Supplementary information

for

Imidazolinium based porous hypercrosslinked ionic polymers for efficient CO_2 capture and fixation with epoxides

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Supplementary information

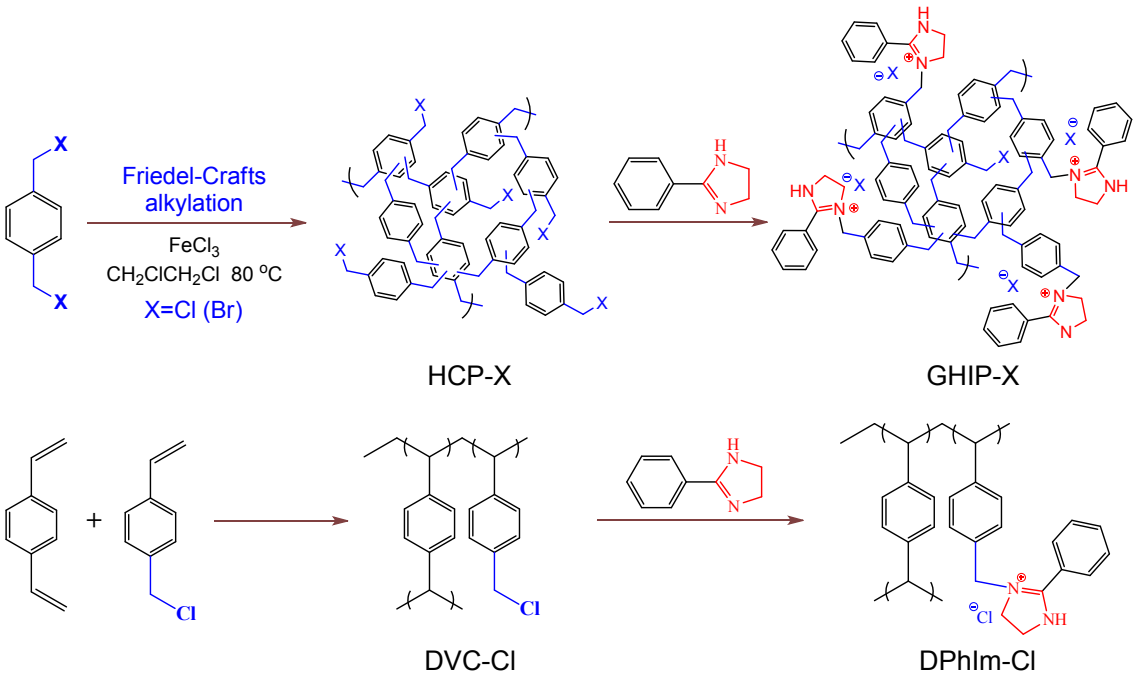
1. Supplementary Experimental

1.1 Synthesis of control samples

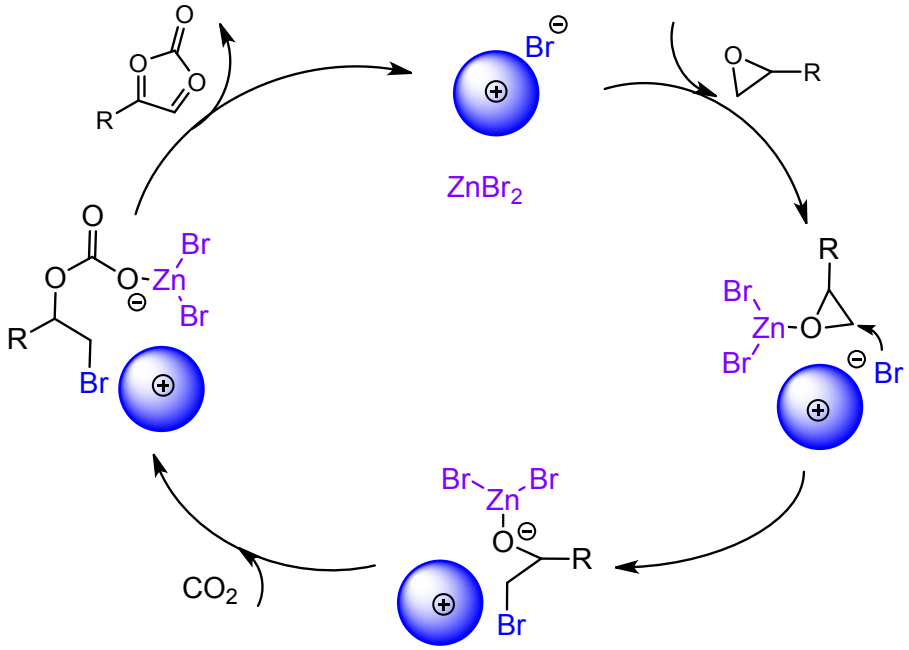
Polystyrene resin supported *2*-phenylimidazolinium salt (DPhIm-Cl) was prepared through the functionalization of chloromethyl tethered polystyrene resin (DVC-Cl) (Scheme S1). The support DVC-Cl was synthesized through the free-radical polymerization of vinylbenzyl chloride (VBC) and divinylbenzene (DVB). VBC (1.53 g, 10 mmol), DVB (0.13 g, 1 mmol) and *2*,*2*'-azobis(isobutyronitrile) (0.008 g, 0.5 wt% based on monomers) were dissolved in 30 mL ethyl acetate solution and stirred at 353 K under nitrogen atmosphere with a reflux condenser. After 24 h, the solid was filtered; washed three times with water, methanol, and diethyl ether, and then dried under reduced pressure at 323 K for 24 h. DVC-Cl (0.3 g), *2*-phenylimidazoline (0.15 g, 1 mmol) and toluene (20 mL) was stirred at 353 K for 24 h in a 25 mL flask. The solid residue was collected by filtration, washed with methanol (3×5 mL) and dried under vacuum at 333 K for 12 h, giving the final product DPhIm-Cl.

2-Phenyl-*3*-butylimidazolinium chloride (PhIm-Cl) was synthesized as follows. *2*-Phenylimidazoline (1.46 g, 10 mmol) was added in a three-necked flask, followed by the slow addition of *1*-chlorobutane (0.93 g, 10 mmol). The mixture was stirred at 353 K for 24 h. The product was recrystallized twice in ethanenitrile-ethyl ethanoate.

2. Supplementary Scheme



Scheme S1 Synthesis of HCP-X, GHIP-X and DPhIm-Cl.



Scheme S2 Proposed mechanism of the cycloaddition of epoxide with CO_2 catalyzed by HIP-Br-2 in the presence of $ZnBr_2$.

3. Supplementary Figures

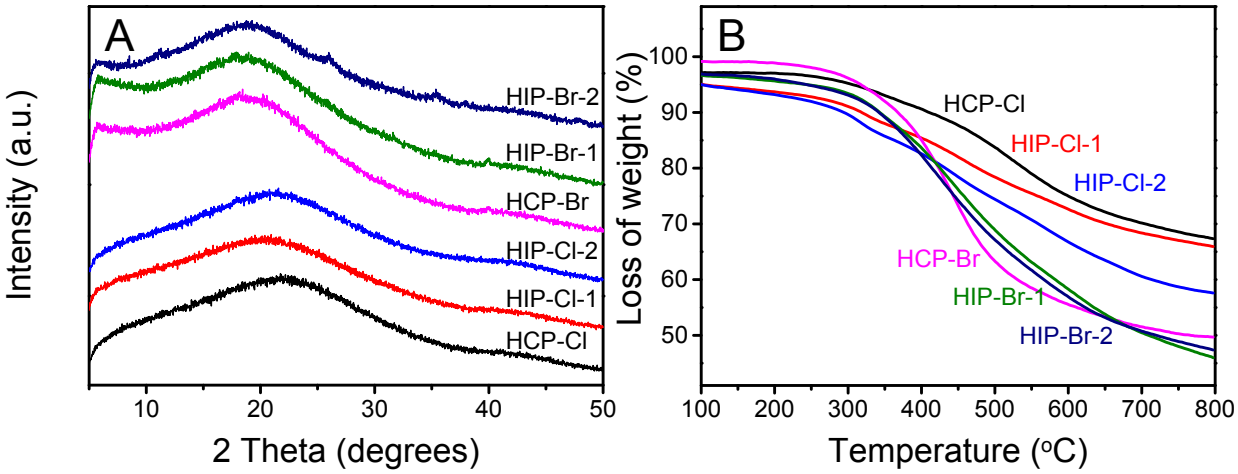


Fig. S1 (A) XRD patterns and (B) TG curves.

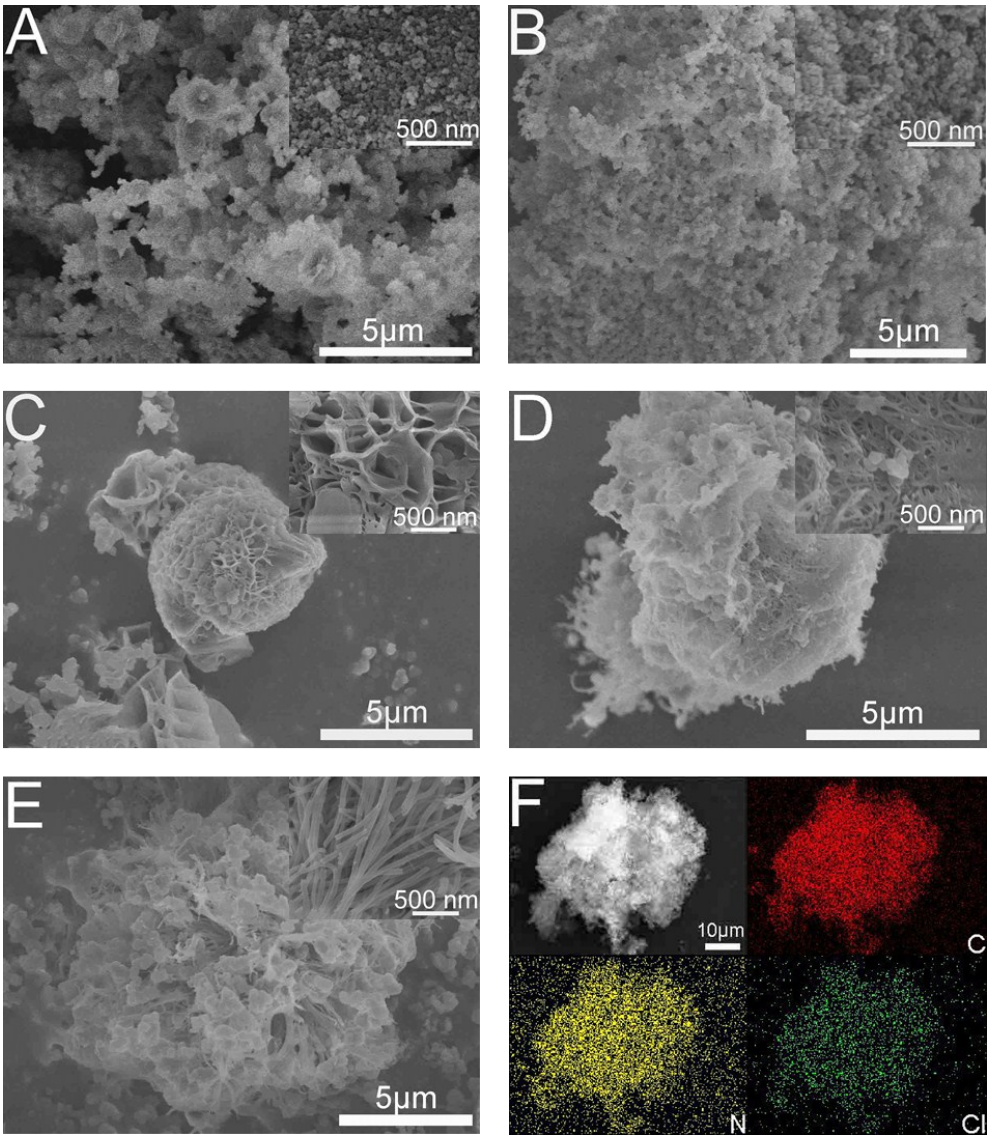


Fig. S2 SEM images of (A) HCP-Cl, (B) HCP-Br, (C) HIP-Cl-1, (D) HIP-Br-1 and (E) HIP-Cl-2. (F) Elemental (C, N and Cl) mapping images of HIP-Cl-2.

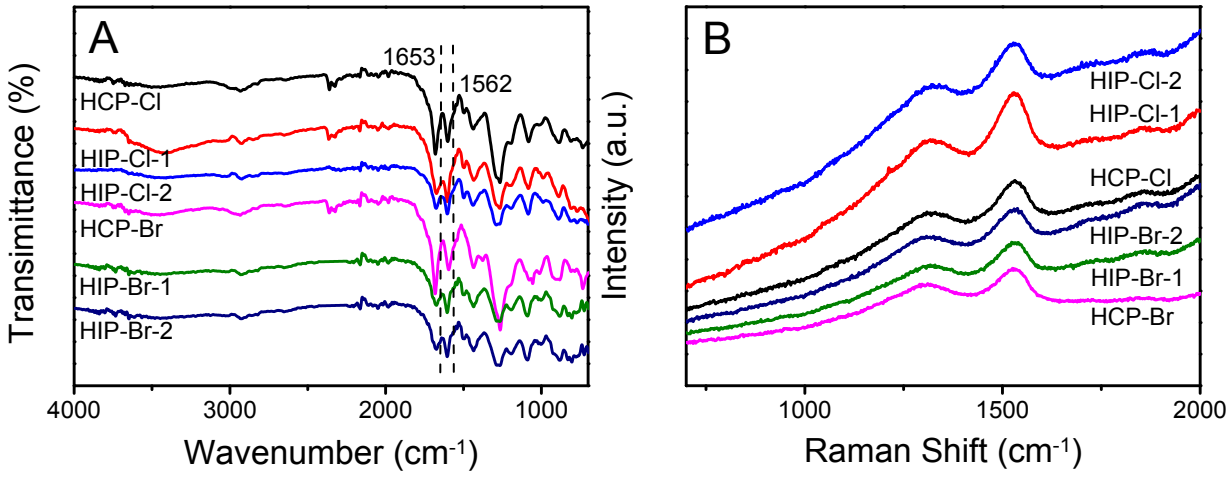


Fig. S3 (A) FT-IR and (B) Raman spectra.

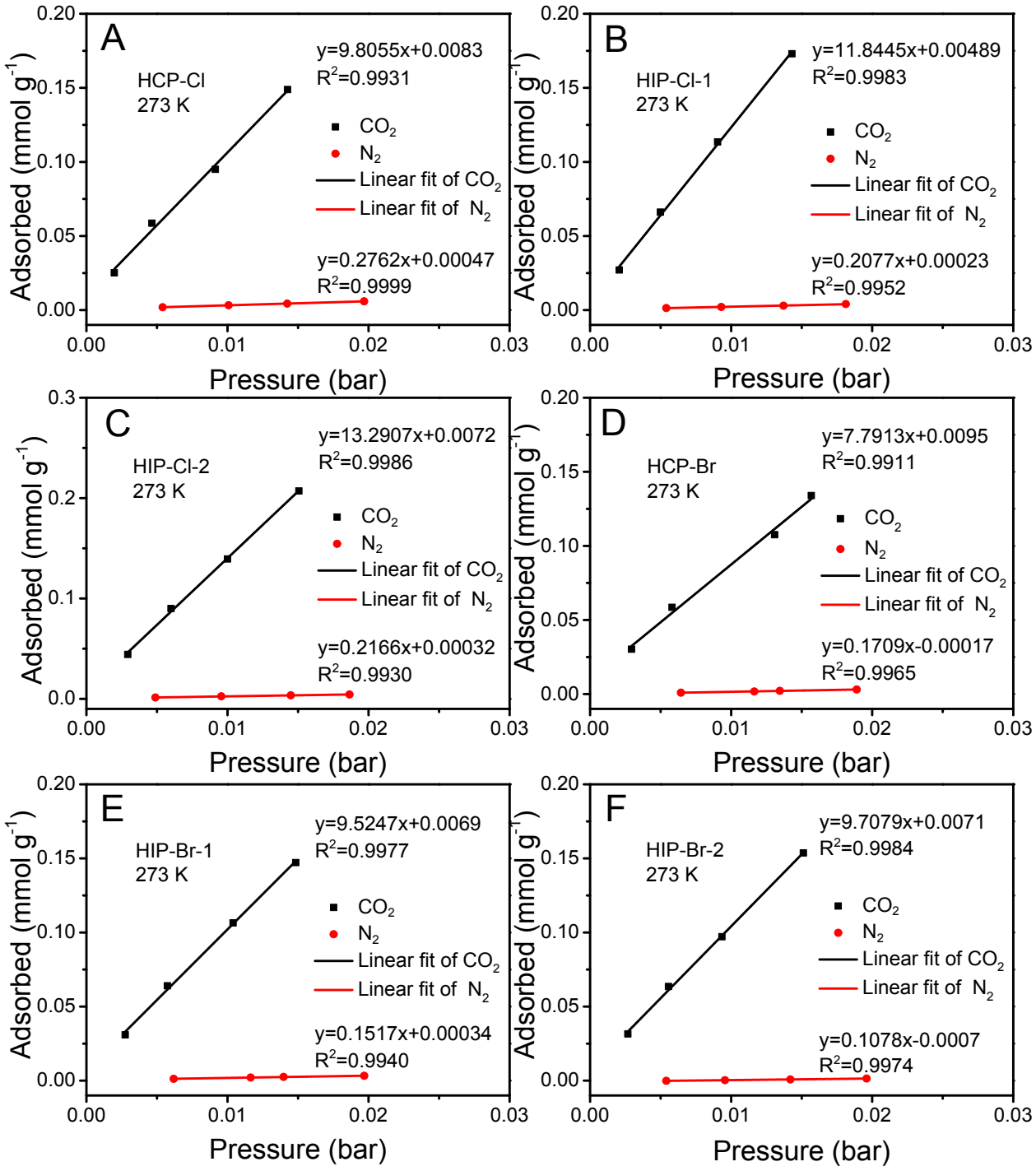


Fig. S4 CO_2/N_2 selectivities calculated by Henry's law constants in the linear low pressure (<0.05 bar) range at 273 K.

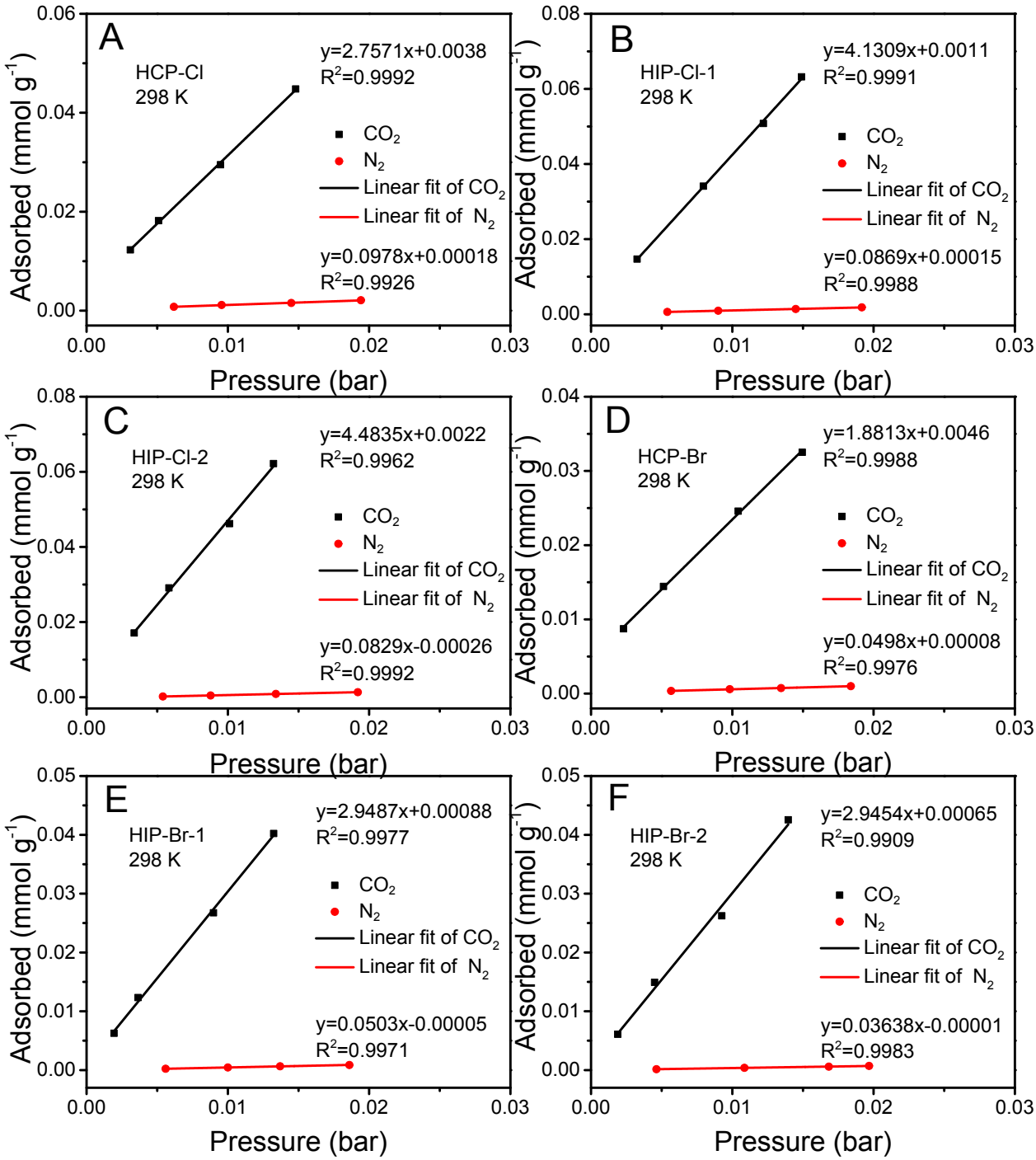


Fig. S5 CO_2/N_2 selectivities calculated by Henry's law constants in the linear low pressure (<0.05 bar) range at 298 K.

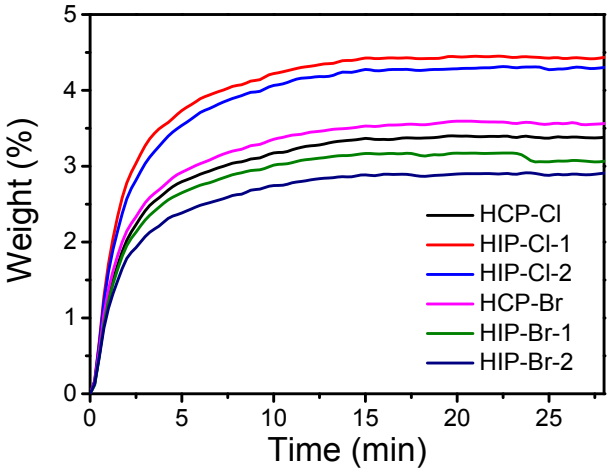


Fig. S6 CO_2 adsorption as a function of time measured by TGA at 308K and 1 bar.

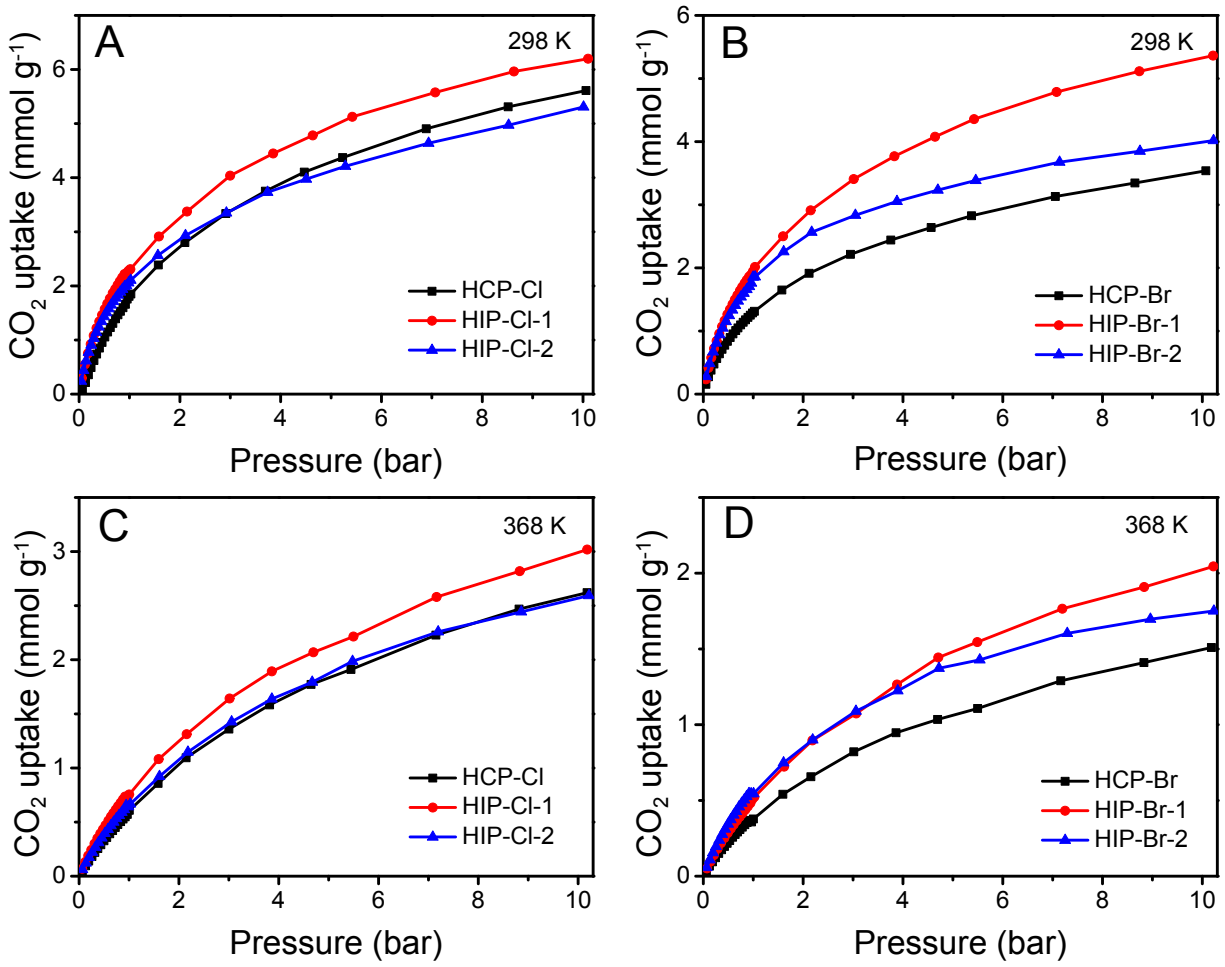


Fig. S7 CO_2 adsorption isotherms at (A,B) 298 K and (C,D) 368 K up to 10 bar.

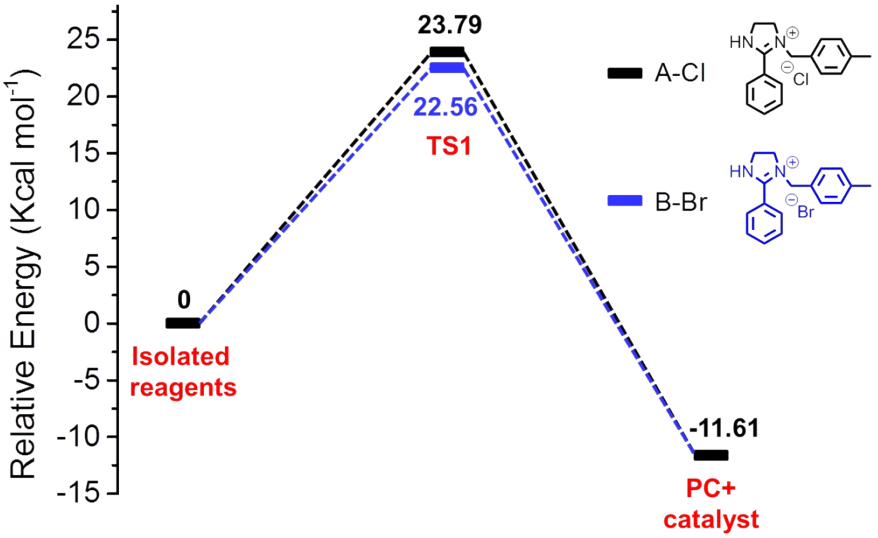


Fig. S8 Relative energies of ring-opening step for fixation of CO_2 with propylene oxide catalyzed by A-Cl and B-Br calculated at the Hybrid B3LYP/DZP level (PC: propylene carbonate).

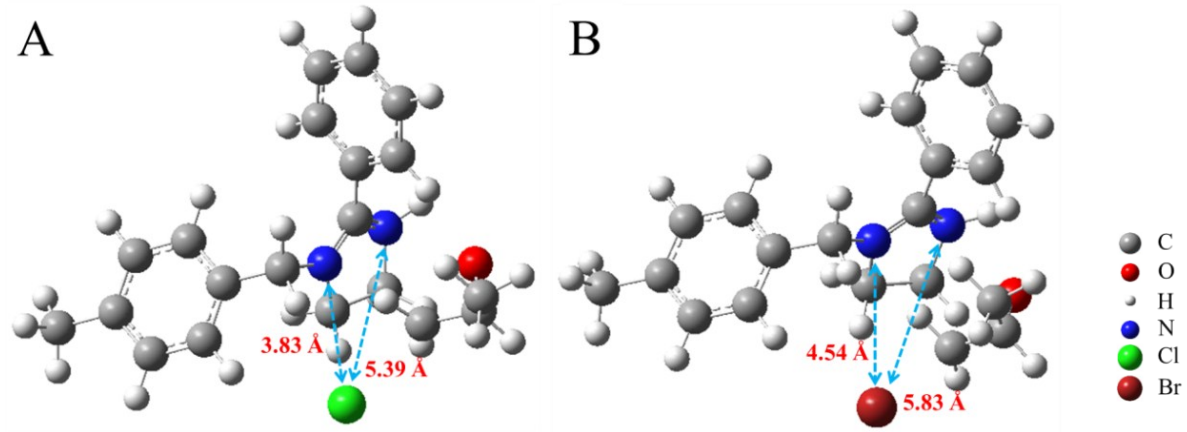


Fig. S9 Optimized geometries for the transition states together with the most calculated distances (in Å) of (A) A-Cl and (B) B-Br.

Additional explanation of Fig. S8 and S9

A simple calculation using A-Cl and B-Br in the absence of $ZnBr_2$ is performed to reveal the higher leaving ability of Br anions than Cl anion in our catalytic system. Fig. S8 displays the relative energies of ring-opening step for CO_2 fixation with propylene oxide catalyzed by A-Cl and B-Br. In the catalytic cycle, the first step (ring opening through the attack of a nucleophile on epoxide) is generally considered to be the rate-determining step with high activation energy (*J. Am. Chem. Soc.*, 2014, 136, 15270; *Catal. Sci. Technol.*, 2014, **4**, 1585; *Green Chem.*, 2012, **14**, 2410; *ACS Catal.*, 2016, **6**, 4871). The energy barrier of the first transition state (TS1) for B-Br (ΔE=22.56 kcal/mol) is lower than the one for A-Cl (ΔE=23.79 kcal/mol, Fig. S8). Besides, the distance between the imidazolinium ring and halogen anions in TS1 of B-Br is longer than that in TS1 of A-Cl (Fig. S9), reflecting a weaker interaction between the imidazolinium ring and Br than the one in the case of Cl. All of these reveal that higher leaving ability of Br anion than Cl anion that reduces the energy barrier in the ring open step and subsequently allows the reaction to be more easily performed.

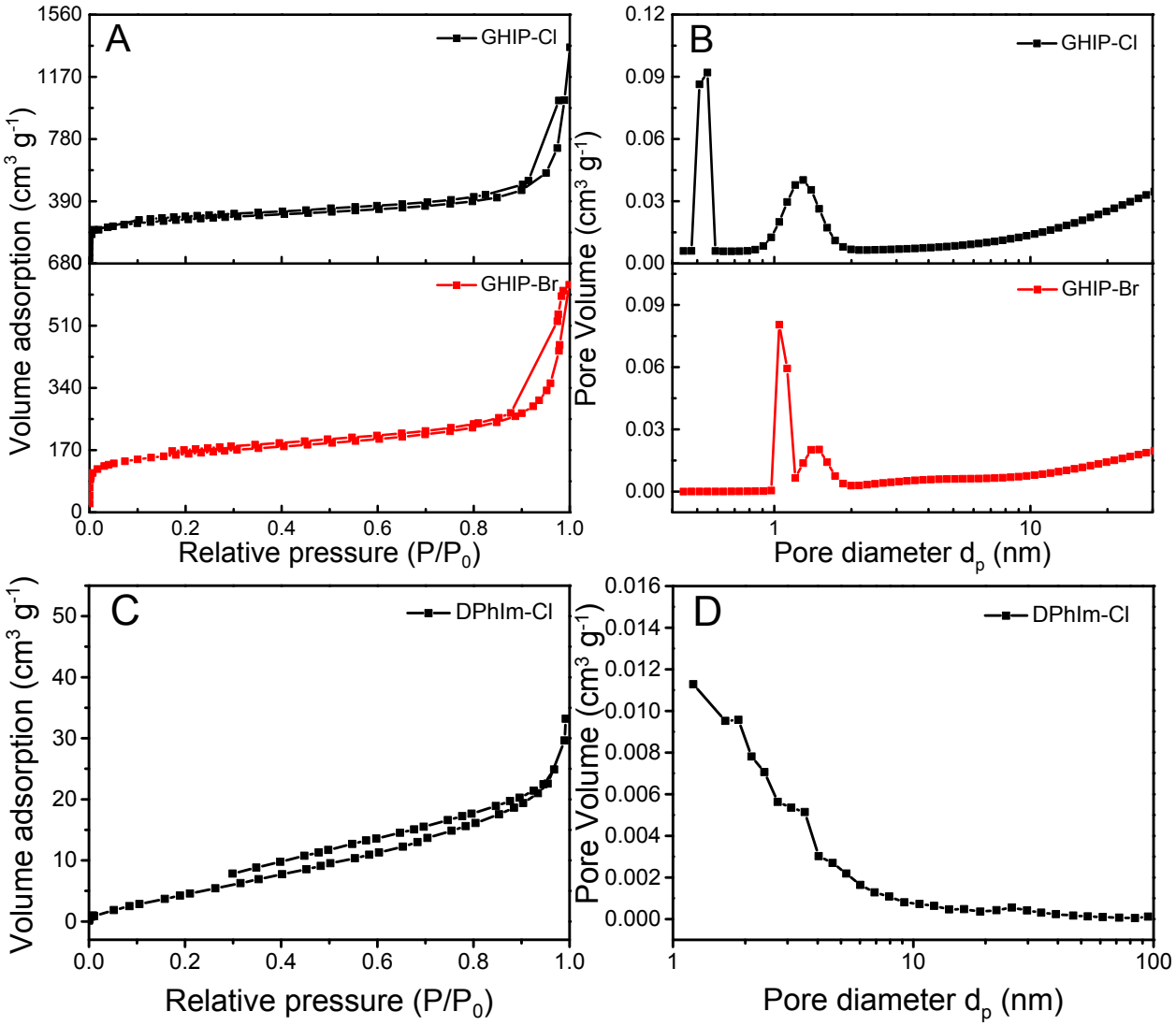


Fig. S10 (A,C) N_2 sorption isotherms and (B,D) pore size distribution curves of GHIPs and DPhIm-Cl.

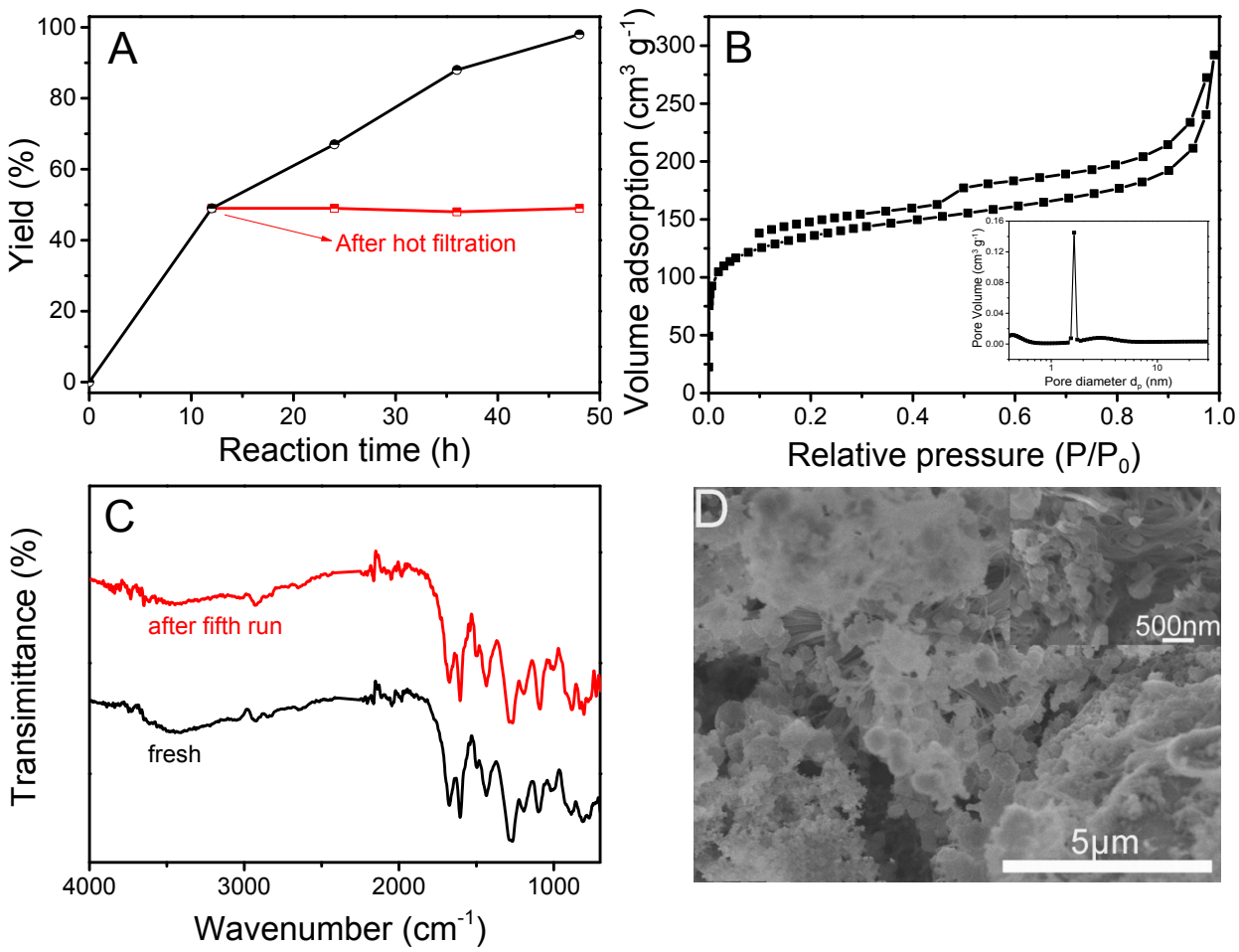


Fig. S11 (A) Hot filtration test for the HIP-Br-2 catalyzed cycloaddition of styrene oxide with CO_2. Reaction conditions: styrene oxide (5 mmol), HIP-Br-2 (10 μmol ionic sites), CO_2 (1 bar), 393 K, 48 h. (B) N_2 sorption isotherm of reused HIP-Br-2 (The inset is the pore size distribution curve). (C) FT-IR of fresh and reused HIP-Br-2 after 5th run. (D) SEM image of reused HIP-Br-2.

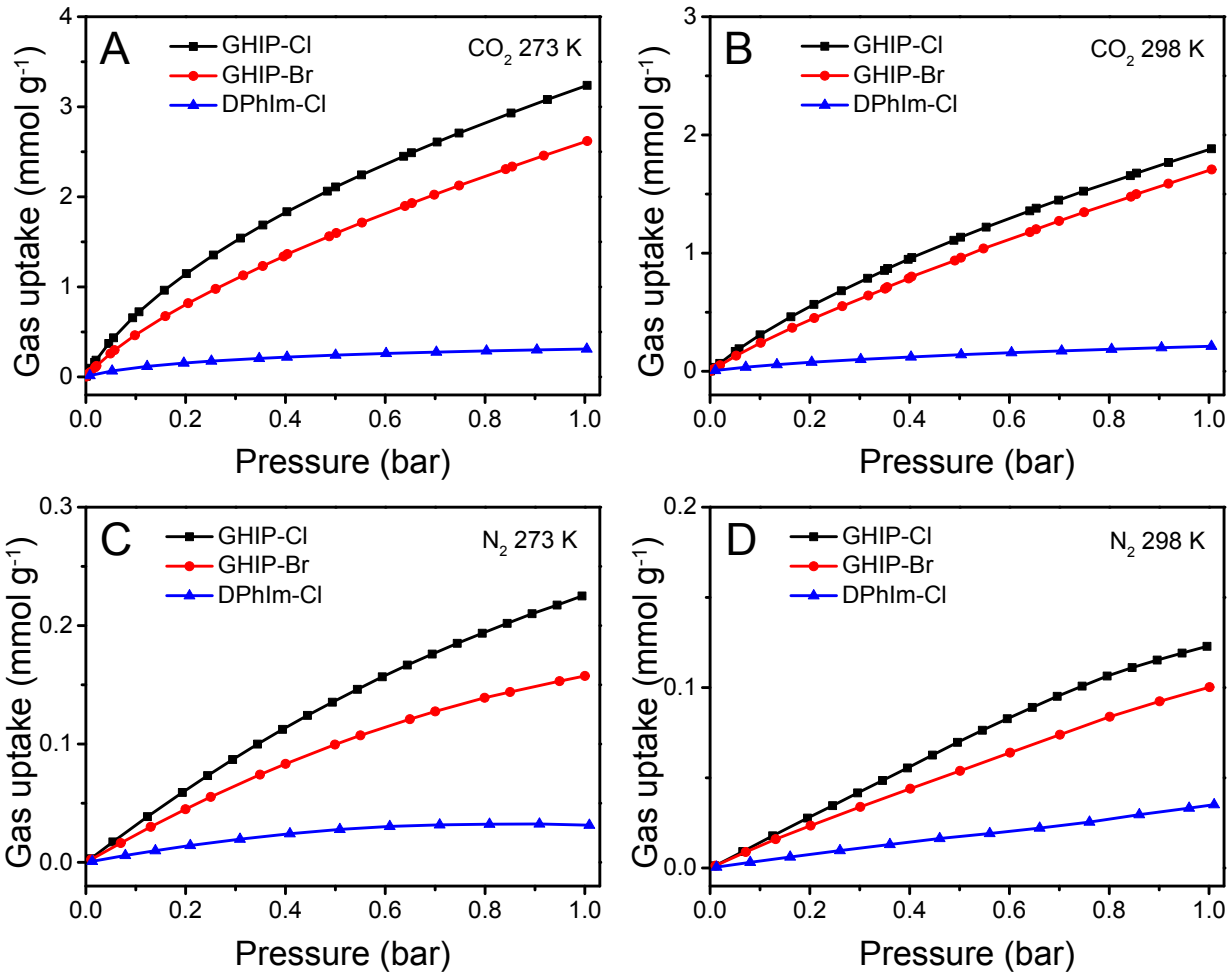


Fig. S12 (A, B) CO_2 and (C, D) N_2 adsorption isotherms of GHIPs and DPhIm-Cl up to 1 bar.

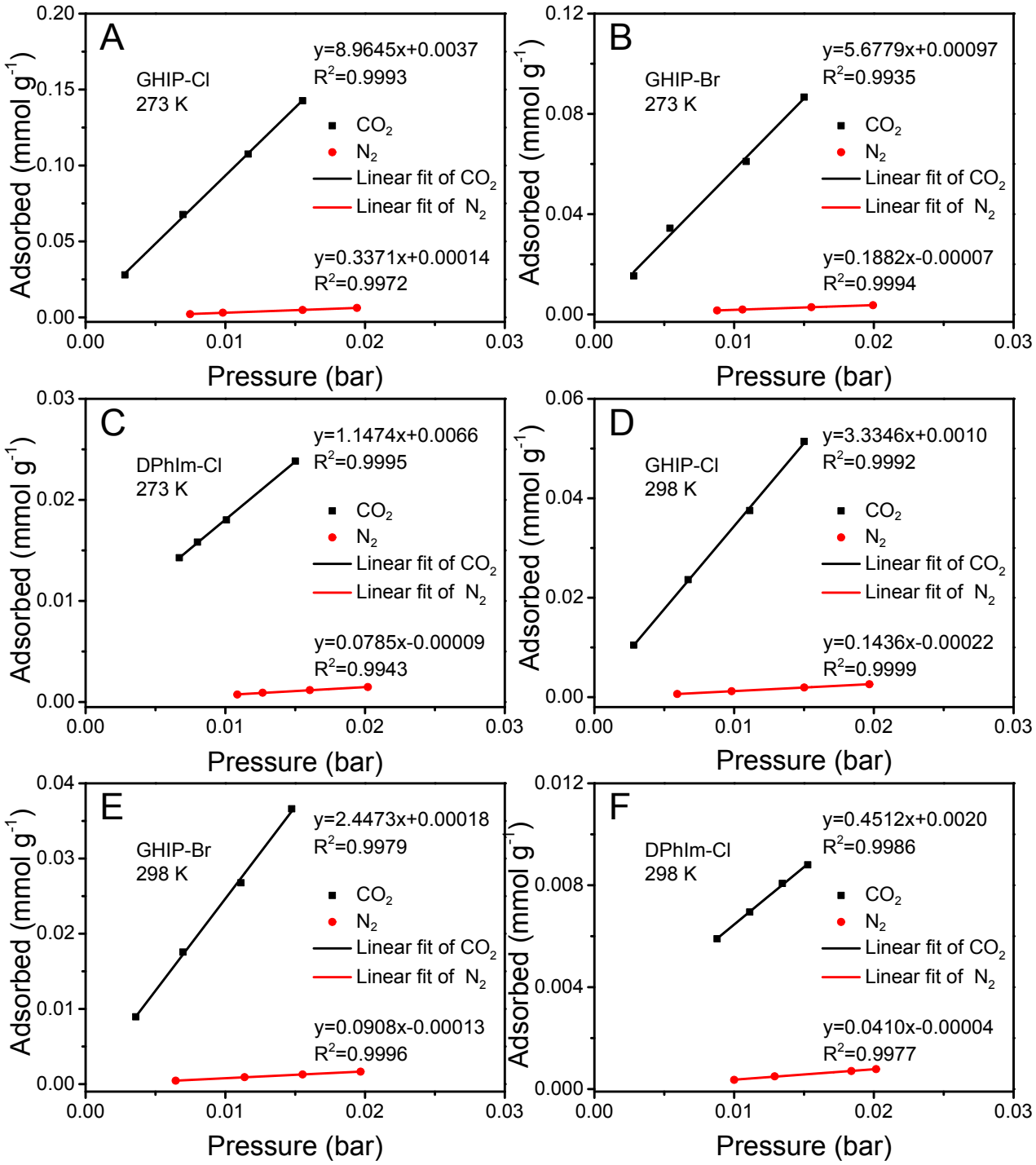


Fig. S13 CO_2/N_2 selectivities calculated by Henry's law constants in the linear low pressure (<0.05 bar) range at (A-C) 273 K and (D-F) 298 K.

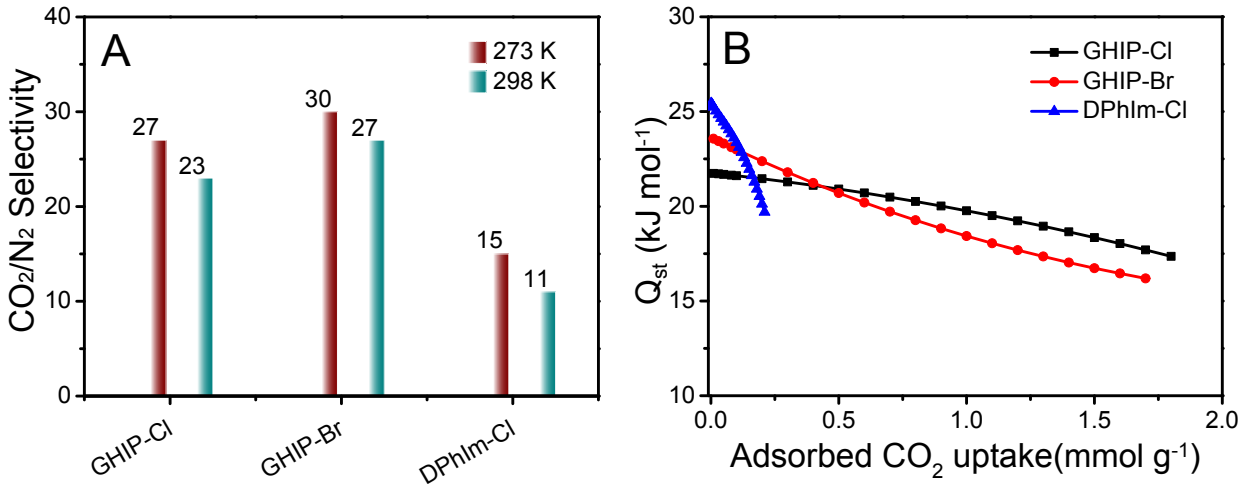


Fig. S14 (A) CO_2/N_2 selectivities calculated using Henry's law constants in the linear low pressure range (<0.05 bar) at 273 K (wine) and 298 K (cyan). (B) Isosteric heats (Q_{st}) calculated from the Clausius-Clapeyron equation.

4. Supplementary Tables

Table S1 Elemental analysis.

Entry	Sample	Found		
		C [%]	H [%]	N [%]
1	HCP-Cl	79.3	4.26	0.00
2	HIP-Cl-1	73.8	4.37	1.09
3	HIP-Cl-2	72.6	4.68	1.91
4	HCP-Br	77.2	4.70	0.00
5	HIP-Br-1	62.2	3.94	1.18
6	HIP-Br-2	62.3	4.62	1.69
7[a]	Reused HIP-Br-2	65.9	4.65	1.67
8	GHIP-Cl	65.4	3.98	1.15
9	GHIP-Br	61.8	3.78	1.22
10	PhIm-Cl	65.3	8.01	11.7
11	DPhIm-Cl	80.6	6.34	5.09

[a] The reused HIP-Br-2 recovered after 5th run during the recycling test.

Table S2 CO_2 adsorption performance of porous ionic polymers.

Sample	CO_2 uptake (mmol g^{-1}) (273K/298K, 1 bar)	CO_2/N_2 selectivity		Ref.
		Method	(273K/298K, 1 bar)	
PCP-Cl	2.3/1.4	IAST[a]	48/36	S1
POM2-IM	3.3/-	Henry[b]	13/-	S2
Polymer-4	2.9/1.7	Henry	-/28	S3
red-POP-V2	-/1.1	-	-/-	S4
TAPOP-1	3.5/-	Henry	8/-	S5
HCP-IL	1.7/1.2	Henry	48/-	S6
CB-PCP-1	2.05/1.2	-	-/-	S7
P(SVImTf$_2$N)	0.46/-	-	-/-	S8
P(CMVImBr1.03-co-AA)	0.64/-	-	-/-	S9
PDMBr	1.02/-	-	-/-	S10
NP-imidazolium	1.74/-	-	-/-	S11
[Et_4NBr]50%-Py-COF	3.74/-	-	-/-	S12

[a] IAST measured from simulated CO_2/N_2 (0.15/0.85) mixture at 1 bar.
[b] Henry's selectivity was calculated by initial slope method below 0.1 bar.

Table S3 CO_2 adsorption performance of nonionic hypercrosslinked polymers.

Sample	CO_2 uptake (mmol g^{-1}) (273K/298K, 1 bar)	CO_2/N_2 selectivity		Ref.
		Method	(273K/298K, 1 bar)	
NOP-50A	4.3/2.7	IAST[a]	72/-	S13
P-PCz-3	5.8/3.4	Henry[b]	22/-	S14
InCz-HCP2	3.6/2.1	Henry	29/-	S15
P-PCz	5.6/3.0	IAST	42/-	S16
HCP-3	2.3/-	Henry	31/-	S17
PHAP-2	2.4/1.5	Henry	34/31	S18
THPS	3.6/-	Henry	38/-	S19
PTPA-1	2.6/1.5	Henry	55/-	S20
Gal-2	2.4/1.4	Henry	42/34	S21
TB-MOP	4.1/2.6	Henry	45/51	S22
TSP-2	4.1/2.6	Henry	38/-	S23
C1M2-Al	3.4/-	IAST	32/-	S24
TB-MOP	1.0/0.5	Henry	38/25	S25
CBZ	2.1/-	Henry	100/76	S26

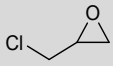
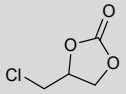
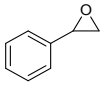
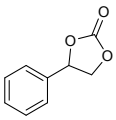
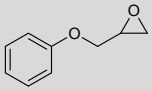
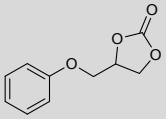
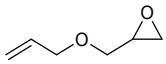
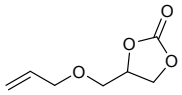
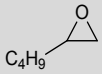
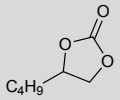
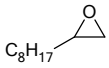
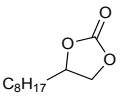
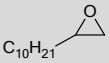
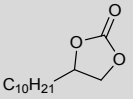
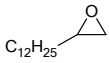
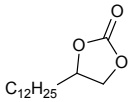
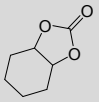
[a] IAST measured from simulated CO_2/N_2 (0.15/0.85) mixture at 1 bar.
[b] Henry's selectivity was calculated by initial slope method below 0.1 bar.

Table S4 Textural properties and CO_2 adsorption performance of PHIPs and DPhIm-Cl.

Sample	S_{BET}[a] (m^2/g)	V_p[b] (cm^3/g)	D_{ave}[c] (nm)	IL content[d] (mmol/g)	CO_2 uptake	
					(mmol/g)[e] 273/298 K	(μmol/m^2)[f] 273/298 K
GHIP-Cl	979	1.63	6.66	0.41	3.2/1.9	3.3/1.9
GHIP-Br	559	0.85	6.07	0.44	2.6/1.7	4.6/3.0
DPhIm-Cl	21	0.05	8.71	1.82	0.3/0.2	14/9.5

[a] BET surface area.
[b] Total pore volume.
[c] Average pore size.
[d] IL content obtained from elemental analysis.
[e] CO_2 adsorption amount per gram at 273 and 298 K (1 bar).
[f] CO_2 adsorption amount per square meter at 273 and 298 K (1 bar).

Table S5 Cycloaddition of CO_2 with epoxides catalyzed by HIP-Br-2.[a]

Entry	Substrate	Product	P_{CO2} (bar)	T (K)	t (h)	Yield (%)	Sel. (%)
1			10	393	6	99	>99
2			10	298	20	99	>99
3			10	393	4	97	98
4			10	298	16	90	97
5			1	393	48	99	>99
6			1	343	96	90	96
7			10	393	6	99	>99
8			20	298	96	90	97
9			1	393	48	98	98
10			1	343	96	98	>99
11			10	393	5	99	>99
12			15	298	96	91	>99
13			1	393	48	96	>99
14			1	343	120	95	>99
15			10	393	4	99	>99
16			20	298	96	84	>99
17			1	393	48	97	>99
18			1	343	96	82	>99
19			10	393	8	94	>99
20			20	298	120	91	>99
21			1	393	96	99	>99
22			1	343	120	85	>99
23			10	393	12	99	>99
24			1	393	96	99	>99
25			10	393	16	99	>99
26			1	393	96	99	>99
27			10	393	16	97	>99
28			1	393	96	99	>99
29			10	393	50	93	>99

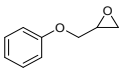
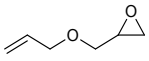
[a] Reaction conditions: epoxides (5 mmol), catalyst (10 μmol ionic sites). Yield and selectivity were determined by GC using *n*-dodecane as the internal standard.

Table S6 Cycloaddition of CO_2 with epichlorohydrin under ambient conditions.[a]

Entry	Catalyst	Co-catalyst	Yield (%)	Sel. (%)
1	HIP-Br-2	-	30	99
2	-	$ZnBr_2$	23	99
3	HIP-Br-2	$ZnBr_2$	96	99
4		$FeCl_3$	<1	99
5	HIP-Br-2	$FeCl_3$	30	99

[a] Reaction conditions: epichlorohydrin (1 mmol), HIP-Br-2 (40 μmol ionic sites), $ZnBr_2$ (0.01 g, 40 μmol), $FeCl_3$ (0.006 g, 40 μmol), DMF (4 mL), CO_2 (1 bar), 298 K, 96 h. Yield and selectivity were determined by GC using *n*-dodecane as the internal standard.

Table S7 Catalytic activity of porous ionic polymers in the cycloaddition of CO_2 with epoxides.

Catalyst	Epoxide	Solvent	CO_2 (bar)	Temp. (K)	Time (h)	Yield (%)	Ref.
PCP-Cl		-	30	373	12	80.4	S1
POM3-IM		ethanol	10	393	12	89	S2
polymer (A2 + A6)/$ZnBr_2$		DMF	10	403	12	96	S3
poly-imidazolium salts		-	10	383	2	96	S27
mlc-SILP		-	100	423	3	55	S28
CLPN		-	30	433	48	83.7	S29
fluorous polymers supported phosphonium chloride		-	80	423	8	95	S30
P–FDIILs		-	25	403	4	99.4	S31
mlc-SILP		-	80	423	3	99	S32
PS-Cat 5		-	10	338	18	98	S33
PSIL		-	60	383	72	93.1	S34
ABMDFP		-	20	403	5	99	S35
CS-EMImBr		-	20	393	4	85	S36
F-PIL-Br		-	10	393	9	96	S37
FDU-HEIMBr		-	20	383	24	95	S38
MCM-41-Imi/Br		-	30	373	4	97.7	S39
PDVB-CEIMBr		-	20	413	4	92.6	S40
PSIL-NTf_2^-		-	8	373	8	88	S41
magnetic supported imidazolium salts		-	30	393	8	42	S42
IM-MPs-EtBr		-	10	383	3	99	S43
n-butBr/mp-C_3N_4		-	25	413	6	92.6	S44
PPh3-ILBr-ZnBr2@POPs		-	30	313	48	53	S45
PP-Br		DMF	1	413	20	98.5	S46
T-IM		-	10	423	10	60	S47
Al-CPOP		-	1	393	24	95	S48
PIP-Bn-Cl		-	20	298	48	73.2	S49
(Zr-MOF), (I)Meim-UiO-66		-	1	393	24	75	S50
PPS⊂COF-TpBpy-Cu		-	1	313	36	93	S51
PAD-3		-	1	363	24	90	S52
PDMBr		-	1	343	48	89	S53

Additional activity comparison

Careful comparison is made between HIP-Br-2 and previous porous ionic polymers or HCPs.

Herein, it should be pointed out that different catalysts are usually evaluated under varied reaction conditions (substrate, reaction temperature, CO_2 pressure, co-catalyst, solvent, etc.), and it is difficult to directly compare the activity between different catalytic systems. Therefore, the reaction conditions should be considered in a reasonable comparison.

The HIP-Br-2 sample can efficiently convert various epoxides into corresponding cyclic carbonates under metal-solvent-additive free conditions (Table S5). High yield can be obtained by using atmospheric CO_2. Compared with previous HCPs (*Chem. Commun.*, 2015, **51**, 12076; *Chem. Commun.*, 2015, **51**, 15708), the HIP-Br-2 demonstrates high activity under milder conditions and better substrate compatibility (high yields are achieved even for the aliphatic long carbon-chain alkyl epoxides and the challenging internal epoxides such as cyclohexene oxide).

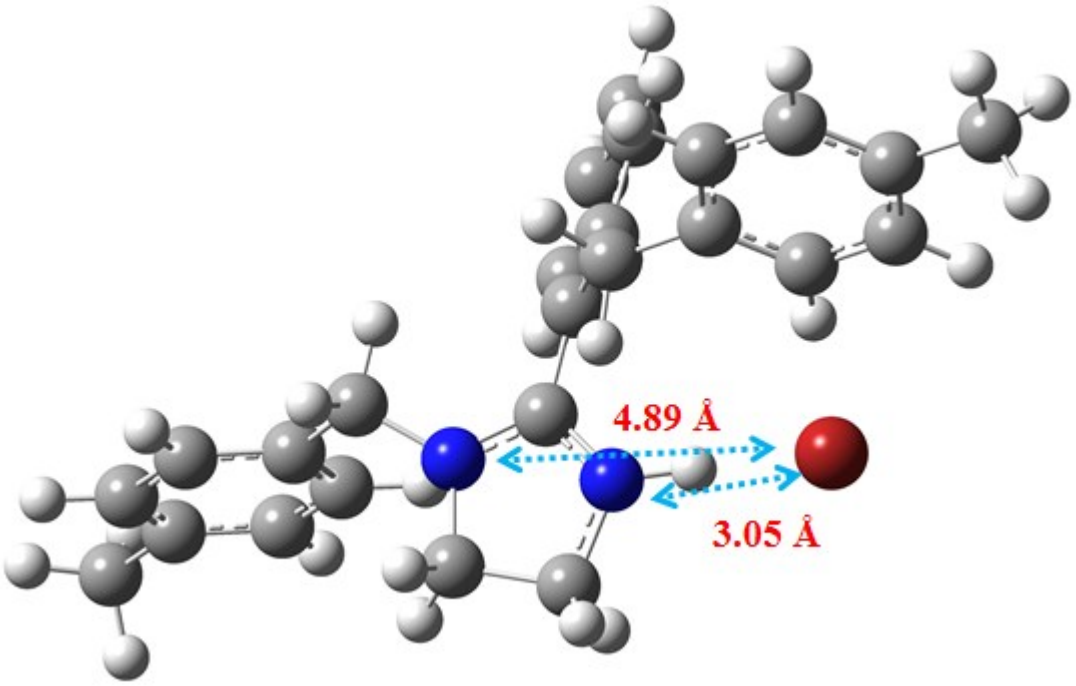
Further, the activity of HIP-Br-2 under metal-solvent-additive free conditions is comparable to the previous efficient porous ionic polymers by comparing the data in Table S5 and S7. For example, compared with recently reported mesoporous poly(ionic liquid) catalyst PAD-3 (*ACS Appl. Mater. Interfaces*, 2016, **8**, 12812) with the activity superior to almost all the previous single component heterogeneous metal-free catalysts, HIP-Br-2 exhibits similar high yields in the cycloaddition of CO_2 with series epoxides and gives a much higher turnover number (TON). HIP-Br-2 demonstrates a high yield of 90% in the cycloaddition of CO_2 with epichlorohydrin under the conditions of 298 K, 1 MPa CO_2 and 16 h. This activity is superior to the one of recently reported efficient porous ionic polymer PIP-Bn-Cl with the yield of 73.2% under the conditions of 298 K, 2 MPa CO_2 and 48 h (*ChemSusChem*, 2017, **10**, 1160). These comparisons prove that HIP-Br-2 is an efficient heterogeneous catalyst compared to previous porous ionic polymers.

In the presence of $ZnBr_2$, HIP-Br-2 affords high yields in catalyzing the conversion of various epoxides under ambient conditions and this performance is also comparable to previous most efficient catalytic systems (*Chem. Mater.*, 2016, **28**, 6276; *J. Am. Chem. Soc.*, 2016, **138**, 2142). By contrast, none of such activity is observed over previous porous ionic polymers. More importantly, HIP-Br-2 displays high yield in the cycloaddition of diluted CO_2 (0.15 bar CO_2 and 0.85 bar N_2)

with various epoxides. Though mixture of CO_2 and N_2 has been used in the CO_2 fixation with epoxides, no such mild condition is reported before, reflecting the specialty and significance of HIP-Br-2 in the cycloaddition reactions by using the flue gas as CO_2 source under mild conditions.

These above step-by-step comparisons reveal that the obtained HIP-Br-2 is a promising heterogeneous catalyst for the chemical conversion of CO_2 with epoxides.

5. Cartesian coordinates for the optimized geometries



Unit I

C	-0.60783090	0.19156359	-0.52776512
C	-2.07012618	0.76618973	-2.21868703
H	-2.03281738	0.09907967	-3.09167675
H	0.75161878	1.73697882	-0.69144930
C	-0.88227804	1.75106883	-2.18183588
H	-0.39458656	1.87356969	-3.15166893
C	-0.02582636	-0.47077248	0.66019373
C	-0.70106765	-0.29690783	1.88244197
C	1.18366885	-1.19569772	0.60198039
C	-0.19289351	-0.84248619	3.05550764
H	-1.60175353	0.30904275	1.91415012
C	1.66501306	-1.74756948	1.79885958
C	0.99508818	-1.57765883	3.00826960
H	-0.70729207	-0.67931742	3.99803505
H	2.59802783	-2.30376711	1.77459987
H	1.40692965	-2.00774347	3.91748671
C	-2.68058102	-1.20744099	-0.72025660
H	-2.61473455	-1.89572511	-1.57631129
H	-2.23847754	-1.71875143	0.13987620
C	-4.13642492	-0.86909526	-0.45302153
C	-5.14735131	-1.70052032	-0.94502017
C	-4.50438004	0.24068848	0.32116947

C	-6.49082818	-1.44049993	-0.65857885
H	-4.88861858	-2.56413091	-1.55511796
C	-5.84585346	0.50029258	0.59940471
H	-3.73919666	0.90967036	0.70733115
C	-6.86539338	-0.33632386	0.11689792
H	-7.25752674	-2.10475606	-1.05124175
H	-6.10531695	1.36796835	1.20270436
C	-8.31648085	-0.04048975	0.41899170
H	-8.97133913	-0.83953728	0.05665291
H	-8.48497068	0.06924972	1.49725801
H	-8.63876874	0.89549887	-0.05520425
N	-1.85620549	-0.03313942	-0.99394907
N	0.02471274	1.12369710	-1.21173767
C	1.94154618	-1.46202724	-0.69394040
H	1.75407092	-2.50418586	-0.99030862
H	1.53611337	-0.83893819	-1.49597870
C	3.44522834	-1.24774767	-0.61010748
C	4.32977427	-2.29797503	-0.87760724
C	3.97981780	0.01098225	-0.28616764
C	5.71502189	-2.10335126	-0.83048526
H	3.93841917	-3.28256241	-1.13018426
C	5.36044086	0.19797215	-0.24623457
H	3.32610045	0.85183784	-0.05682767
C	6.25485042	-0.85154574	-0.51540370
H	6.37976758	-2.93883592	-1.04227336
H	5.74787020	1.18363697	0.00485417
C	7.74942361	-0.62700905	-0.46705369
H	8.06408161	-0.24115440	0.51089503
H	8.29994327	-1.55547964	-0.65384790
H	8.06727059	0.10686060	-1.21909129
H	-3.04793362	1.25284562	-2.19586967
H	-1.16599539	2.74077208	-1.80562228
Br	1.65497766	2.98234674	0.57398081

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2 3 1.0 5 1.0 34 1.0 53 1.0

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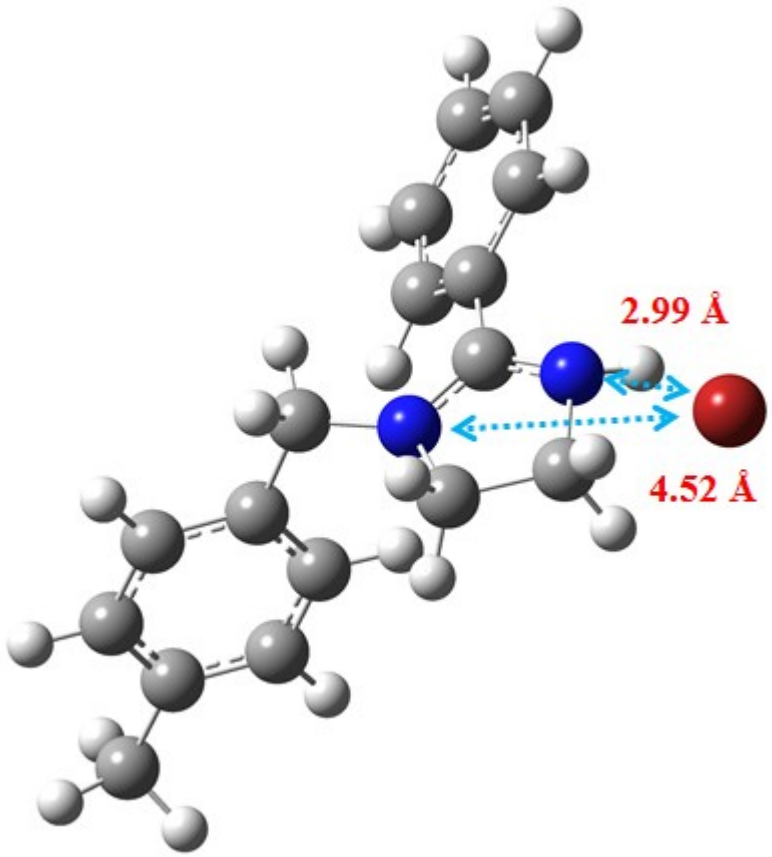

Unit II

C	0.99871561	-0.02367573	1.11703959
C	-0.34808185	-1.62645583	2.09355815
H	-1.14752315	-2.21779011	1.63991575
H	2.54818417	-1.22425942	0.58889791
C	1.06452011	-2.19456242	1.83868614
H	1.08279250	-2.93837557	1.03492060
C	1.47776846	1.20969326	0.47686985
C	0.74446850	1.85316949	-0.53382704
C	2.73746166	1.70774536	0.84851222
C	1.26501940	2.98636367	-1.15524274
H	-0.19864774	1.44046064	-0.87412802
C	3.24338973	2.85135689	0.23460921
H	3.31049250	1.19643279	1.61411838
C	2.51005556	3.49073152	-0.76811085
H	0.70527530	3.46535946	-1.95239289
H	4.21757257	3.23096793	0.52545131
H	2.91295259	4.37295727	-1.25649347
C	-1.37857711	0.64894540	1.59833857
H	-1.69525945	0.66477655	2.65038131
H	-0.99672503	1.64740818	1.36771421
C	-2.57047327	0.31350231	0.71500568

C	-3.85444779	0.70784658	1.10985168
C	-2.42257356	-0.34929931	-0.50965167
C	-4.95965993	0.45905157	0.29437188
H	-3.99672415	1.21033677	2.06421945
C	-3.53221176	-0.60097214	-1.31933586
H	-1.44109332	-0.68530157	-0.83333862
C	-4.81923057	-0.19656910	-0.93750190
H	-5.94701553	0.77159922	0.62507556
H	-3.39061437	-1.12441889	-2.26143286
C	-6.01135327	-0.44494958	-1.83187009
H	-6.94040061	-0.49454221	-1.25616245
H	-6.12410829	0.36072223	-2.56823220
H	-5.90525651	-1.38131225	-2.38814188
N	-0.27343211	-0.29078549	1.46754840
N	1.83080914	-1.01992380	1.38556997
H	-0.56631118	-1.50739523	3.16289940
H	1.51457838	-2.63055115	2.73321845
Br	3.03678436	-1.70667546	-1.26331816

1 7 1.0 35 1.5 36 1.5
2 3 1.0 5 1.0 35 1.0 37 1.0
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The transition states of A-Cl

C	1.183183	0.206747	1.014591
C	-0.275975	-1.267380	1.980831
H	-0.855125	-1.834205	1.248889
H	2.882876	-0.856311	1.214083
C	1.159522	-1.787927	2.137848
H	1.259414	-2.840934	1.887477
C	1.784978	1.422962	0.432458
C	1.678021	1.686102	0.933181
C	2.478277	2.284430	1.285342
C	2.255046	2.838811	-1.450472
H	1.154838	0.997480	-1.584059
C	3.045610	3.435775	0.750191
H	2.554834	2.034459	2.345923
C	2.933193	3.714920	-0.607592
H	2.175601	3.052121	-2.508272
H	3.578889	4.115882	1.401761
H	3.376785	4.615578	-1.012554
C	-1.124409	1.104036	1.386793
H	-1.305046	1.468546	2.400779
H	-0.760777	1.929189	0.776388
C	-2.398994	0.510685	0.840192
C	-3.473132	0.287938	1.700520
C	-2.520315	0.153320	-0.501958
C	-4.642059	-0.292990	1.221542
H	-3.388558	0.572085	2.745204
C	-3.690227	-0.428400	-0.973220
H	-1.698906	0.328504	-1.187413
C	-4.769421	-0.664522	-0.117706
H	-5.466587	-0.459789	1.904411

H	-3.768221	-0.700430	-2.018996
C	-6.047191	-1.271800	-0.631772
H	-6.490512	-1.941008	0.106089
H	-6.780354	-0.492284	-0.852573
H	-5.878118	-1.839182	-1.546787
N	-0.045905	0.096872	1.449548
N	1.874829	-0.933812	1.163523
H	-0.834468	-1.223264	2.913656
H	1.559319	-1.574182	3.131737
Cl	-1.889002	1.648596	5.121090
C	1.615765	1.182918	5.187034
C	0.406449	1.300612	4.340796
O	2.312105	0.860512	4.015924
C	2.079009	2.441321	5.895466
H	2.113703	3.278997	5.195108
H	3.082954	2.288787	6.296061
H	1.404005	2.697914	6.714954
H	1.547574	0.351483	5.903839
H	0.313269	2.191189	3.743444
H	-0.008620	0.383474	3.987224

The transition states of 2-Br

C	2.070726	0.321370	1.047027
C	1.291315	-1.718842	1.761671
H	0.816705	-2.348462	1.007934
H	4.048914	-0.087996	1.002011
C	2.830500	-1.752839	1.690992
H	3.202392	-2.606366	1.128724
C	2.159715	1.738665	0.646900
C	2.832394	2.630399	1.482881
C	1.611524	2.159095	-0.565920
C	2.929343	3.963676	1.099202
H	3.238788	2.252474	2.421741
C	1.729071	3.490595	-0.940684
H	1.114907	1.450251	-1.216002
C	2.382129	4.393049	-0.104983
H	3.434306	4.668376	1.747192
H	1.315102	3.822252	-1.883734
H	2.466155	5.431867	-0.397819
C	-0.327660	0.300460	1.769945
H	-0.361323	0.495764	2.844937
H	-0.388382	1.252273	1.245725
C	-1.451932	-0.629319	1.394889
C	-2.101542	-1.361558	2.386716
C	-1.824090	-0.810402	0.063531
C	-3.097294	-2.269398	2.043881
H	-1.815440	-1.233629	3.426740
C	-2.817774	-1.720095	-0.271558
H	-1.333516	-0.241993	-0.718480
C	-3.466799	-2.469394	0.713898
H	-3.586810	-2.835484	2.827267

H	-3.093429	-1.851420	-1.310986
C	-4.553835	-3.445319	0.352722
H	-4.592491	-4.271009	1.063291
H	-5.530101	-2.954395	0.360985
H	-4.398524	-3.860699	-0.643063
N	0.986716	-0.298808	1.455851
N	3.122859	-0.493209	0.984262
H	0.899376	-1.982019	2.742851
H	3.290621	-1.708620	2.677702
Br	-0.091222	-0.737385	5.846652
C	2.798661	1.015491	5.022786
C	2.017795	-0.173916	4.651177
O	3.521093	0.750491	3.856710
C	2.056297	2.338345	5.084597
H	1.419943	2.470156	4.205926
H	2.770368	3.164712	5.119997
H	1.421424	2.381288	5.971705
H	3.381308	0.869738	5.943869
H	1.388810	-0.056408	3.799775
H	2.434637	-1.142943	4.864322

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