Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Unique allosteric effect driven rapid absorption of carbon dioxide on a new ionogel [P_{4444}][2-Op]@MCM-41 with excellent cyclic stability and loading-dependent capacity

Chunfeng Xue[a], Hongye Zhu[a], Xiao Du[a], Xiaowei An[a], Enyang Wang[a], Donghong Duan[a], Lijuan Shi[a], Xiaogang Hao[a*], Bo Xiao[b], Changjun Peng[c]*

[a] Department of Chemical Engineering, Taiyuan University of Technology, Taiyuan 030024, Shanxi, P. R. China

[b] School of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast, BT7-1NN, Northern Ireland, UK

[c] State Key Laboratory of Chemical Engineering and Department of Chemistry, East China University of Science and Technology, Shanghai, 200237, P. R. China

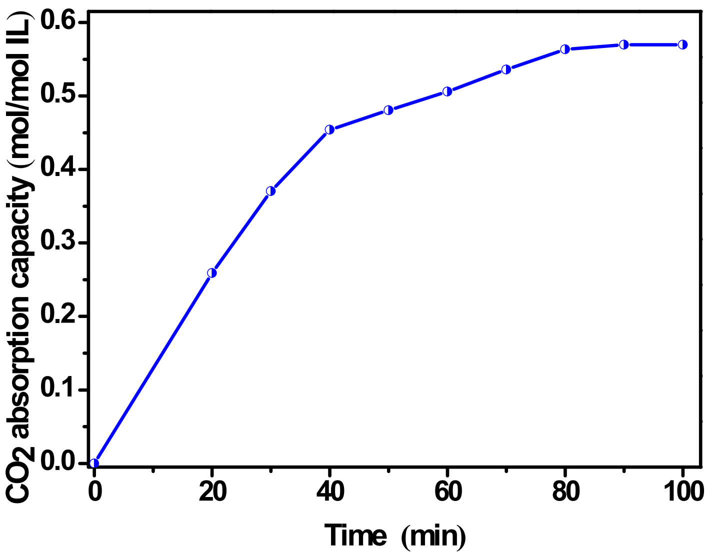


Fig. S1 Absorption isotherm curve from bubble CO_2 in the pure IL [P_{4444}][2-Op] at 50 °C and ordinary pressure

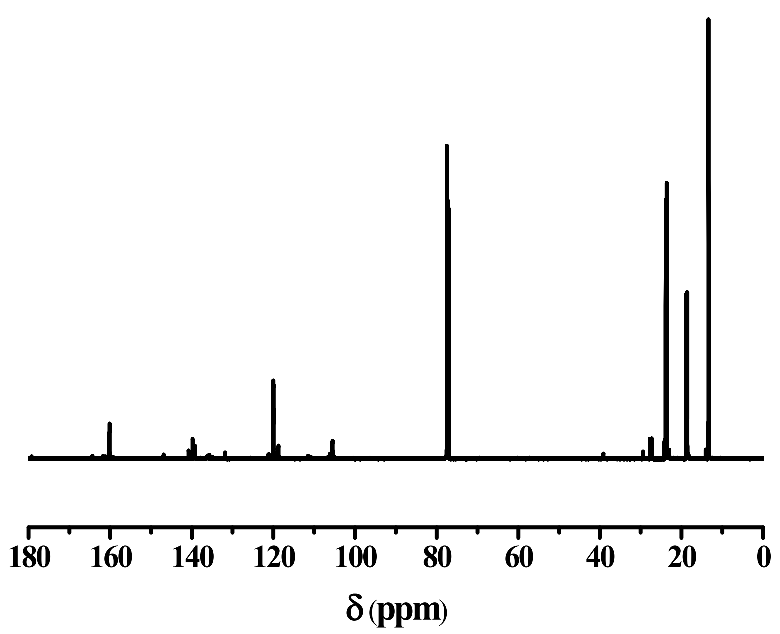
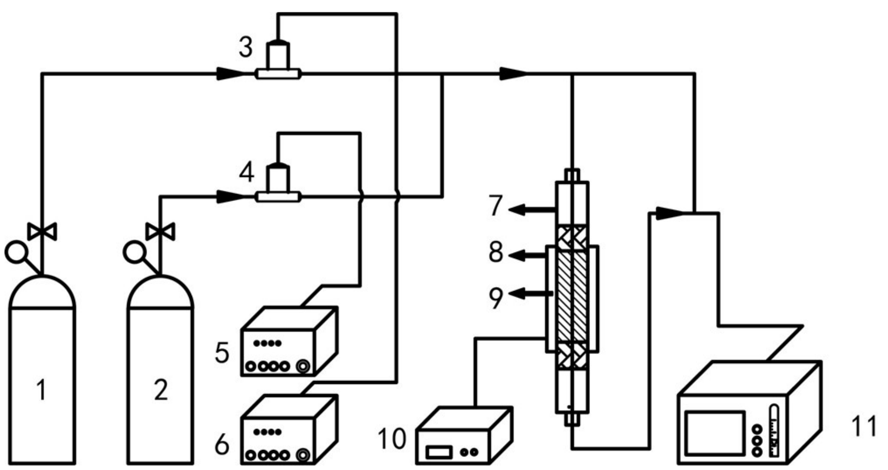
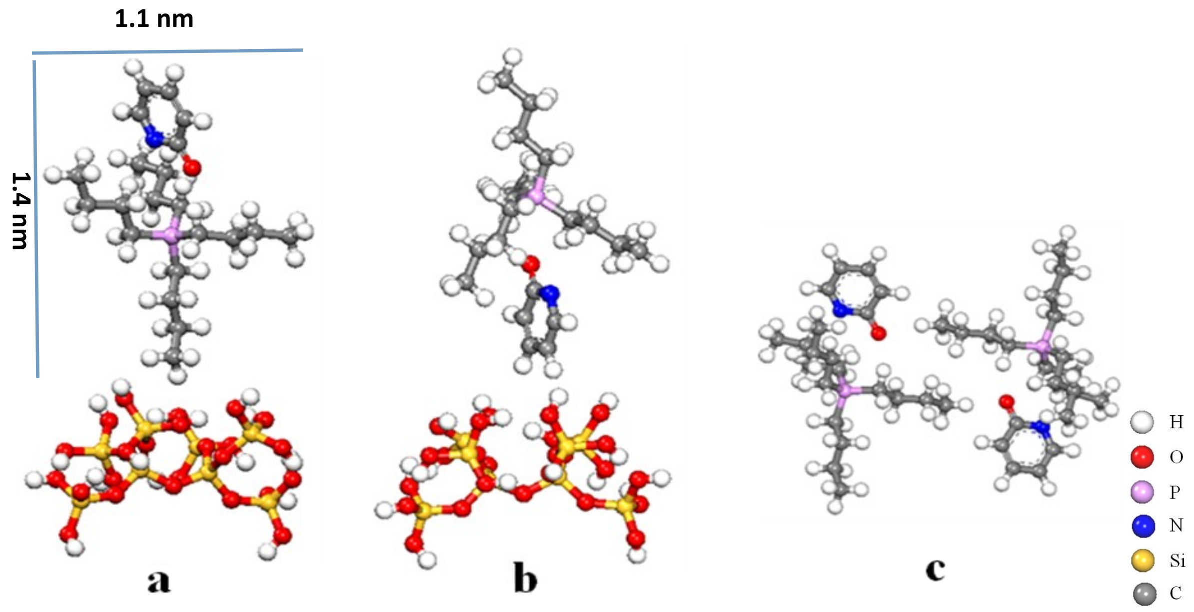


Fig. S2 ^{13}C NMR of the IL [P_{4444}][2-Op]



1. CO_2 cylinder; 2. N_2 cylinder; 3. CO_2 mass flow controller; 4. N_2 mass flow controller; 5. Flow readout box; 6. Flow readout box; 7. Sample cell; 8. Heating jacket; 9. Adsorbent; 10. Temperature controller; 11. Gas analyzer.

Fig. S3. Diagram of the CO_2 adsorption setup at atmospheric pressure



–41.8 kJ·mol^{-1} –37.7 kJ·mol^{-1} –22.3 kJ·mol^{-1}

Fig. S4. Bonding styles and bounding energy: (a) [P_{4444}] cation of IL [P_{4444}][2-Op] close to the surface of silica MCM-41, (b) [2-Op] anion IL [P_{4444}][2-Op] close to the surface of silica MCM-41, and (c) the two IL pair of [P_{4444}][2-Op] arranged with staggered structure.

Table S1. Mulliken atomic charges in different circumstance of materials

Material	Group	Mulliken atomic charge	
		Before loading	After loading
[P_{4444}][2-Op]	N	-0.452	-0.478
	O	-0.638	-0.643
MCM-41	OH(1)	-0.365	-0.368
	OH(2)	-0.364	-0.365
	OH(3)	-0.420	-0.422
	OH(4)	-0.392	-0.395
	OH(5)	-0.407	-0.410
	OH(6)	-0.329 c	-0.368

Table S2 Comparison of CO_2 absorption capacities of absorbents at ordinary pressure

Sample	Adsorption Temperature	Adsorption time (min.)	Capacity, (mmol/g)	Reference
5%[P_{4444}][2-Op]/MCM-41	50 °C	4.67	1.21	This study
33.3%BMIMCl/ZrP	60 °C	180	0.73	[1]
33.3%BMIMCl/MMT	70 °C		0.42	
15%PAP/MCM-41	120 °C	Unavailable	0.48	[2]
15%PA/MCM-41			0.37	
50%[P_{66614}][2-Op]/MCM-41	19 °C	240	0.905	[3]
[$P(C_4)_4$][Gly]/8SiO_2	25 °C	800	0.205	[4]
50% [EMIM][Arg]/PMMA	40 °C	45	1.01	
50% [EMIM][Ala]/PMMA	40 °C	45	1.38	
50% [EMIM][Gly]/PMMA	25 °C	45	1.71	[5]
50% [EMIM][Gly]/PMMA	40 °C	45	1.53	
50% [EMIM][Gly]/PMMA	80 °C	45	1.02	
25%SALG-AT-EZT3/SiO_2	40 °C	333.33	2.01	[6]
25%EZT3/ZSM-5	40 °C	333.33	2.93	
25%EZT3/Nano-SiO_2	40 °C	333.33	3.38	[7]
25%EZT3/Fumed SiO_2	40 °C	333.33	2.74	
25%Arg/PMMA	40 °C	333.33	1.3	[8]
50%DBUOH/silica gel	25 °C	300	1.93	[9]
40% DBUOH/MCM-41	25 °C	300	1.85	
60% DBUOH/SBA-15	25 °C	300	2.49	
50%EZT3/SBA-15	40 °C	Unavailable	4.7	[10]
60%TM/MCM-41	55 °C	60	3.706	[11]

The quantum chemical calculation was performed using the DMOL3 module included in the Accelrys Material Studio 6.0 software package. GGA/PBE/DNP+ with an all-electron method was used for these calculations.

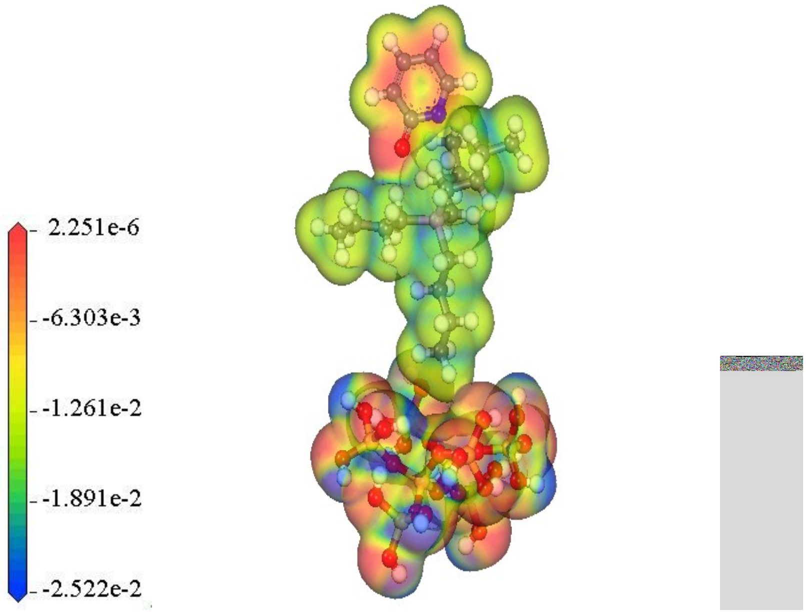


Fig. S5 The surface electrostatic potential of $[P_{4444}]$ cation of $[P_{4444}]$[2-Op] IL close to the surface of silica MCM-41.

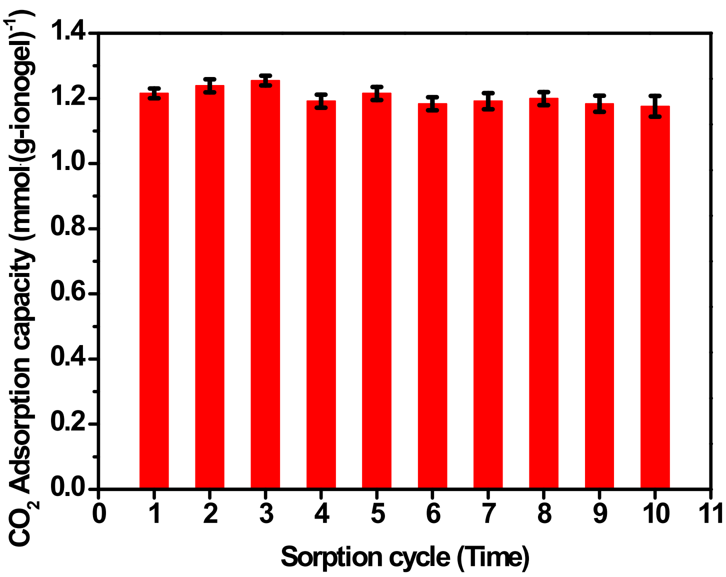


Fig. S6 Ten cycles of CO_2 adsorption/desorption capacity of the ionogel PM-5 at 50 °C

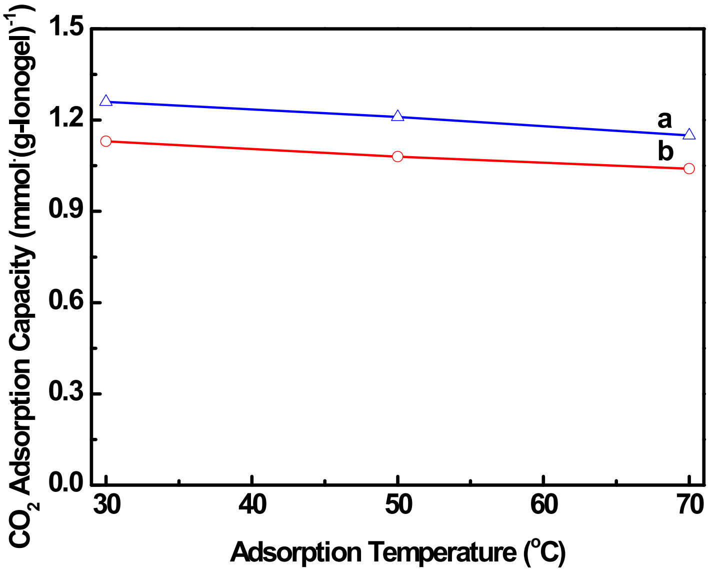


Fig. S7. CO_2 adsorption capacity of ionogel PM-5 recorded in gas mixture with CO_2 partial pressure of 0.1435 (a) and 0.0988 (b) at different temperatures of 30, 50, and 70 °C.

References:

1. Y. Zhou, J. Liu, M. Xiao, Y. Meng and L. Sun, *ACS Applied Materials & Interfaces*, 2016, **8**, 5547-5555.
2. M. M. Wan, H. Y. Zhu, Y. Y. Li, J. Ma, S. Liu and J. H. Zhu, *ACS Applied Materials & Interfaces*, 2014, **6**, 12947-12955.
3. J. Cheng, Y. Li, L. Hu, J. Zhou and K. Cen, *Energy & Fuels*, 2016, **30**, 3251-3256.
4. J. Zhang, S. Zhang, K. Dong, Y. Zhang, Y. Shen and X. Lv, *Chemistry – A European Journal*, 2006, **12**, 4021-4026.
5. X. Wang, N. G. Akhmedov, Y. Duan, D. Luebke and B. Li, *Journal of Materials Chemistry A*, 2013, **1**, 2978-2982.
6. I. H. Arellano, S. H. Madani, J. Huang and P. Pendleton, *Chemical Engineering Journal*, 2016, **283**, 692-702.

7. I. H. Arellano, J. Huang and P. Pendleton, *RSC Advances*, 2015, **5**, 65074-65083.

8. B. Jiang, X. Wang, M. L. Gray, Y. Duan, D. Luebke and B. Li, *Applied Energy*, 2013, **109**, 112-118.

9. S. Lee, S.-Y. Moon, H. Kim, J.-S. Bae, E. Jeon, H.-Y. Ahn and J.-W. Park, *RSC Advances*, 2014, **4**, 1543-1550.

10. I. H. Arellano, J. Huang and P. Pendleton, *Chemical Engineering Journal*, 2015, **281**, 119-125.

11. X. Zhang, X. Zheng, S. Zhang, B. Zhao and W. Wu, *Industrial & Engineering Chemistry Research*, 2012, **51**, 15163-15169.