Synthesis of $Li_{4+x}Si_{1-x}Fe_xO_4$ solid solution by dry ball milling and its highly efficient CO_2 chemisorption in a wide temperature range and low CO_2 concentrations

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Supplementary Information

Table S.1. $Li_{4+x}Si_{1-x}Fe_xO_4$ unit cell atomic positions. (x=0.1, 0.2, 0.3, 0.4 and 0.5)

Atom symbol (occ.)	Wyckoff site	x (fracc.)	y (fracc.)	z (fracc.)
Si(1-x), Fe(x)	E	0.34200	0.25000	0.00560
Si(1-x), Fe(x)	E	0.75400	0.25000	0.13860
Si(1-x), Fe(x)	E	0.47720	0.25000	0.71520
Si(1-x), Fe(x)	E	0.20100	0.25000	0.29240
Si(1-x), Fe(x)	E	0.04000	0.25000	0.57730
Si(1-x), Fe(x)	E	0.8941	0.25000	0.8567
Si(1-x), Fe(x)	E	0.61500	0.25000	0.42900
O	F	0.3560	0.0265	0.0579
O	F	0.7860	0.0342	0.1956
O	F	0.4994	0.0305	0.7715
O	F	0.2185	0.0283	0.3484
O	F	0.0668	0.0316	0.6344
O	F	0.9269	0.0330	0.9175
O	F	0.6530	0.0283	0.4811
O	E	0.1998	0.25	0.9638
O	E	0.6186	0.25	0.0977
O	E	0.3352	0.25	0.6744
O	E	0.0626	0.25	0.2447
O	E	0.9082	0.25	0.5278
O	E	0.7611	0.25	0.8143
O	E	0.4745	0.25	0.3985
O	E	0.4194	0.25	0.9341
O	E	0.8436	0.25	0.0682
O	E	0.5526	0.25	0.6386
O	E	0.2842	0.25	0.2228
O	E	0.1308	0.25	0.5114
O	E	0.9918	0.25	0.7957
O	E	0.6967	0.25	0.3561
Li	F	0.3823	0.0072	0.4068
Li	F	0.8123	0.0006	0.5448
Li	F	0.6605	0.0112	0.8270

Li	F	0.5255	0.9981	0.1173
Li	E	0.2722	0.25	0.8558
Li	E	0.4176	0.25	0.5491
Li	E	0.1321	0.25	0.1464
Li	E	0.9695	0.25	0.4271
Li	E	0.4490	0.25	0.278
Li	E	0.7272	0.25	0.6977
Li	E	0.5940	0.25	0.9794
Li	F	0.1962	0.9631	0.0192
Li	F	0.3309	0.9681	0.7279
Li	F	0.9515	0.0298	0.7108
Li	F	0.0790	0.0278	0.8663
Li	F	0.2373	0.0379	0.5977
Li	E	0.1407	0.25	0.7360
Li	E	0.0082	0.25	0.0076
Li	E	0.8701	0.25	0.2956

Table S2. Specific surface area obtained using BET model

Sample	Li_4SiO_4 SS	Li_4SiO_4 DBM	Li_5FeO_4 SS	Li_5FeO_4 DBM	SiFe01 DBM	SiFe02 DBM	SiFe03 DBM	SiFe04 DBM	SiFe05 DBM
Surface area (m^2/g)	1.1	3.1	1	2.9	3	3.1	3.1	3.2	3.3

Figure S1. N_2 adsorption-desorption isotherms of Li_4SiO_4, Li_5FeO_4 and $Li_{4.5}Si_{0.5}Fe_{0.5}O_4$ samples.

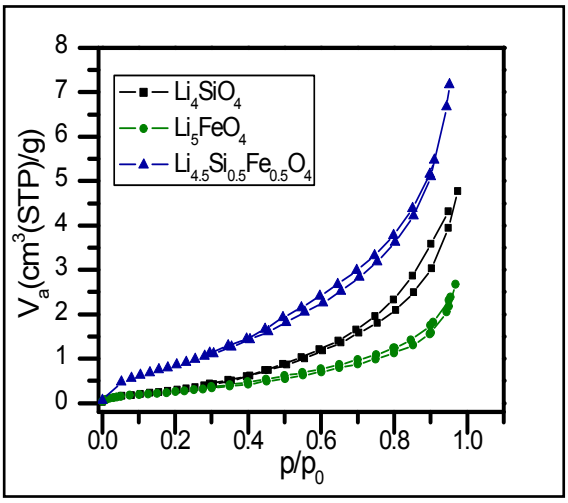

Figure S2. Maximum isothermal capture at each temperature in the $Li_{4.5}Si_{0.5}Fe_{0.5}O_4$ using a CO_2 partial pressure of 0.2 and a saturated atmosphere of CO_2

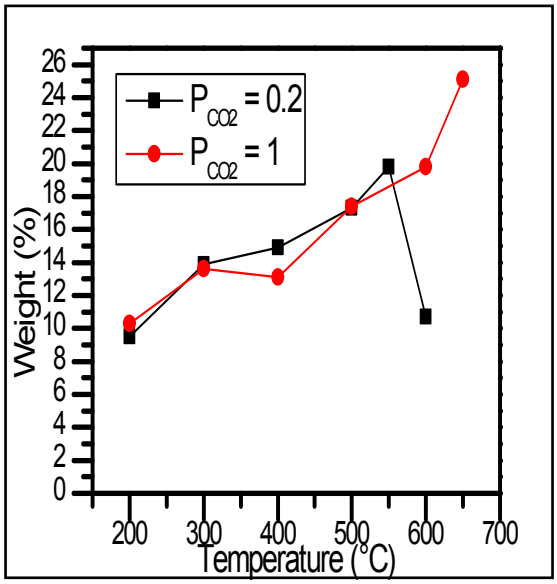

Figure S3. Eyring-type plot of ln(k/T) versus 1/T for data obtained using a double exponential reaction model in the isotherms performed using a CO_2 partial pressure of 0.2.