Electronic Supporting Informations (ESI):

Chabazite and zeolite 13X for CO₂ capture under high pressure moderate temperature conditions

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Experimental

1. Chabazite synthesis and ion-exchange

K⁺-form Chabazite was hydrothermally synthesized following the procedure reported by Bourgogne *et al.*¹using KOH (reagent grade 90%, Aldrich).

K⁺-form chabazite having mesopores (KCHA(M)) was prepared following the same procedure as the microporous chabazite but with addition of [3-(trimethoxysilyl)propyl]octadecyldimethylammonium chloride (TPOAC; 72%, Aldrich) as a mesopore forming agent. A typical procedure involved addition of 25 g of zeolite Y powder in 198.2 mL of DI water and 45% solution (26.8 mL) of KOH in a polypropylene bottle (500 mL, glass, SCHOTT). The mixture was stirred by a magnetic bar until a homogeneous mixture was obtained. TPOAC in a range of about 5- 15 mol% of silicon in the mixture was then added dropwise. The homogeneous mixture was placed in an oven for 15 d at 368 K. The product obtained was filtered, washed with 1 litre of DI water twice and dried in an oven at 373 K.

K⁺-form chabazite samples were ion-exchanged to Na⁺ form (NaCHA). Typically, 5 g of KCHA was introduced to 300 mL M NaCl solution (pH 6.5) under reflux at 353 K with stirring for 12 h. The solution was decanted and fresh solution was added, which was repeated three times. After the final exchange step, the solution was filtered and washed with 1L of DI water twice. The resulting NaCHA samples were dried at 373 K overnight. Mg²⁺, Ca²⁺, and Li⁺ chabazite were prepared from NaCHA by single ion exchange of NaCHA with 1 M MgCl₂ (5 g NaCHA: 300 mL MgCl₂), 1 M LiCl (3 g NaCHA: 100 mL LiCl) and 1 M CaCl₂ (5 g NaCHA: 300 mL CaCl₂). Direct ion-exchanges using K⁺-form chabazite samples produced products with far less surface areas due to incomplete ion-exchange of large K⁺ ions.

2. Mg(OH)₂ impregnation over zeolite 13X or chabazite

Mg(OH)₂ impregnation in nano-sized petals form on zeolite 13X was conducted as follow.^{2,3} A 0.04 M MgCl₂ solution was prepared by adding DI water to 0.67 g of MgCl₂ crystals (95%, Aldrich), to make 20 mL of solution. 60 mL of NH₄OH solution (0.04 M) was also prepared by diluting 2.07 g of NH₄OH (30%, Aldrich) with DI water. First, zeolite 13X (0.2 g) was added to the MgCl₂ solution (20 mL). NH₄OH solution (60 mL) was then introduced into the above mixture with constant stirring, and lastly, the resulting mixture was allowed to remain at ambient conditions (298 K) for 72 h. The product was separated by vacuum filtration, re-dispersed in 50 mL of DI water, sonicated for 10 s, separated once more by vacuum filtration, and dried in a vacuum oven at 323 K. The precipitation of Mg(OH)₂ on chabazite particles were followed the same procedure as on zeolite 13X

3. Characterization

The XRD (Rigaku) patterns of the zeolite samples were obtained using Cu K α (k = 1.54 Å) radiation. The N₂ adsorptiondesorption isotherms (BELsorp-mini, BEL, Japan) were measured at 77 K. Before the isotherm measurements, the samples were pre-treated at 623 K for 12 h under high vacuum. The specific surface areas of the samples were calculated using the BET method. The mesopore volumes were determined using the Barrett–Joiner–Halenda (BJH) method. The sample morphologies were examined by scanning electron microscopy (SEM, Hitachi S-4300). High-resolution transmission electron microscopy (TEM, JEM-2100F) images were obtained at 200 kV. The concentrations of cations in the zeolite samples were determined via Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES; Optima 7300DV). The FT-IR spectra of the $Mg(OH)_2$ -impregnated zeolite samples were obtained on a Nicolet Is10 FT-IR spectrometer (Thermo Scientific) at ambient temperature.

For the structural analysis of $Mg(OH)_2$ loaded NaX zeolite, the X-ray powder diffraction pattern was collected with X'Pert-Pro (PANalytical) diffractometer using Cu K $\alpha_{1,2}$ radiation ($\lambda = 1.5406$ Å and 1.5443 Å). Data were obtained on the sample at room temperature in the Bragg-Brentano geometry mode in parafocusing mode with a step size of 0.017° for a scan time of 3600 s per step over the 20 range 5 – 100°. Profile refinement of the structure model was performed via the Rietveld method with the Jana2006 package.⁴ Other extraframework species were found using the difference fourier method. During the Rietveld refinement, a pseudo-Voigt, together with a manually interpolated background, was used to describe the peak shape. The framework was modelled as completely siliceous. Isotropic displacement parameters of all Si and Al atoms were constrained to be equal to minimize the number of parameters, as were those of all O atoms and those of all cation atoms. The data collection and crystallographic parameters are summarized in Table S5 and S6.

The Multinuclear MAS NMR spectra were measured using UnityInova 600 (Varian) spectrometer at a spinning rate of 8 kHz and 20 kHz, respectively for the ²⁹Si and ²⁷Al nuclei at Korea Basic Science Institute at Daegu Branch.. The ²⁹Si MAS NMR spectra were measured at a ²⁹Si frequency of 119.182 MHz with a $\pi/2$ rad pulse length of 5.0 µs, a recycle delay of 30 s, and an acquisition of about 1200 pulse transients. The ²⁹Si chemical shift is reported relative to TMS. The ²⁷Al MAS NMR spectra were measured at a ²⁷Al frequency of 156.320 MHz with a $\pi/8$ rad pulse length of 1.8 µs and a recycle delay of 0.5 s. Approximately 6000 pulse transients were accumulated, and the ²⁷Al chemical shifts are reported relative to an Al(H₂O)₆³⁺ solution. The ¹H-²⁹Si CP MAS NMR spectra were measured on the same UnityInova 600 (Varian) spectrometer at a spinning rate of 20 kHz. The ¹H-²⁹Si CP MAS NMR spectra were also recorded at a ²⁹Si frequency of 119.182 MHz with $\pi/2$ rad pulse length of 6.5 µs, a recycle delay of 6.5 s, a contact time of 3 ms, and an acquisition of ca. 10000 pulse transients. All spectral deconvolution and simulation were performed using the PeakFit curve-fitting program. The Q_n peaks in which *n* indicated the number of the neighboring Si atoms were assigned following the literature.⁵

4. CO₂ adsorption measurement

1) Volumetric measurements

 CO_2 adsorption isotherms over zeolite under static conditions were obtained using a BELsorp(II)-mini (BEL, Japan) at 298 K with activated solid samples. Before the adsorption measurements, the samples were also activated at 623 K for 12 h in a vacuum.

2) TGA runs

 CO_2 adsorption/desorption cyclic experiments were conducted using a TGA unit (SCINCO, thermal gravimeter S-1000) connected to a gas flow panel. Ultra-high purity N₂ was used as a purge gas in the initial activation and desorption experiments, and adsorption was carried out using ultra-high purity CO_2 (99.999%). A feed flow rate of 30 mL min⁻¹ to the sample chamber was controlled using an MFC.

5. CO₂ adsorption isotherms at high pressure ambient temperature conditions using a magnetic suspension balance

High-pressure CO₂ adsorption isotherms were obtained using a magnetic suspension balance (Rubotherm, Germany) with in situ density measurement in a closed system. Activated samples were initially conditioned at 623 K under vacuum (3×10^{-3} torr) for 12 h. Prior to commencing measurement of the CO₂ adsorption capacity, buoyancy was corrected in ultra high purity He. High pressure adsorption was carried out using ultra high purity CO₂ (99.999%) in a pressure range of 0–20 bar at 298 K.

6. High pressure and high temperature breakthrough experiments

Experiments to evaluate CO_2 separation from a gas mixture were carried out using a custom-made breakthrough apparatus shown below, which can accommodate high pressure and high temperature conditions. The apparatus has a tubular adsorption column within a tube furnace. The column is made of stainless steel with a total length of 350 mm (12.7 mm diameter and 1 mm wall thickness). Gas flow rates were monitored by mass flow controllers installed upstream of the adsorption bed. A back-pressure controller between the adsorption bed and the product exit was installed to maintain constant adsorption pressure in the bed and adsorption pressure in column was monitored with pressure gauge. The relative amounts of the gases passing through the column were monitored by using a Hiden Analytical HPR20 mass spectrometer.

0.5 g of pretreated zeolite samples were placed inside the column. The gas mixture of 30 vol% CO₂ with N₂ balance was fed into the column at a flow rate of 100 mL/min. The relative intensity of each gas component was normalized to the same level by purging gas mixtures through the bypass before they passed through the column. The working capacity was calculated by the formula of CO₂ flow rate (mL/min) × CO₂ breakthrough time (min)/sample weight (g), which is then converted to a value in mgCO₂/g sorbent unit by using the ideal gas law.

7. References

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Scheme. S1 Schematic diagram of modified TGA adsorption unit.



Scheme. S2 Schematic diagram of breakthrough experimental unit.



Fig. S1 Powder X-ray diffraction patterns of ion-exchaged microporous chabazites.



Fig. S2 N₂ isotherms of ion-exchanged microporous chabazites at 77 K.



Fig. S3 SEM image of KCHA.



Fig. S4 CO₂ adsorption isotherms of ion-exchanged microporous chabazites (a) LiCHA, (b) CaCHA, (c) NaCHA, (d) KCHA and (e) MgCHA at 1 bar, 298 K.



Fig. S5 Recycle runs of CO₂ adsorption–desorption on (a) KCHA, (b) NaCHA, (c) CaCHA, (d) LiCH A and (e) MgCHA at 1 bar, 473 K.



Fig. S6 Powder X-ray diffraction patterns of mesoporous chabazites prepared using different amount of TPOAC (0-10%).



Fig. S7 N₂ adsorption isotherms of mesoporous chabazites at 77 K: diamond; 0%, triangle; 3%, squar e; 5%, circle; 10% in TPOAC.



Fig. S8 TEM images of mesoporous K-chabazite: (a) TPOAC 0% (b) TPOAC 3% (c) TPOAC 5% an d (d) TPOAC 10%.



Fig. S9 Powder X-ray diffraction patterns of ion-exchanged mesoporous chabazites.



Fig. S10 TEM images of ion-exchanged mesoporous chabazite: (a) KCHA (b) KCHA(M) (c) NaCHA (M) and (d) CaCHA(M).



Fig. S11 N₂ adsorption isotherms of ion-exchanged mesoporous chabazites at 77 K.



Fig. S12 Pore size distributions of ion-exchanged mesoporous chabazites .



Fig. S13 Breakthrough curves of (a) KCHA, (b) NaCHA and (c) CaCHA for CO_2 (30% CO_2 , N_2 as a balance, 100 mL min⁻¹) at 1-20 bar, 298 K: square; N_2 at 20 bar, triangle; CO_2 at 1 bar, circle; CO_2 at 20 bar.



Fig. S14 Breakthrough curves of (a) KCHA, (b) NaCHA and (c) CaCHA for CO_2 (30% CO_2 , N_2 as a balance, 100 mL min⁻¹) at 1-20 bar, 473 K: square; N_2 at 20 bar, triangle; CO_2 at 1 bar and circle; CO_2 at 20 bar.



Fig. S15 Breakthrough curves of (a) KCHA(M), (b) NaCHA(M) and (c) CaCHA(M) for CO₂ (30% C O₂, N₂ as a balance, 100 mL min⁻¹) at 1-20 bar, 298 K: square; N₂ at 20 bar, triangle; CO₂ at 1 bar and circle; CO₂ at 20 bar.



Fig. S16 Breakthrough curves of (a) KCHA(M), (b) NaCHA(M) and (c) CaCHA(M) for CO₂ (30% C O_2 , N_2 as a balance, 100 mL min⁻¹) at 1-20 bar, 473 K: square; N_2 at 20 bar, triangle; CO₂ at 1 bar and circle; CO₂ at 20 bar.



Fig. S17 High-pressure CO_2 isotherms of the chabazites at 1-20 bar, 298 K; micro-KCHA and meso-KCHA.



Fig. S18 High-pressure CO_2 isotherms of the chabazites at 1-20 bar, 298 K; micro-NaCHA and meso-NaCHA.



Fig. S19 High-pressure CO_2 isotherms of the chabazites at 1-20 bar, 298 K; micro-CaCHA and meso-CaCHA.



Fig. S20 (a) ²⁹Si magic angle spinning NMR with (blue solid line) and without (black solid line) cross polarization for (1) the microporous and (2) mesoporous CaCHA zeolites, respectively, (b) ²⁹Si magic angle spinning NMR of (1) the microporous and (2) mesoporous CaCHA zeolites with the correspond ing Q_n peaks obtained from deconvolution of the experimental spectrum. The Q_n peak was assigned fo llowing the literature⁵, and (c) ²⁷Al magic angle spinning NMR of (1) the microporous and (2) mesoporous CaCHA zeolites. The tetrahedral Al peak, T_d was obtained at 58.3 ppm in the absence of octahed ral Al peak at 0 ppm.



Fig. S21 Experimental CO_2 adsorption isotherm obtained at 298 K on (a) the microporous CaCHA ze olite (open circle), which was also fitted with the single adsorption site model (solid line) and (b) mes oporous CaCHA zeolite (open circle), which was also fitted with the dual adsorption sites model (soli d line). The corresponding calculated strong and weak adsorption isotherms were shown (dashed lines). Refer to Table S3 for model description.



Fig. S22 High-pressure CO₂ adsorption isotherm of MCM-41 at 298 K measured by Rubotherm.



Fig. S23 SEM-EDX of (a), (b) 13X and (c), (d) $Mg(OH)_2$ impregnated on 13X.



Fig. S24 TEM-EDS mapping of $Mg(OH)_2$ impregnated on 13X.



Fig. S25 FT-IR spectra of 13X and $Mg(OH)_2$ impregnated on 13X. The $Mg(OH)_2$ peak was obtained a t 3700 (cm⁻¹): Seec. P. Y. Koh, J. Yan, J. Ward, W. J. Koros, A. S. Teja and B. Xu, *Materials Researc h Bulletin*, 2011, **46**, 390 for peak assignment.



Fig. S26 Final Rietveld refinement plot for $Mg(OH)_2$ loaded NaX zeolite. The corresponding phases were indexed with the colored bar. The inset shows the magnification of the high angle region around 35-45°. The background (green solid line) with the phase indexing at 38° shows the presence of the br oad peak corresponding to $Mg(OH)_2$ phase.



Fig. S27 Breakthrough curves for CO_2 (30% CO_2 , 10% H_2O , N_2 as a balance, 100 mL min⁻¹) at 10 bar, 473 K: square; N_2 , circle; CO_2 over Mg(OH)₂ impregnated on 13X, triangle; CO_2 over 13X and diamo nd; CO_2 over Mg(OH)₂.



Fig. S28 Recycle runs of Mg(OH)₂ impregnated on 13X using breakthrough instrument (60% CO₂, 10% H₂O, N₂ as a balance, 350 mL min⁻¹) at 10 bar, 473 K: square; N₂, circle; CO₂ (1st cycle), triangle; CO₂ (2nd cycle), hexagonal; CO₂ (3rd cycle), and diamond; CO₂ (4th cycle).



Fig. S29 Powder X-ray diffraction pattern on $Mg(OH)_2$ impregnated on 13X after 4 recycle runs of C O_2 sorption–desorption at moisture conditions, 10 bar, 473 K.



Fig. S30 N_2 adsorption isotherm of Mg(OH)₂ impregnated on 13X at 77 K after 4 recycle runs of CO₂ sorption–desorption at moisture conditions, 10 bar, 473 K.



Fig. S31 Pore size distribution of $Mg(OH)_2$ impregnated on 13X after 4 recycle runs of CO_2 sorption-desorption at moisture conditions, 10 bar, 473 K.



Fig. S32 SEM image of $Mg(OH)_2$ impregnated on 13X after 4 recycle runs of CO_2 sorption–desorptio n at moisture conditions, 10 bar, 473 K.



Fig. S33 Recycle runs of 13X using breakthrough instrument (30% CO₂, 10% H₂O, N₂ as a balance, 1 00 mL min⁻¹) at 20 bar, 473 K: square; N₂, circle; CO₂ (1st cycle), triangle; CO₂ (2nd cycle), and diam ond; CO₂ (3rd cycle).



Fig. S34 Powder X-ray diffraction pattern of 13X after 3 recycle runs of CO₂ sorption–desorption at moisture conditions, 20 bar, 473 K.



Fig. S35 N_2 adsorption isotherm of 13X at 77 K after 3 recycle runs of CO_2 sorption–desorption at mo isture conditions, 20 bar, 473 K.



Fig. S36 Pore size distribution of 13X after 3 recycle runs of CO₂ sorption–desorption at moisture con ditions, 20 bar, 473 K.



Fig. S37 SEM images of (a) CaCHA and (b) $Mg(OH)_2$ impregnated CaCHA.



Fig. S38 SEM images of (a) CaCHA(M) and (b) $Mg(OH)_2$ impregnated CaCHA(M).



Fig. S39 Powder X-ray diffraction patterns on (a) $Mg(OH)_2$ impregnated CaCHA, (b) CaCHA and (c) $Mg(OH)_2$.



Fig. S40 Powder X-ray diffraction patterns of (a) $Mg(OH)_2$ impregnated CaCHA(M), (b) CaCHA(M) and (c) $Mg(OH)_2$.



Fig. 41 SEM images of impregnated Mg(OH)₂ on different support materials.



Fig. 42 Powder X-ray diffraction patterns of impregnated Mg(OH)₂ on different support materials.

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Fig. S43 CO₂ breakthrough curves (30% CO₂, 10% H₂O, N₂ as a balance, 100 mL min⁻¹) at 20 bar, 47 3 K: square; N₂, circle; CO₂ over Mg(OH)₂ impregnated on CaCHA, triangle; CO₂ over CaCHA and d iamond; CO₂ over Mg(OH)₂.



Fig. S44 CO₂ breakthrough curves (30% CO₂, 10% H₂O, N₂ as a balance, 100 mL min⁻¹) at 20 bar, 47 3 K: square; N₂, circle; CO₂ over Mg(OH)₂ impregnated on CaCHA(M), triangle; CO₂ over CaCHA(M) and diamond; CO₂ over Mg(OH)₂.

Table S1 Textural properties of mesoporous chabazites prepared using different amount of TPOAC (0 -10%)

Sample	$S_{BET} (m^2/g)$	V_{Pore} (cm ³ /g)	V_{meso} (cm ³ /g, BJH plot)
Mesochabazite (TPOAC 10%)	70	0.08	0.07
Mesochabazite (TPOAC 5%)	73	0.10	0.09
Mesochabazite (TPOAC 3%)	54	0.06	0.06
chabazite	17	0.04	0.04

Table S2 $\mathrm{CO}_2/\mathrm{N}_2$ selectivity over 13X and CHA

	Selectivity (CO ₂ /N ₂)			
Sample	1 bar		20	bar
-	298 K	473 K	298 K	473 K
13X	37	35	-	11
NaCHA	43	41.5	18	15.5
CaCHA	47	42	20.5	17
CaCHA(M)	39	32.5	24	19

Estimated by integrating the respective breakthrough pattern of CO_2 and N_2

	CaCHA (Micro)	CaCHA (Meso)
$q_{sat.A}$ (mg CO ₂ /g adsorbent)	221.1	196.7
b_A (bar ⁻¹)	23.981	5.149
$q_{sat.B}$ (mg CO ₂ /g adsorbent)	-	92.5
$b_{\rm B}$ (bar ⁻¹)	-	0.079
R _{sqr}	0.999	0.999

Table S3 Dual-site Langmuir parameters for adsorption of CO_2 in CHA samples at 298 K

	$a \rightarrow b P$	$a = b_{\rm D} P$
$Q_{1} = a_{1} + a_{2} =$	⁴ Sat.A [~] A ⁻	⁴ Sat.B [~] B ⁻
Vtotal $\Psi A + \Psi B$	$1 + b_{A}P_{A}$	$1 + b_{P}P$
	A +	- D

where $q_{sat,A}$ and $q_{sat,B}$ are the saturation quantities on the site with respective equilibrium constant b_A and b_B at pressure P.

Table S4 Weight percent of Mg(OH)₂ and textual properties before and after impregnation on zeolites

Sample	$Mg(OH)_2 (wt\%)^a$	$S_{BET} \left(m^2/g \right)$	$V_{Pore}(cm^{3}/g)$	$V_{Meso}(cm^{3}/g)$
Mg(OH) ₂ /zeolite 13X	8	804 ^b /750	0.34°/0.45	0.05 ^d /0.19
Mg(OH) ₂ /CaCHA	15	680/610	0.43/0.49	0.07/0.16
Mg(OH) ₂ /CaCHA(M)	18	200/173	0.20/0.30	0.18/0.27

 $Mg(OH)_2 (wt\%)^a$: calculated by weight percent of Mg^{2+} in zeolite from ICP-OES analysis, $S_{BET}^b = sur$ face area before impregnation, $V_{Pore}^c =$ total pore volume before impregnation, and $V_{Meso}^d =$ meso pore volume before impregnation.

Material	Mg(OH) ₂ /NaX
Refined chemical composition	Mg _{64.1} (H ₂ O) ₂₆₀ [TO ₂] ₁₉₂
Formula weight of unit cell	17718.3
Crystal system	Cubic
Space group	F d -3
Cell parameters (Å)	24.9719(2), 24.9719(2), 24.9719(2)
Cell volume (Å ³)	15572.4(2)
Diffractometer	X'Pert-Pro, PANalytical
Diffraction geometry	Bragg-Brentano
X-ray source	Cu Ka _{1,2} radiation (1.5046, 0.15444 Å)
2scan range (°)	5-100
Scan step size (°) and time per step (sec)	0.017, 3600
Data collection temperature (K)	300
Number of data points	5685
Number of geometric restraints	8
Profile function	pseudo-Voigt
Number of variable	51
$R_{\rm p}$ (%)	6.69
$R_{\rm wp}(\%)$	9.36
R_{\exp} (%)	1.32
Goodness of Fit	7.07

Table S5 Data collection and crystallographic parameters for $Mg(OH)_2/NaX$

^aThe abbreviation follows the notation appeared in the Jana2006 program suite.⁴

site	x	у	Ζ	$U_{\rm iso}$	occupancy	type
T1	0.4116(5)	0.1805(4)	0.0020(5)	0.0174	1	Si/Al
T2	0.3227(4)	0.0894(5)	0.0029(5)	0.0174	1	Si/Al
01	0.4534(5)	0.1540(4)	-0.0476(5)	0.0198	1	Ο
02	0.4448(5)	0.1950(4)	0.0567(7)	0.0198	1	Ο
03	0.2731(7)	0.1298(11)	-0.0166(7)	0.0198	1	Ο
04	0.3714(5)	0.1318(5)	0.0212(4)	0.0198	1	Ο
Mg1	0.4541(7)	0.0459(7)	-0.0459(7)	0.08	0.509	Mg
Mg2	0.0606(4)	0.0606(4)	0.9394(4)	0.08	1.044	Mg
Mg3	0.3992(14)	0.1008(14)	0.1008(14)	0.08	0.229	Mg
Mg4	-0.1097(13)	0.1097(13)	0.8903(13)	0.08	0.261	Mg
Ow1	0.625	0.125	0.125	0.08	1.22	Ο
Ow2	0.4645(7)	0.0355(7)	0.0355(7)	0.08	0.69	Ο
Ow3	-0.0390(9)	0.1929(10)	0.9037(9)	0.08	0.796	Ο
Ow4	-0.1173(13)	0.1255(13)	0.9786(7)	0.08	0.772	Ο
Ow5	0.0412(9)	0.1850(4)	0.9754(8)	0.08	0.899	Ο
Ow6	0.0437(11)	0.0437(11)	1.0437(11)	0.08	0.43	0

Table S6 Atomic Coordinates, Thermal Parameters, and Occupancy Factors for $Mg(OH)_2/Na X$