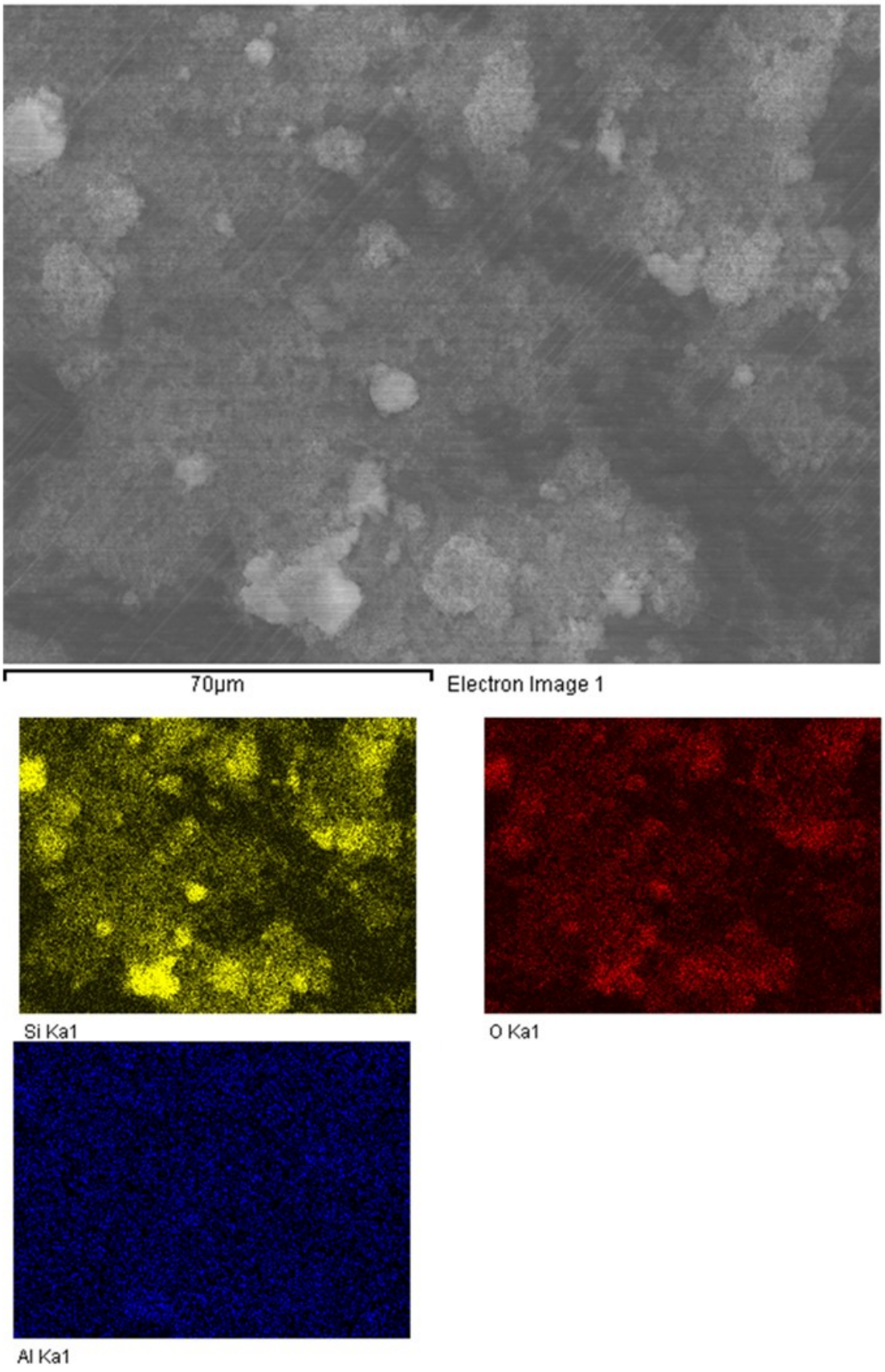

Figure S3. Elemental mapping of mesoporous silica.

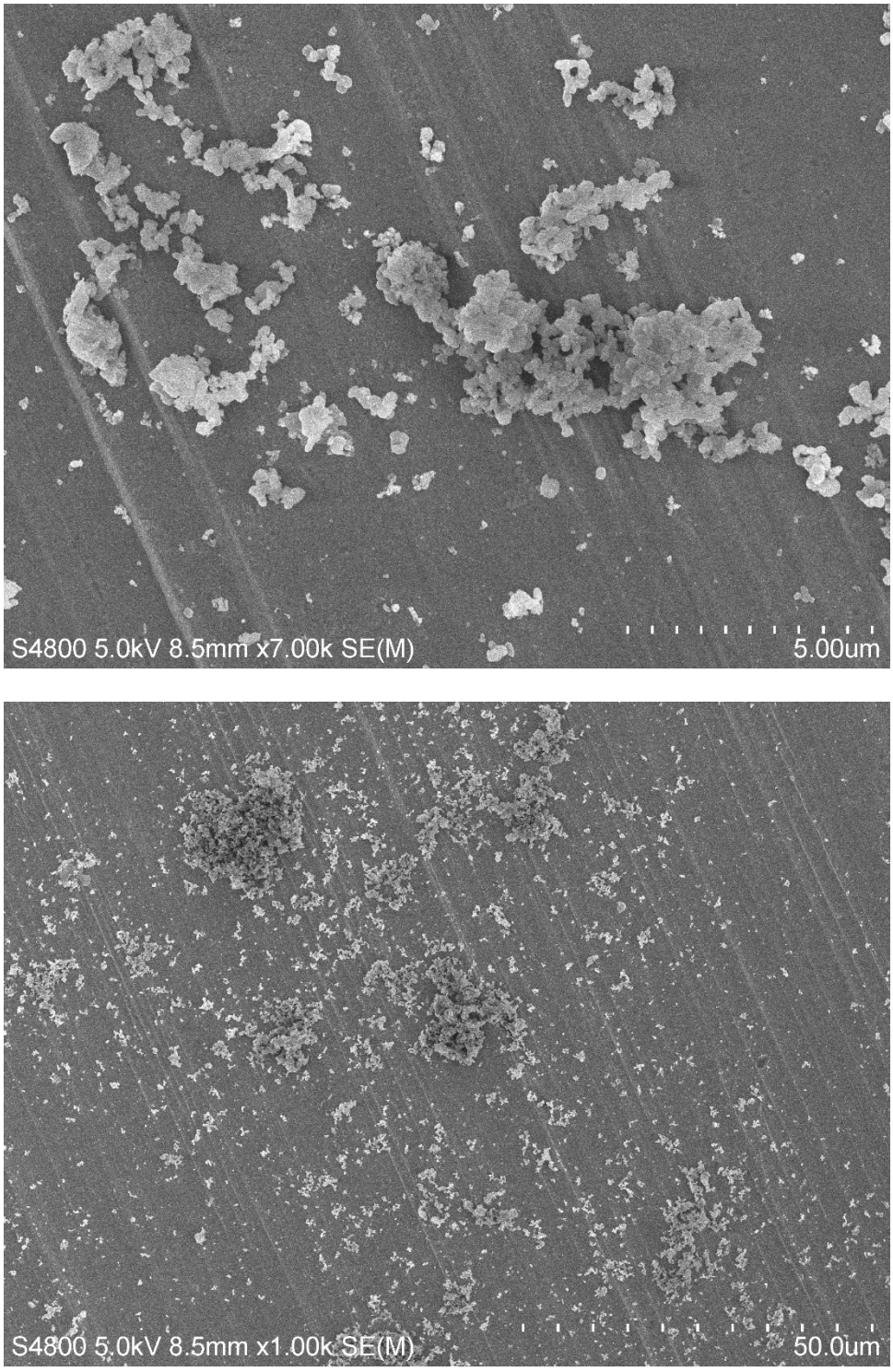

Figure S4. SEM images of mesoporous silica.

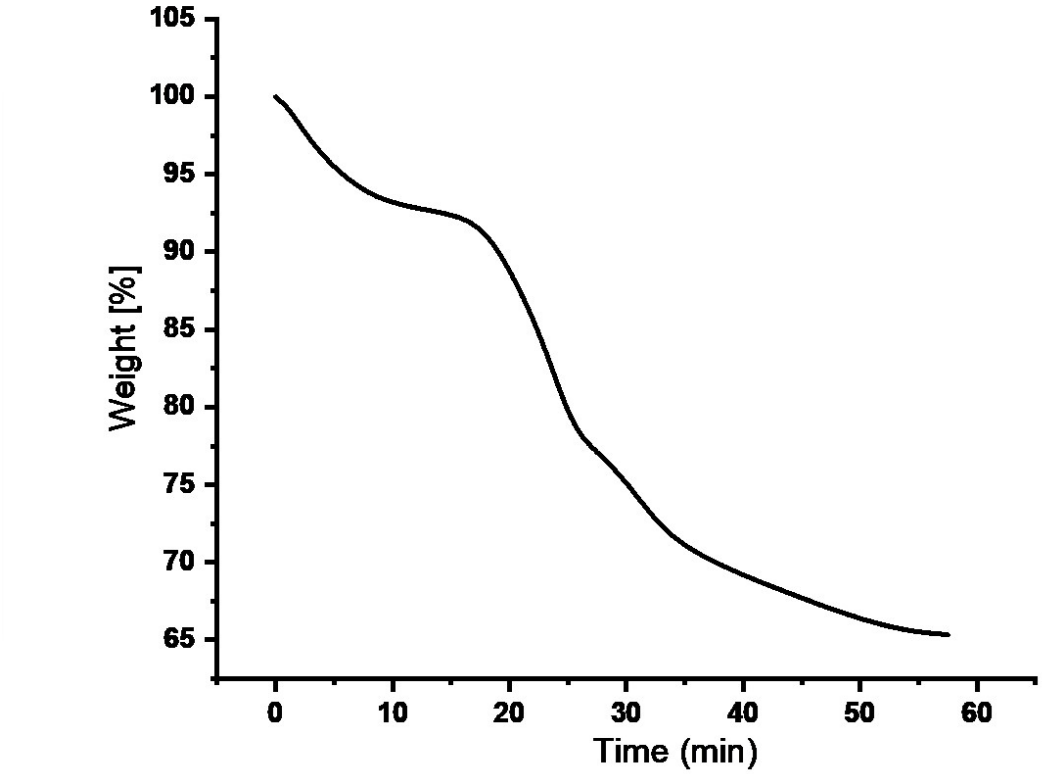

Figure S5. TGA analysis of mesoporous silica. TGA was performed from 25 to 600 °C with rate of 10 °C under the flow of air (50 ml/min).

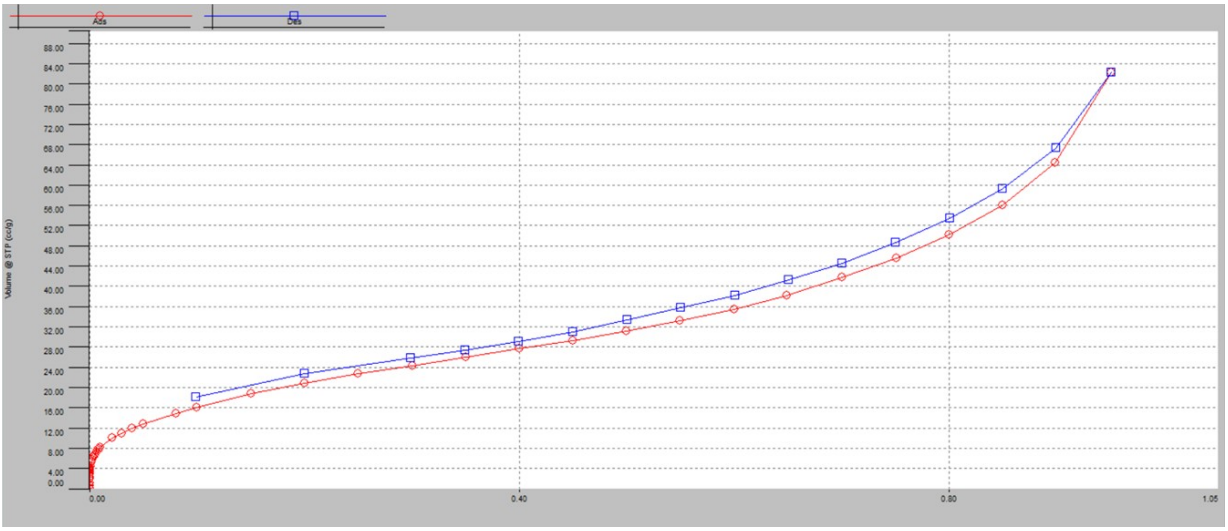

Figure S6. N_2 adsorption isotherm of mesoporous silica.

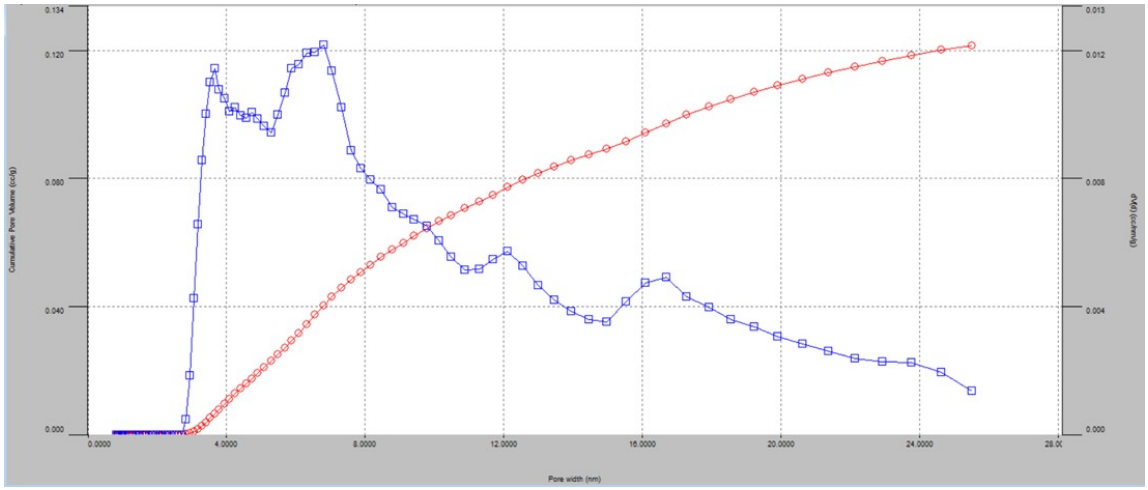

Figure S7. DFT pore size distribution of mesoporous silica.

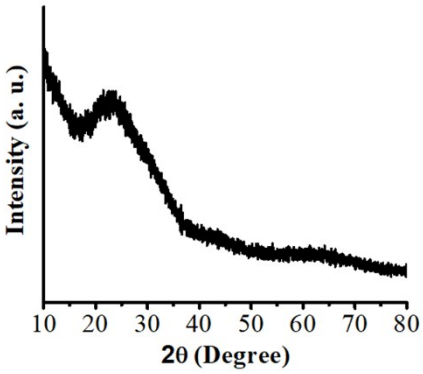

Figure S8. PXRD of mesoporous silica.

Figure S9. Digital image of mesoporous silica beads.

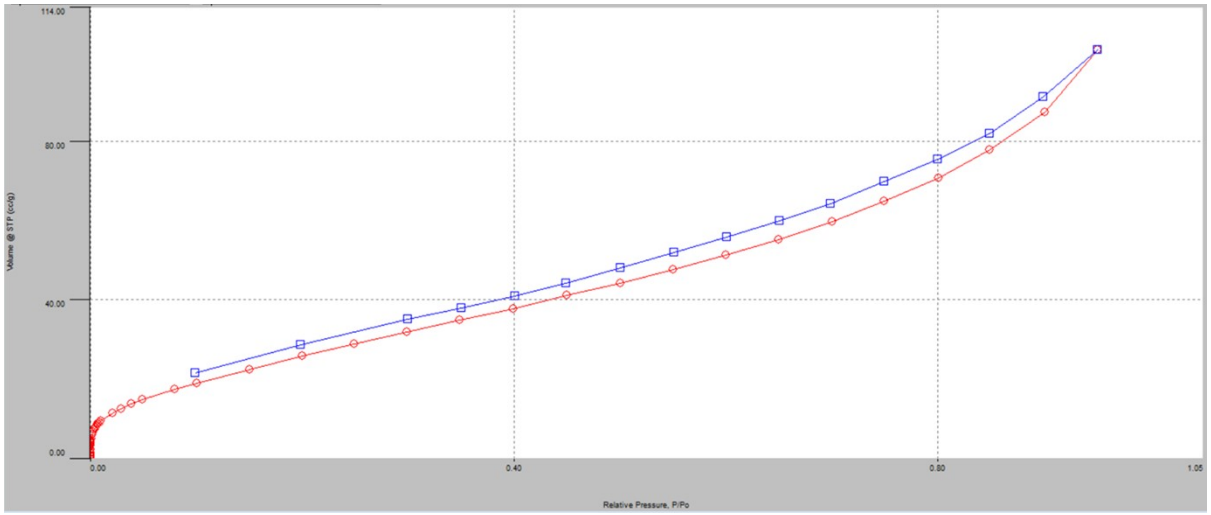

Figure S10. N_2 sorption isotherm of mesoporous silica beads.

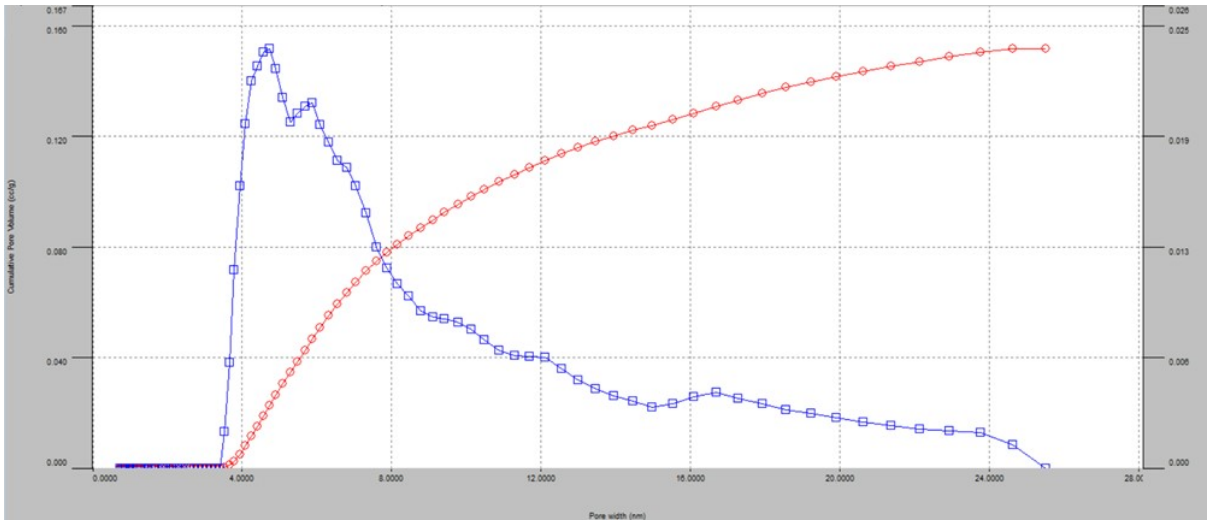

Figure S11. Pore size distribution of mesoporous silica beads.

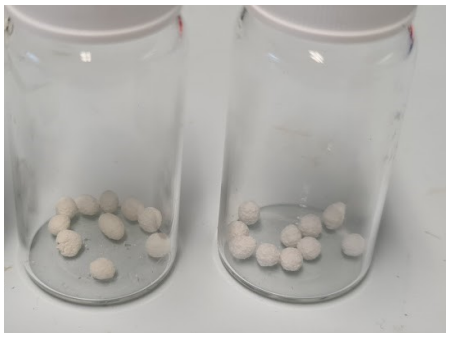

Figure S12. digital image of mesoporous silica beads after HMDA (left) and PEI (right) functionalization.

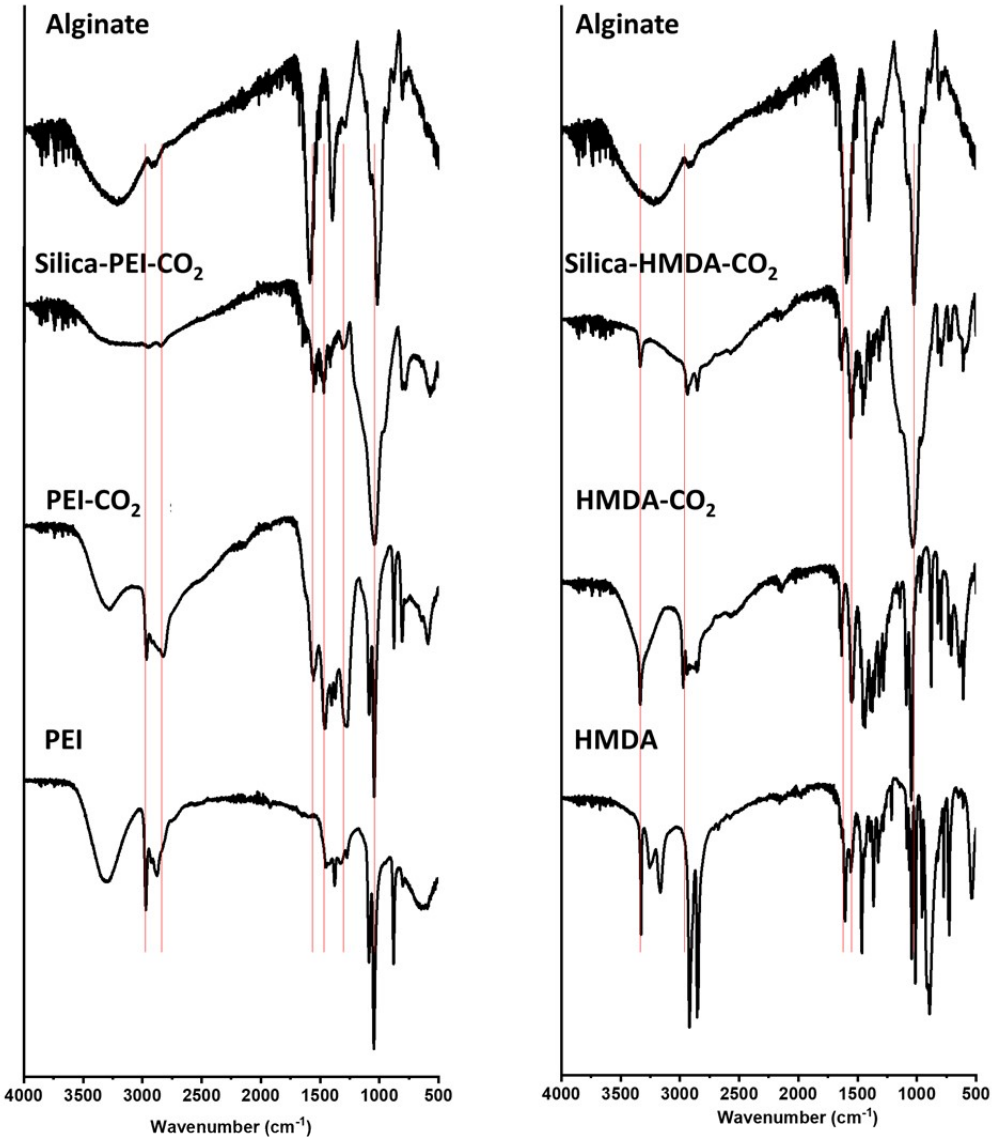

Figure S13. FTIR spectrum of various samples before and after CO_2 adsorption.

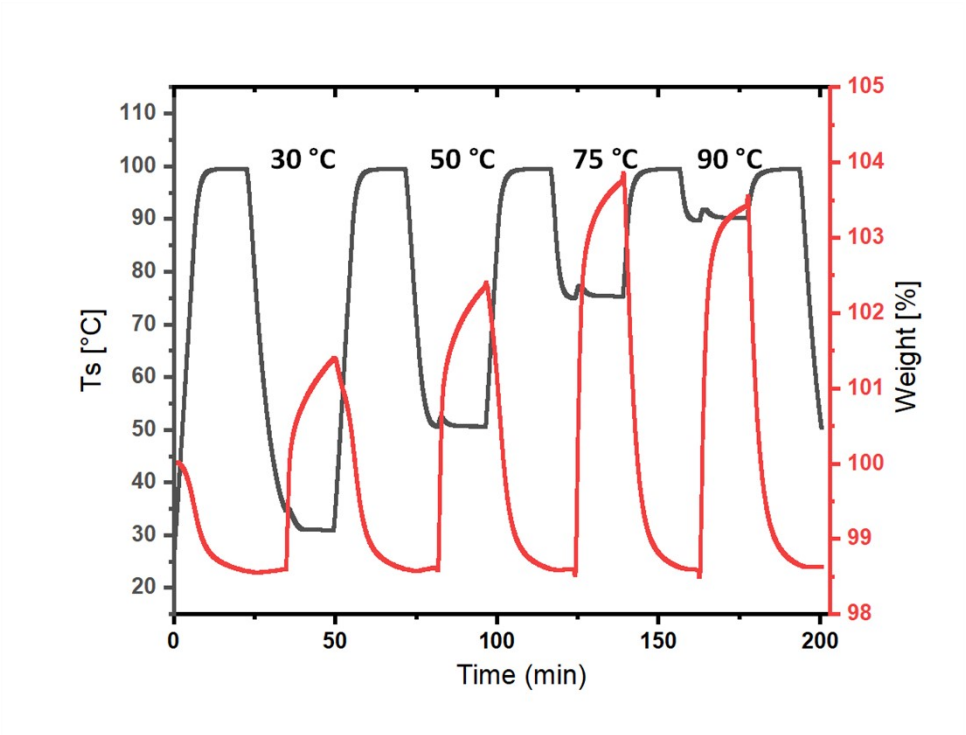

Figure S14. Adsorption temperature optimization. Measurements were performed at 30, 50, 75 and 90 °C.

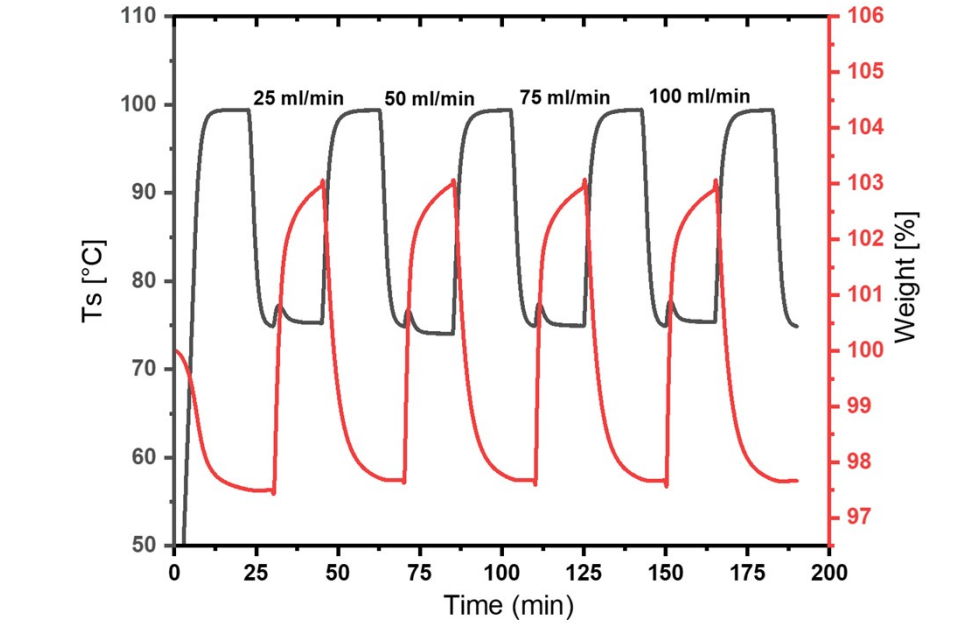

Figure S15. 15% CO_2 flow rate optimization at fixed adsorption temperature i.e. 75 °C.

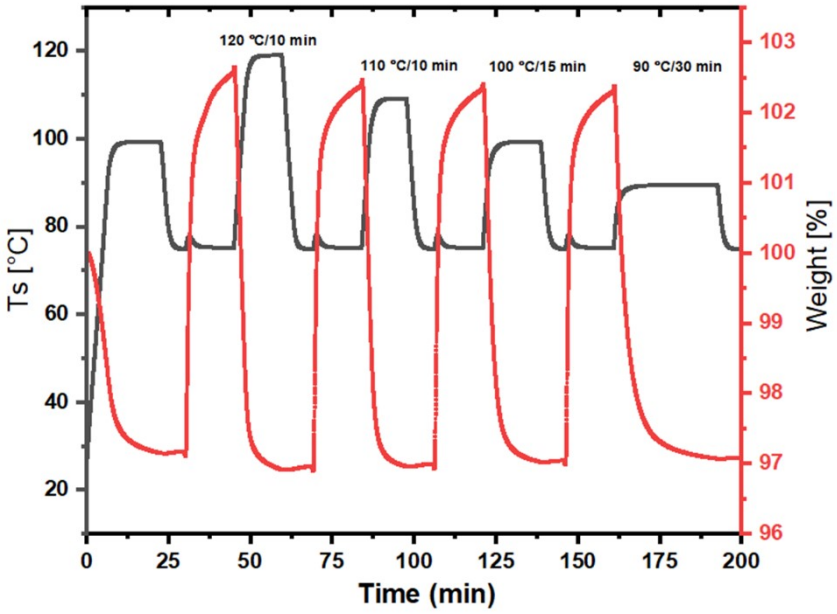

Figure S16. Desorption temperature optimization at a constant flow rate.

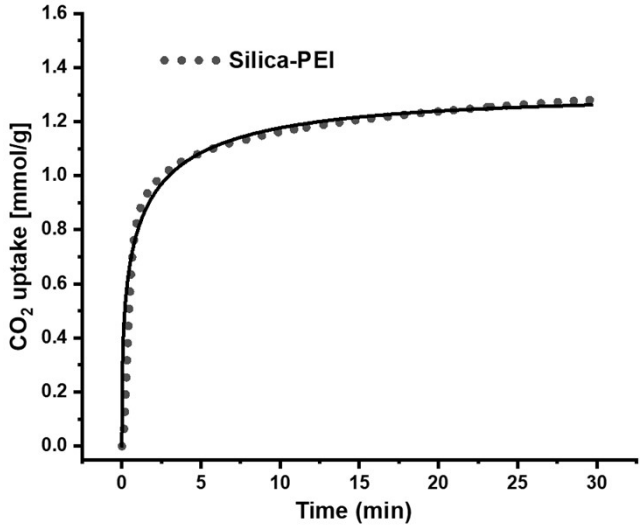

Figure S17. CO_2 adsorption of powder samples at 75 °C for 30 min. 15% CO_2 in N_2 was used for measurement.

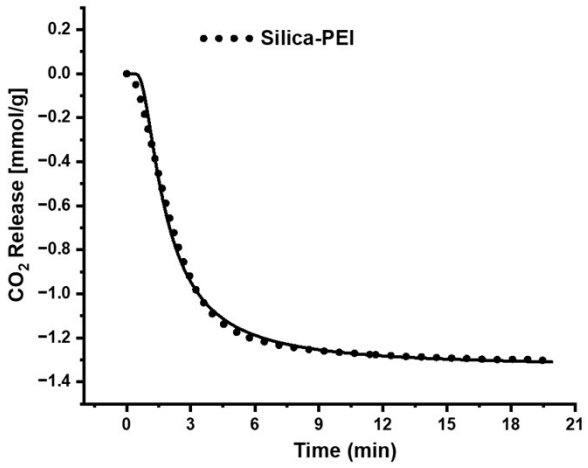

Figure S18. CO_2 desorption of powder samples at 100 °C for 15 min. 15% CO_2 in N_2.

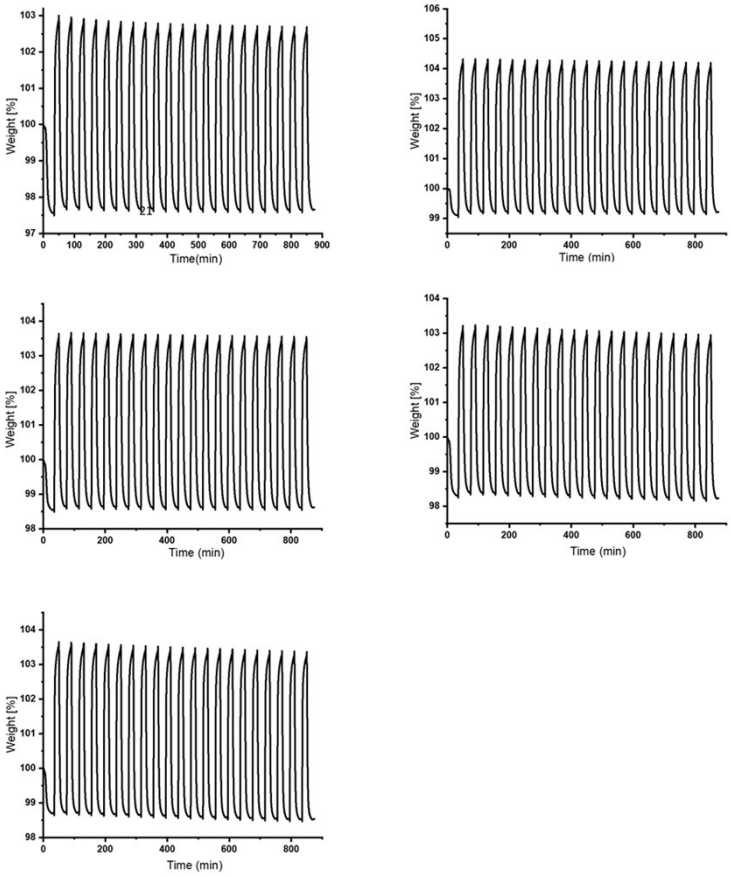

Figure S19. Five sets of 21 adsorption-desorption cycles of Silica-PEI bead (total of 105 cycles were recorded), cycling measurements were performed at 75 °C for 15 min, 25 ml/min Flow, Desorption at 100 °C for 15 min under the flow of N_2 gas (50 ml/min).

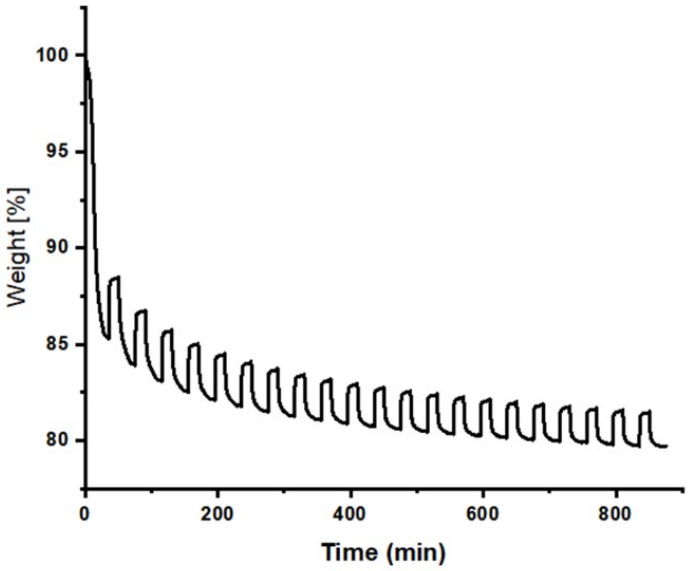

Figure S20. 20 adsorption-desorption cycles of silica-HMDA bead, measurements were performed at 75 °C for 15 min, 15% CO_2 flow: 25 ml/min, desorption at 100 °C for 15 min under the flow of N_2 gas (50 ml/min).

Table S1: SEM-EDX analysis. All data in wt.%.

		Mg	**Al**	**Si**	**Ca**	**Ti**	**S**	**O**
1	**Original**	7.31	9.55	16.19	21.60	1.32	1.11	42.92
2	**Metal dissolution**	1.79	2.42	**41.05**	-	-	-	51.96
3	**Metal Precipitation**	32.02	13.62	3.32	10.06	-	-	40.98
4	**Ca-separation**	-	2.41	-	68.22	-	-	29.01
5	**Mesoporous Silica**	-	5.33	42.04	-	-		52.63

-not detected

Table-S2: CHN analysis of amine-functionalized beads.

Weight(mg)	Name	N (wt. %)	C (wt. %)	H (wt.% %)	S (wt. %)
1.8700	Silica-PEI	12.02	31.34	6.826	0.000
1.8610	Silica-PEI	12.42	31.72	7.109	0.000
2.1850	Silica-PEI	12.86	32.38	7.377	0.000
1.9420	Silica-HMDA	10.27	36.03	8.060	0.000
1.9670	Silica-HMDA	9.92	35.46	7.956	0.000
2.1090	Silica-HMDA	9.46	35.55	7.570	0.000

Table S3. Fitting parameter of Avrami kinetic model for the desorption of CO_2 on silica-PEI bead.

Kinetic Models	Avrami [$Q_e(1-\exp(-(k_A x)^{n^A}))$]			
Parameters	**Q_e**	**k_A**	**n_A**	**R^2**
90 °C	-1.192 ± 0.0003	0.272 ± 0.0003	0.977 ± 0.001	0.9999
100 °C	-1.210 ± 0.0004	0.376 ± 0.0005	1.230 ± 0.003	0.9999
110 °C	-1.239± 0.0004	0.410 ± 0.0005	1.467± 0.004	0.9999
120 °C	-1.289± 0.0005	0.396 ± 0.0006	1.492 ± 0.005	0.9999

Table S4: Powder sample adsorption Kinetic parameters.

Kinetic Models	**Avrami [Qe*(1-EXP(-(ka*x)^nA))**			
Parameters	Q_e	k_a	n_A	R^2
Silica-PEI	1.29 ± 0.003	0.904 ± 0.011	0.399 ± 0.004	0.9999

Table S5: Powder sample desorption Kinetic parameters (desorption temperature 100 °C, 15 min, 50 ml/min N_2 flow).

Kinetic Models	Avrami [$Q_e(1-\exp(-(k_A x)^{n^A}))$]			
Parameters	**Q_e**	**k_A**	**n_A**	**R^2**
Silica-PEI	-1.33 ± 0.006	0.65 ± 0.008	1.57 ± 0.006	0.9999