Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

CO_2 capture by Li_2CaSiO_4 and enhancement with alkali carbonates

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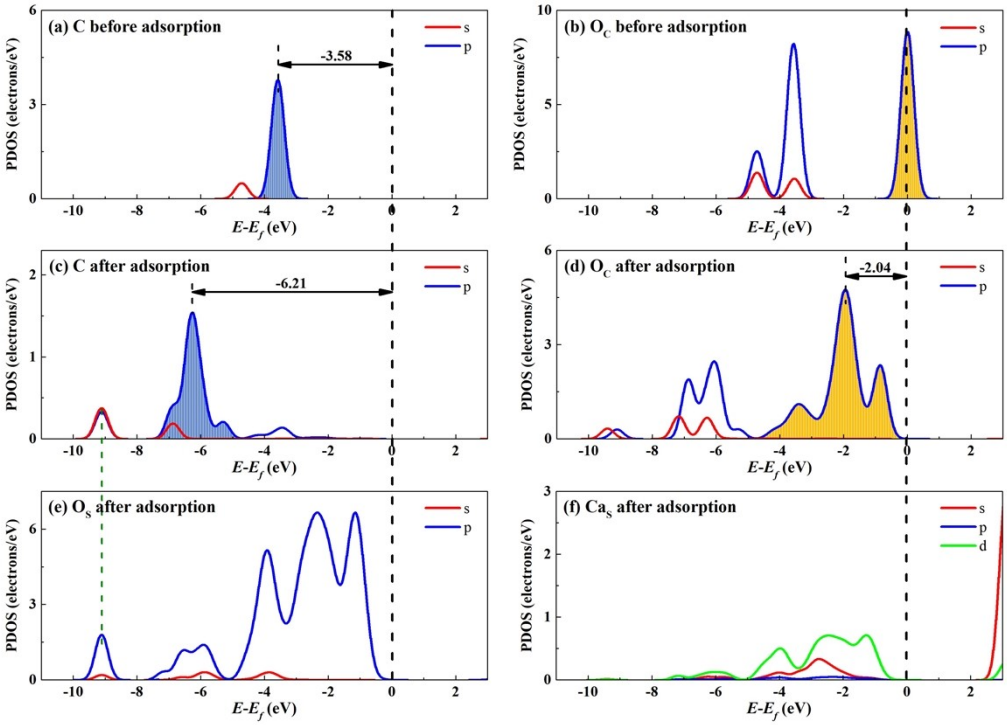

Fig. S1. Density of states analyses of CO_2 before and after adsorption on Li_2CaSiO_4 (101) surface with top atoms of O and Ca.

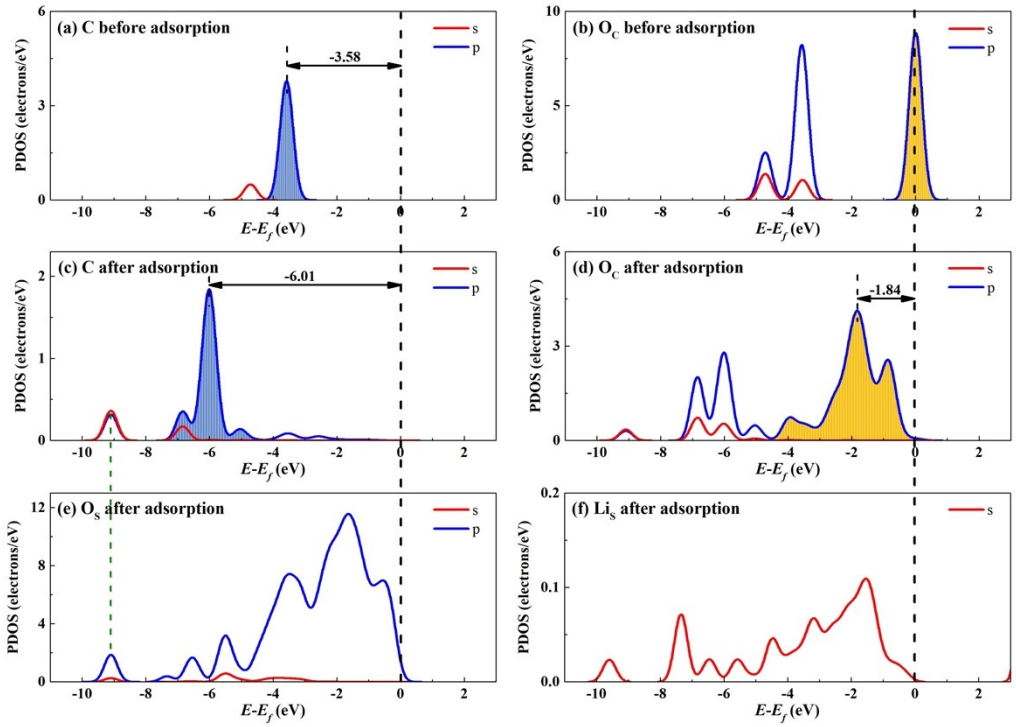

Fig. S2. Density of states analyses of CO_2 before and after adsorption on Li_2CaSiO_4 (101) surface with top atoms of O and Li.

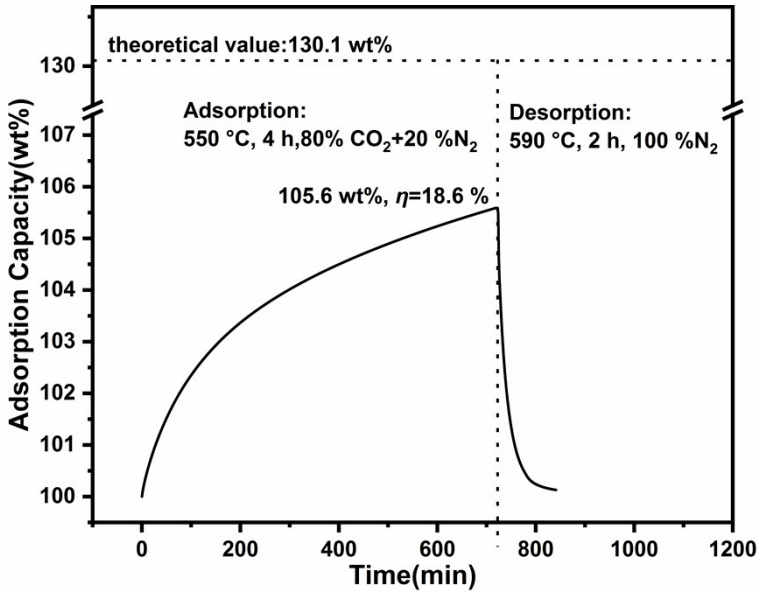

Fig. S3. Isothermal analysis of adsorption at 550 °C in the atmosphere of 80% CO_2 and desorption at 590 °C in 100% N_2.

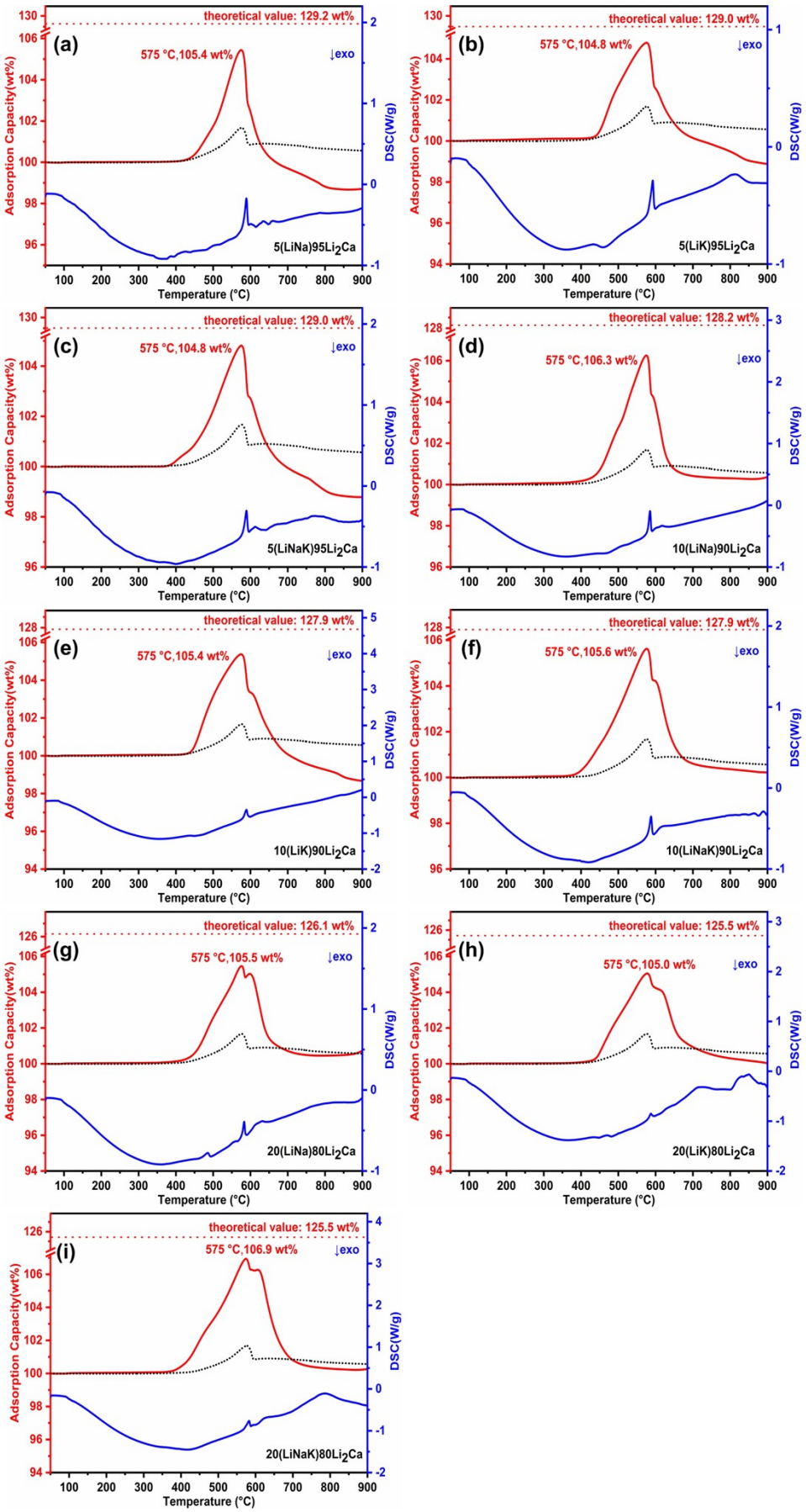

Fig. S4. Dynamic thermal analyses of Li_2CaSiO_4 mixed with different alkali carbonates from 50

to 900 °C with a heating rate of 10 °C·min^{-1} under the atmosphere containing 80% CO_2. Dashed line: TG curve of pristine Li_2CaSiO_4.

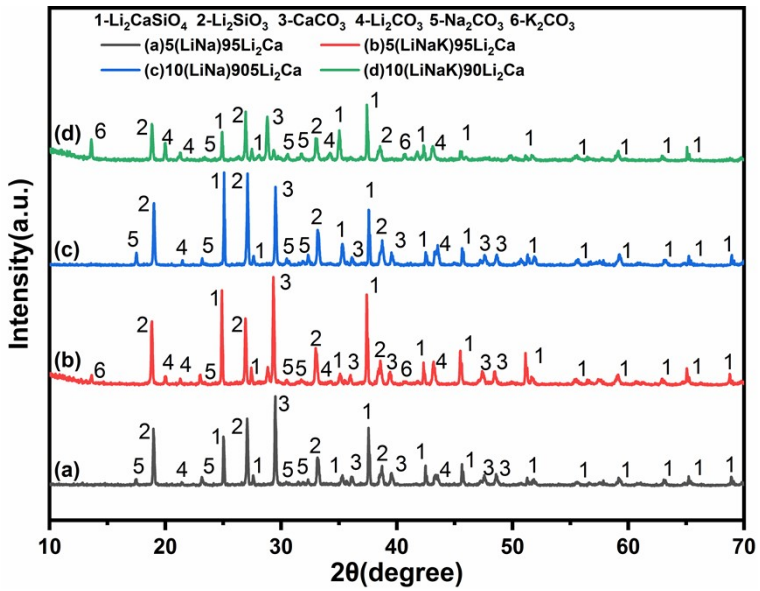

Fig. S5. XRD patterns of the 5(LiNa)95Li_2Ca(a), 5(LiNaK)95Li_2Ca(b), 10(LiNa)90Li_2Ca(c), 10(LiNaK)90Li_2Ca(d), Li_2CaSiO_4 after CO_2 adsorption at 550 °C in the 80 % CO_2 for 4 h.

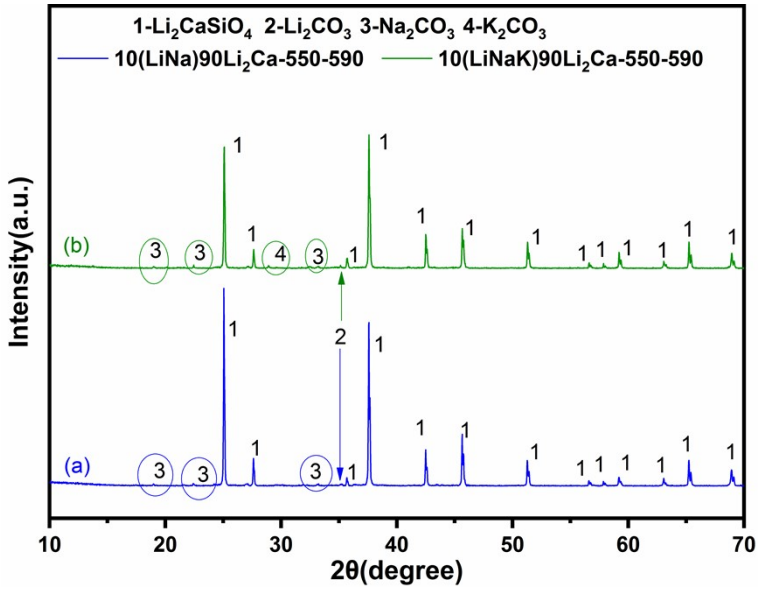

Fig. S6. XRD patterns of the 10(LiNa)90Li_2Ca(a), 10(LiNaK)90Li_2Ca(b) after CO_2 desorption at 590 °C in the 100 % N_2 for 2 h.

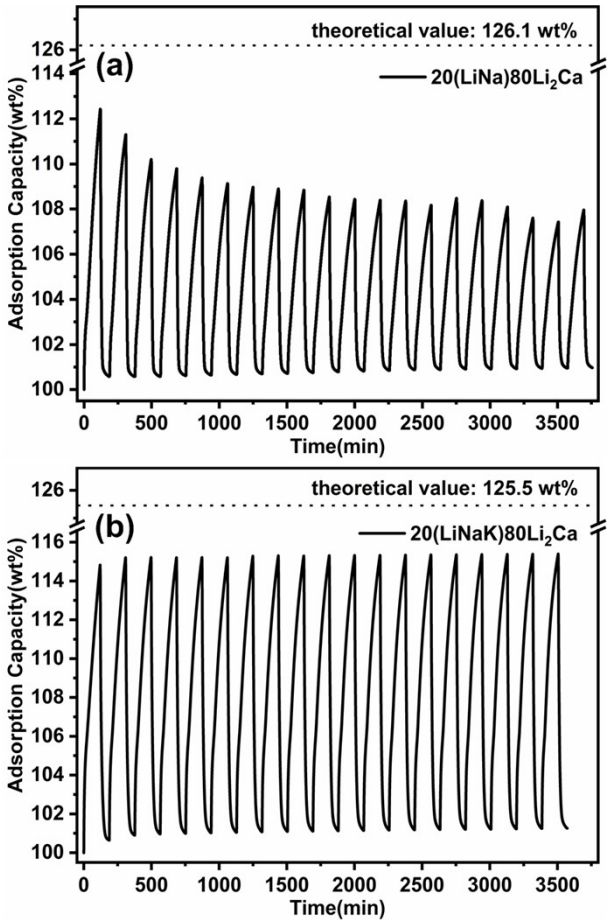

Fig. S7. Cyclic stability of 20(LiNa)80Li_2Ca(a), and 20(LiNaK)80Li_2Ca(b) (adsorption: 550°C, 2h, 80% CO_2，50 mL·min^{-1}; desorption: 590°C, 1h, 100 % N_2，50 mL·min^{-1})

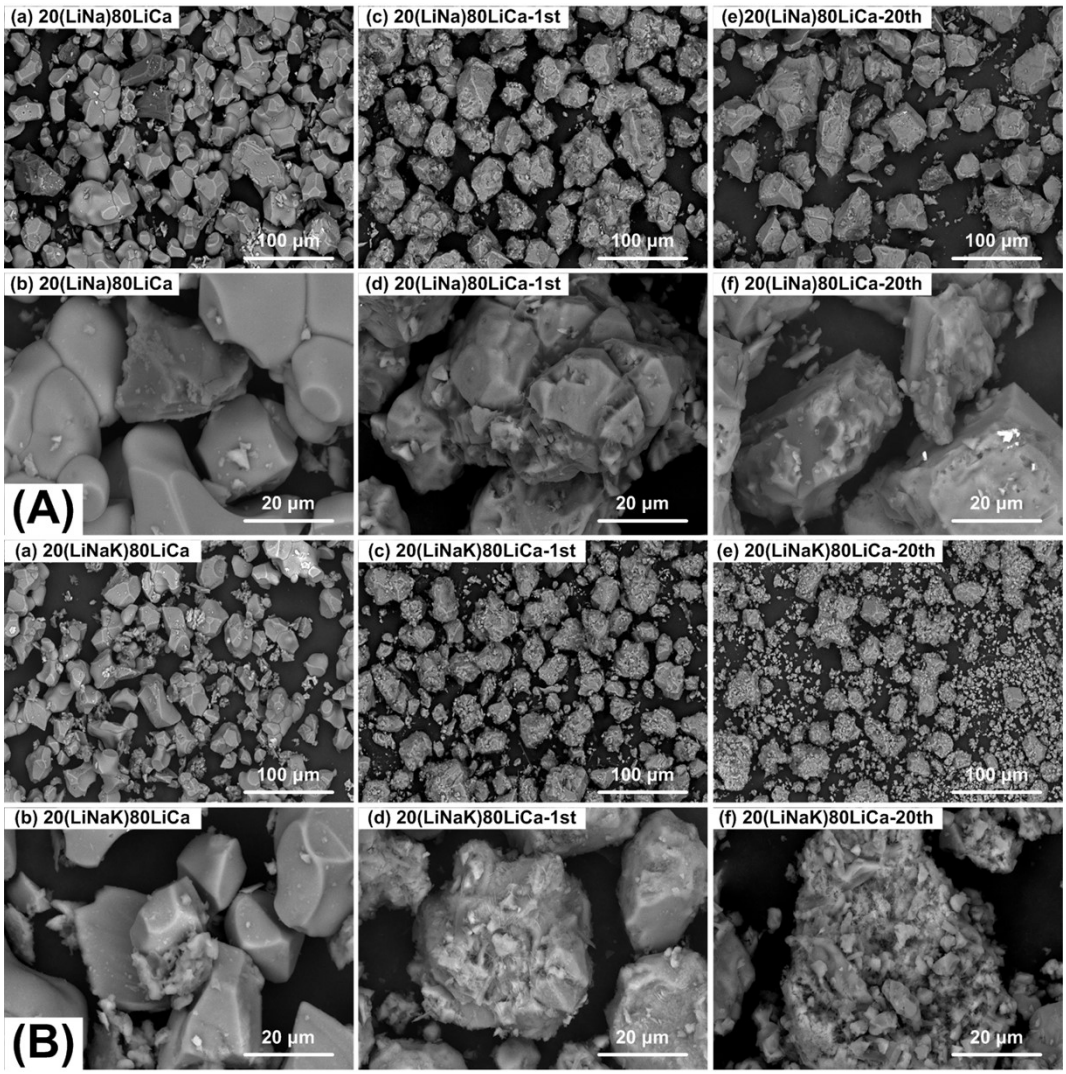

Fig. S8. SEM images of 20(LiNa)80Li_2Ca(A), and 20(LiNaK)80Li_2Ca (B) after different cycles

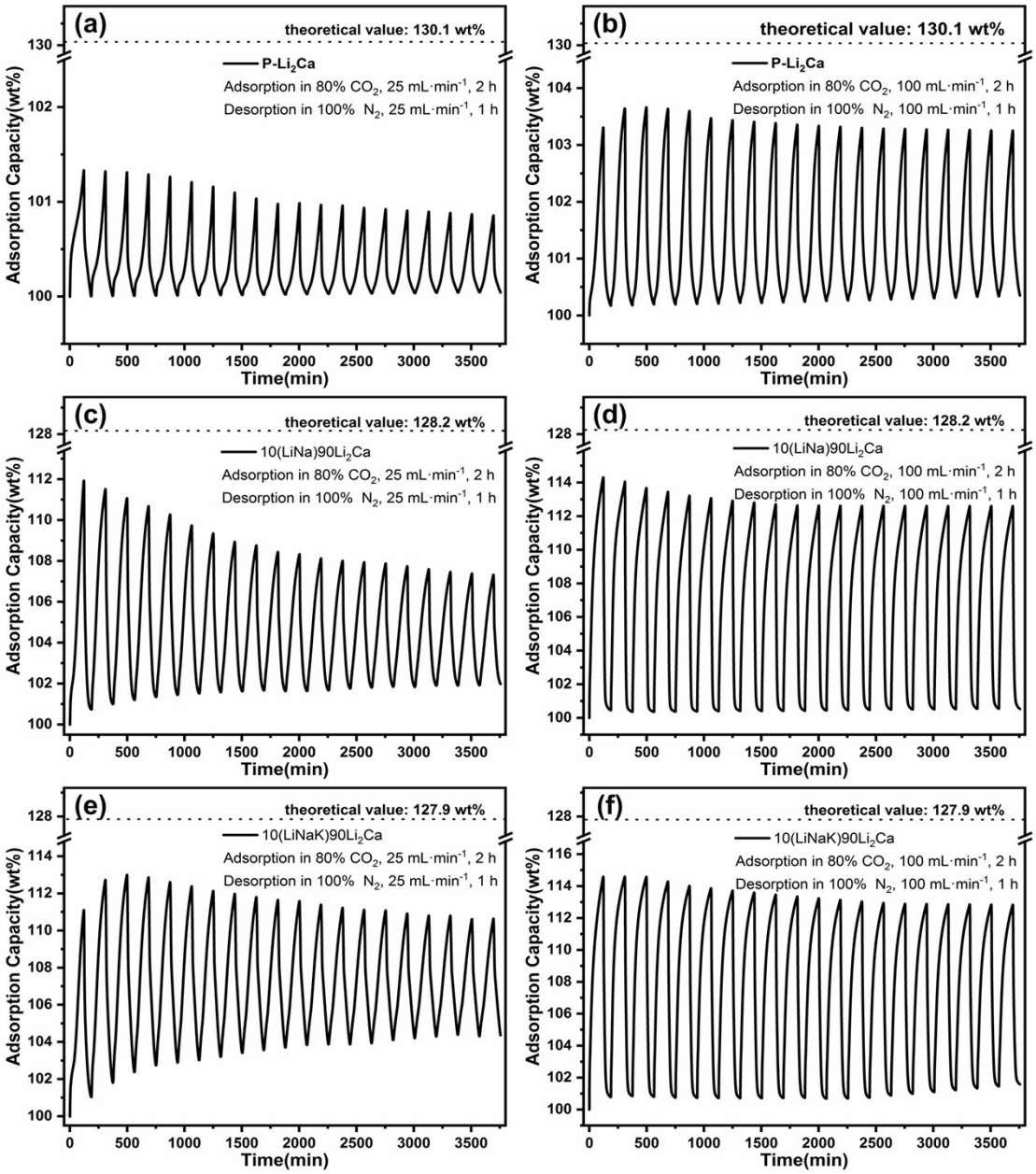

Fig. S9. Cyclic stability of P-Li_2Ca(a,b), 10(LiNa)90Li_2Ca(c,d), and 10(LiNaK)90Li_2Ca(e,f) at different flow rates during 20 capture/release cycles.

Table S1. Weight gain of P-Li_2Ca, 10(LiNa)90Li_2Ca, and 10(LiNaK)90Li_2Ca at different flow rates during 20 capture/release cycles.

Flow rate \ Weight gain \ Samples		P-Li_2Ca	10(LiNa)90Li_2Ca	10(LiNaK)90Li_2Ca
25mL/min	Minimum	0.8 wt%	5.4 wt%	6.3 wt%
	Median	1.0 wt%	7.0 wt%	8.1 wt%
	Maximum	1.3 wt%	11.9 wt%	11.1 wt%
50mL/min	Minimum	1.2 wt%	10.6 wt%	9.6 wt%
	Median	1.4 wt%	10.8 wt%	10.4 wt%
	Maximum	1.6 wt%	12.2 wt%	12.3 wt%
100mL/min	Minimum	2.9 wt%	11.1 wt%	11.4 wt%
	Median	3.1 wt%	11.3 wt%	12.7 wt%
	Maximum	3.3 wt%	14.3 wt%	14.6 wt%