Electronic Supplementary Material (ESI) for Polymer Chemistry.

CO_2 adsorption and catalytic application of imidazole ionic liquid functionalized porous organic polymers

Shuang Hao, Yuchuan Liu, Chuning Shang, Zhiqiang Liang* and Jihong Yu*

State Key Laboratory of Inorganic Synthesis & Preparative Chemistry, Jilin University, Changchun, 130012, P. R. China

Email: liangzq@jlu.edu.cn; jihong@jlu.edu.cn

Supporting Information

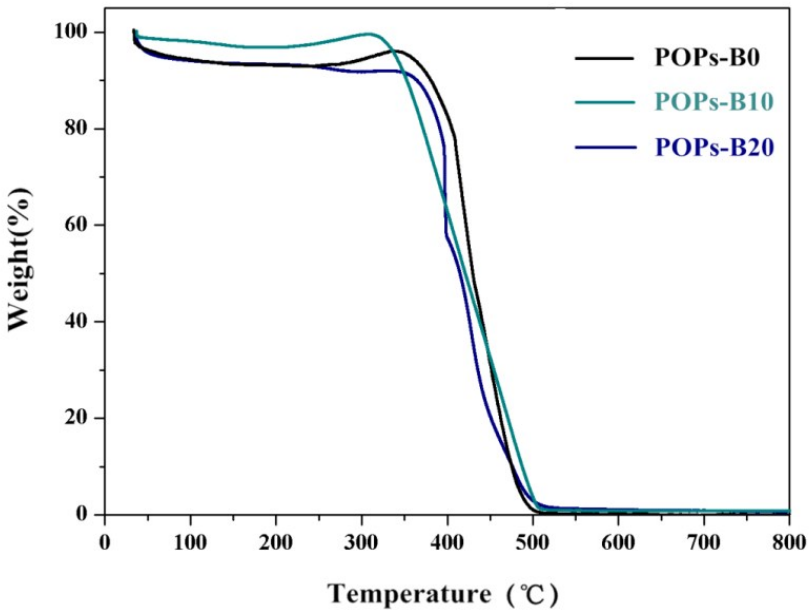

Fig. S1 TG analysis of **POPs-B0**, **POPs-B10** and **POPs-B20**.

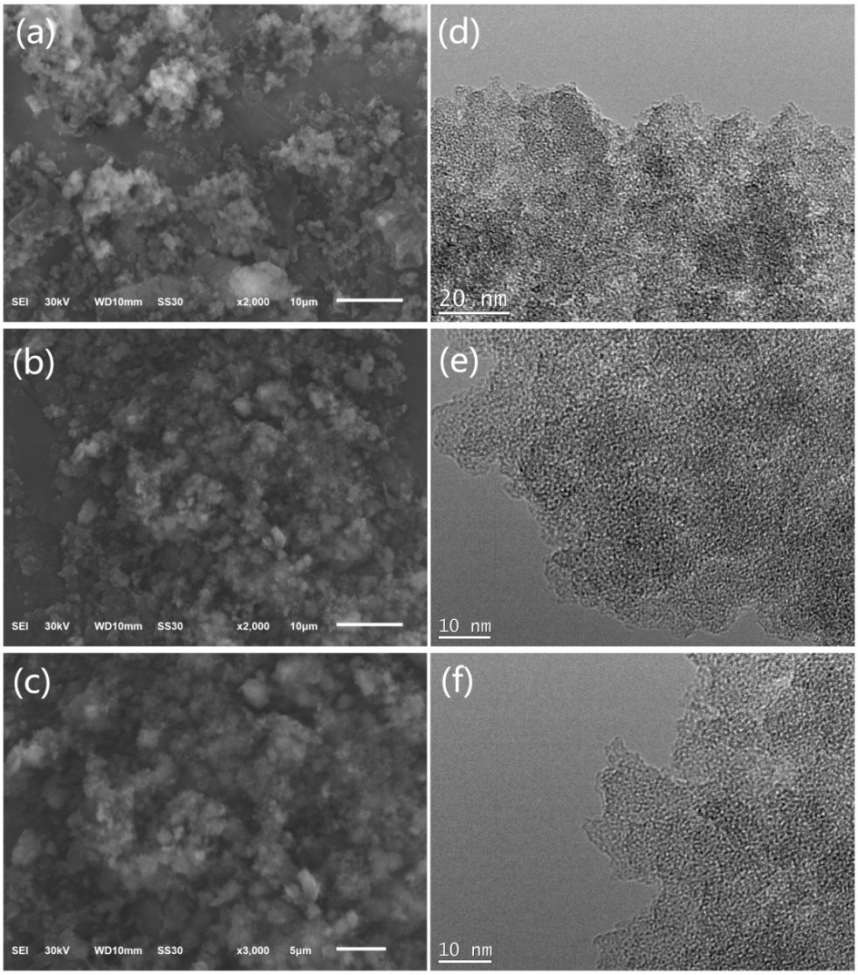

Fig. S2 SEM (a-c) and TEM images (d-f) of **POPs-B0**, **POPs-B10** and **POPs-B20**

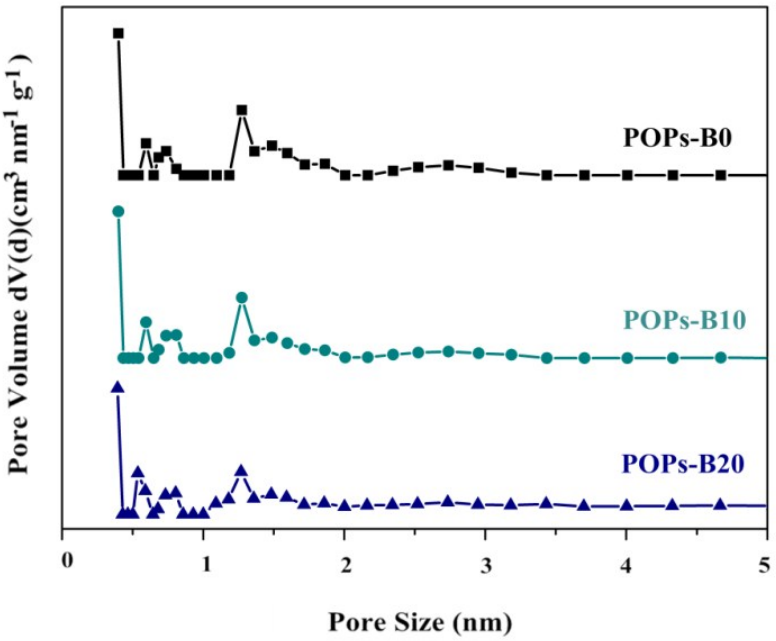

Fig. S3 Pore size distribution of **POPs-B0**, **POPs-B10** and **POPs-B20** calculated using NL-DFT methods.

Heat of CO_2 Adsorption Calculation

The isosteric heats (Q_{st}) of adsorption for **POPs-B0, POPs-B10** and **POPs-B20** were calculated by fitting the CO_2 adsorption isotherms measured at 273 K, 283 K and 298 K to the Viral equation.

$$\ln P = \ln N + {}^{1}/_{T}\sum_{i=0}^{m} a_i N_i + \sum_{i=0}^{n} b_j N_i$$

$$Q_{st} = -R\sum_{i=0}^{m} a_i N_i$$

N: adsorbed volume (cm^3/g);

P: pressure (mmHg);

T: temperature (K);

a_i, b_j: constants;

R: 8.314 $J \cdot mol^{-1} \cdot K^{-1}$

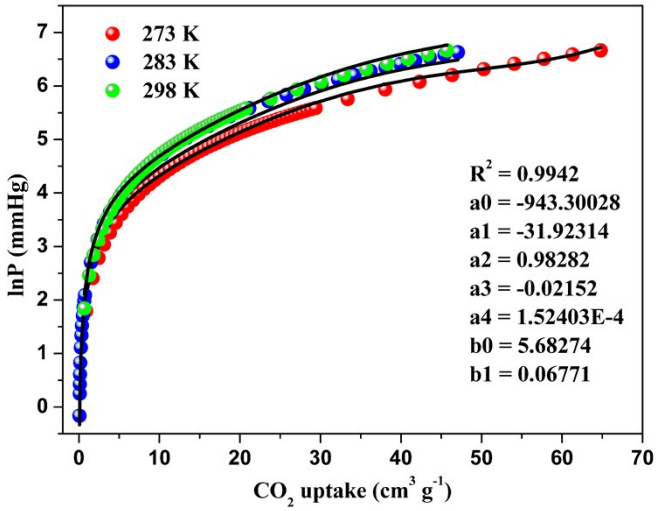

Fig. S4 Virial fitting for CO_2 isotherms of **POPs-B0**.

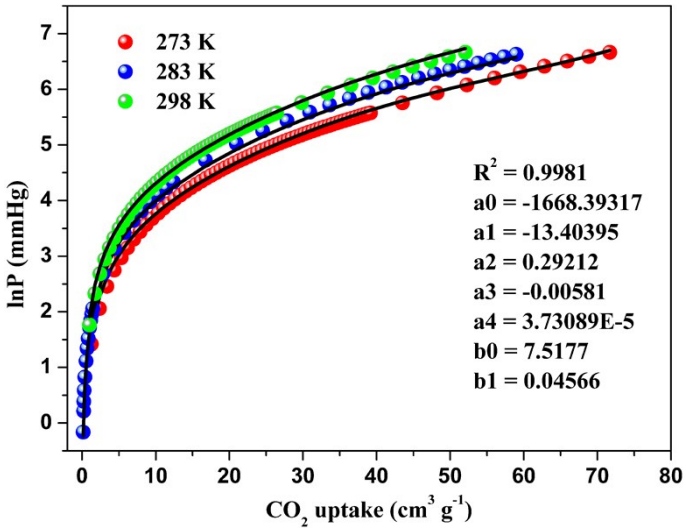

Fig. S5 Virial fitting for CO_2 isotherms of **POPs-B10**.

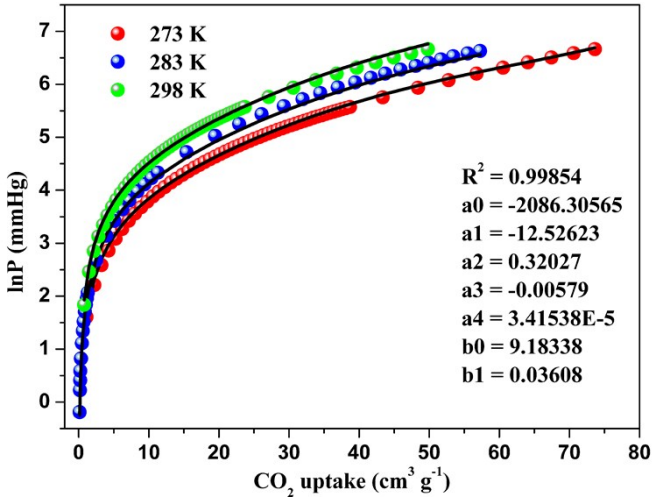

Fig. S6 Virial fitting for CO_2 isotherms of **POPs-B20**.

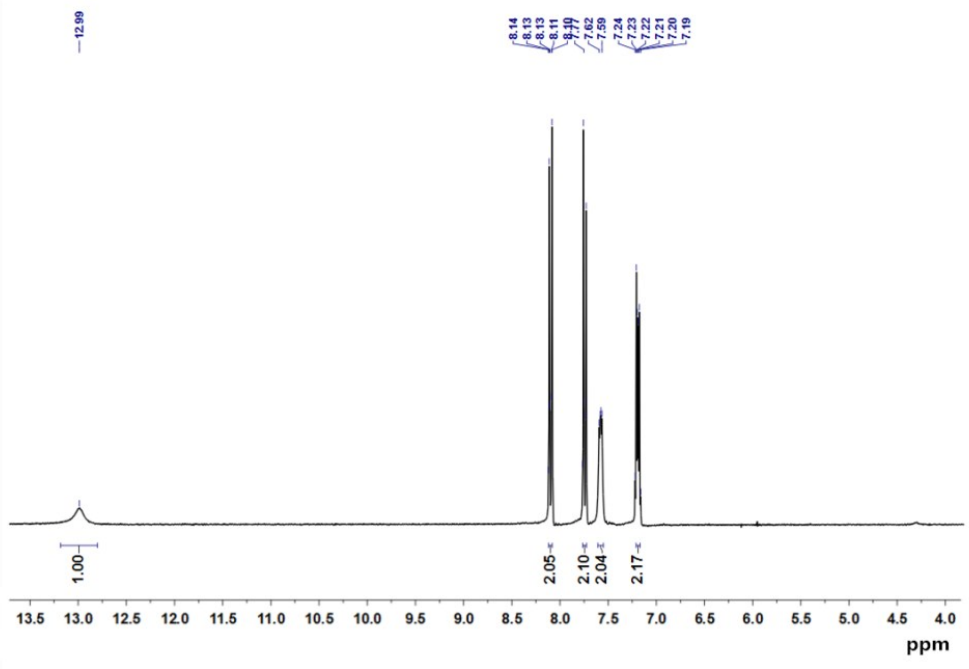

Fig. S7 [1]H NMR spectrum of 2-(4-bromophenyl)-1H-benzoimidazole.

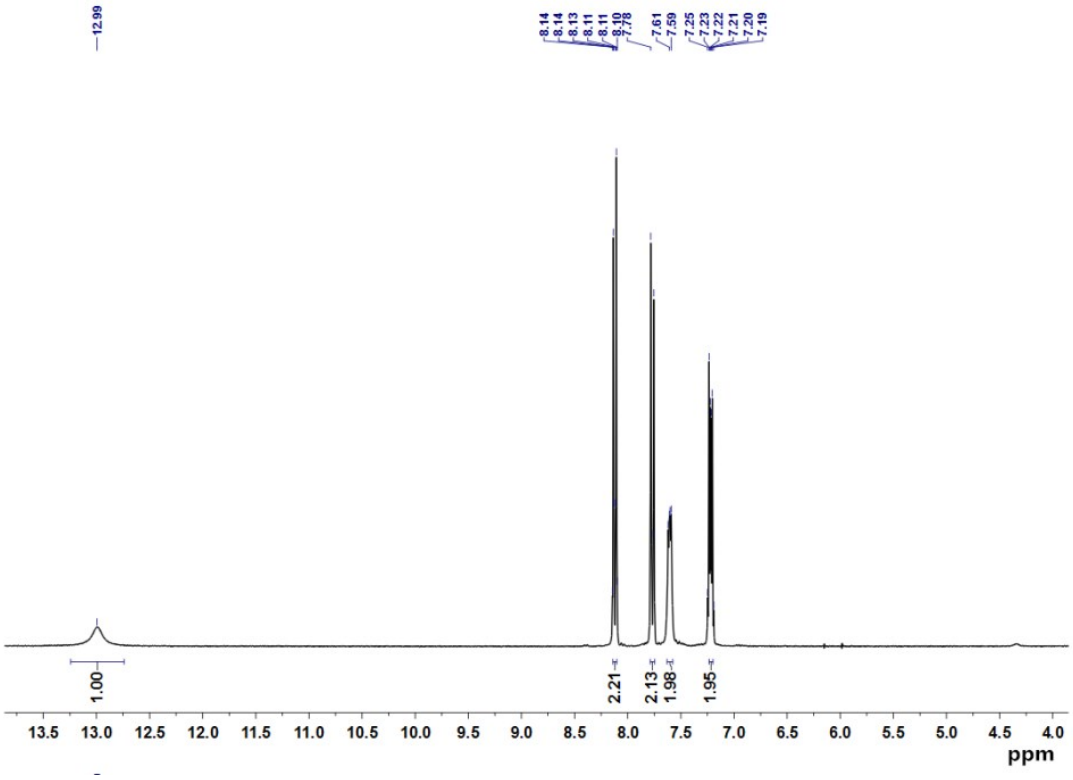

Fig. S8 [1]H NMR spectrum of 2-(4-cyanophenyl)-1H-benzimidazole.

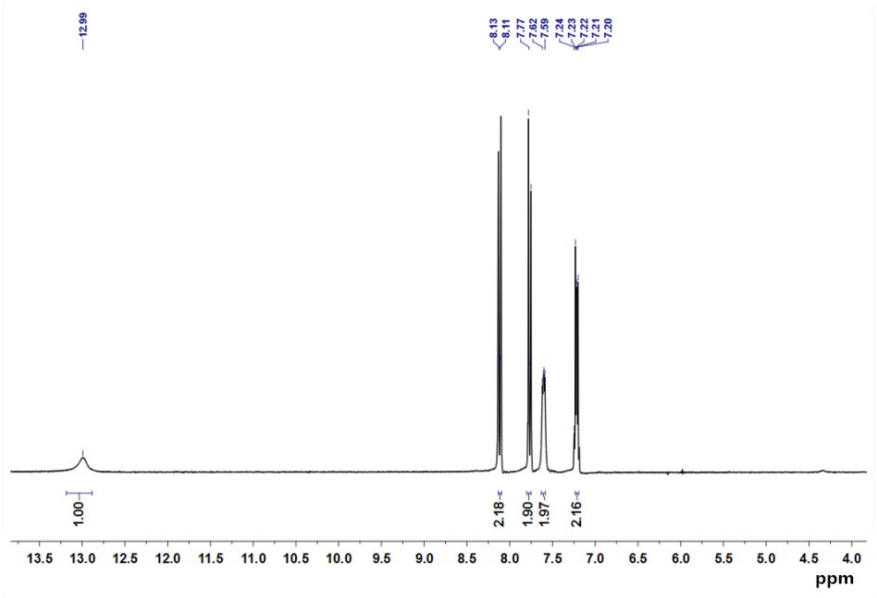

Fig. S9 ^{1}H NMR spectrum of 2-(4-chlorophenyl)-1H-benzimidazole.

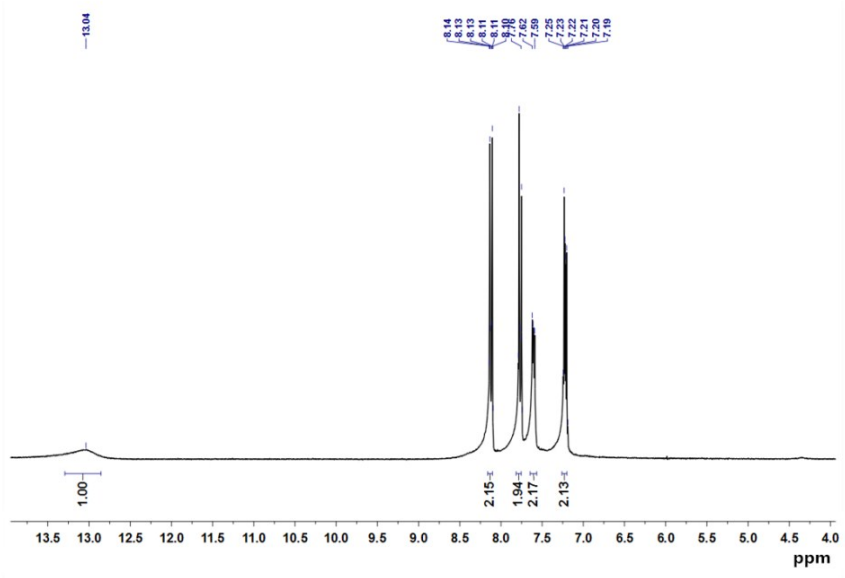

Fig. S10 ^{1}H NMR spectrum of 2-(4-nitrophenyl)-1H-benzimidazole.

Table S1 Elemental analysis of **POPs-B0**, **POPs-B10** and **POPs-B20**.

Sample	Observed Values			Theoretical Values		
	C [%]	H [%]	N [%]	C [%]	H [%]	N [%]
POPs-B0	82.16	5.45	0	94.12	5.88	0
POPs-B10	80.60	5.09	1.41	88.97	5.92	2.26
POPs-B20	86.20	5.96	3.77	85.53	5.93	3.77

Table S2 ICP analyses of **POPs-B0**, **POPs-B10** and **POPs-B20**.

Sample	Fe [‰]
POPs-B0	0.042
POPs-B10	0.031
POPs-B20	0.036

Table S3 The yields of POPs.

POPs	*p*-DCX	N-MI	−HCl	Calculated	Found	Yield (%)
B0	963 mg / 5.5 mmol	-	401.5 mg / 11.0 mmol	561.5 mg	547 mg	97.4
B10	963 mg / 5.5 mmol	41 mg / 0.5 mmol	383.25 mg / 10.5 mmol	620.75 mg	566 mg	91.2
B20	963 mg / 5.5 mmol	75 mg / 0.9 mmol	368.65 mg / 10.1 mmol	669.35 mg	604 mg	90.2

Table S4 Summary of CO_2 uptakes in porous organic polymers at 273 K and 1 atm.

POPs	CO_2 uptake (mmol/g)	Ref.	POPs	CO_2 uptake (mmol/g)	Ref.
POPs-B10	3.20	This work	POM1-IM	3.12	8
POPs-B20	3.29		POM2-IM	3.30	
GPOP-1	2.0	1	POM3-IM	3.23	
GPOP-2	2.39		POM4-IM	2.41	
GPOP-3	2.77		POM5-IM	1.30	
Th-1	2.89	2	POM6-IM	1.25	
Py-1	2.70		Glc-1	2.29	9
Fu-1	2.20		Glc-2	2.37	
THPS	3.57	3	Glc-3	2.41	
PAF-32	1.66	4	Gal-1	2.69	
PAF-32-NH_2	1.62		Gal-1	2.35	
PAF-32-OH	2.27		Ara-1	1.69	
TSP-1	3.0	5	CB-PCP-1	2.05	10
TSP-2	4.1		CMP-1-NH_2	1.64	11
CPOP-16	2.34	6	CMP-1-$(OH)_2$	1.80	
CPOP-17	2.50		CMP-1-COOH	1.60	
CPOP-18	3.43		PAF-1	2.05	12
CPOP-19	3.80		PAF-3	3.48	
HCP-1	3.01	7	PAF-4	2.41	
HCP 2	3.30		PCBZ	1.13	13
Hcp-3	3.24		PCBZL	1.46	
Hcp-4	3.92		CPOP-1	4.82	14

References

1. T. Wang, Y.-C. Zhao, M. Luo, L.-M. Zhang, Y. Cui, C.-S. Zhang and B.-H. Han, *Polymer*, 2015, **60**, 26.
2. Y. L. Luo, B. Y. Li, W. Wang, K. B. Wu and B. E. Tan, *Adv. Mater.*, 2012, **24**,

5703.

3. C. Zhang, P.-C. Zhu, L. X. Tan, J.-M. Liu, B. E. Tan, X.-L. Yang and H.-B. Xu, *Macromolecules*, 2015, **48**, 8509.
4. X. F. Jing, D. L. Zou, P. Cui, H. Ren and G. S. Zhu, *J. Mater. Chem. A*, 2013, **1**, 13926.
5. X. Zhu, S. M. Mahurin, S.-H. An, C.-L. Do-Thanh, C. C. Tian, Y. K. Li, L. W. Gill, E. W. Hagaman, Z. J. Bian, J.-H. Zhou, J. Hu, H. L. Liu and S. Dai, *Chem. Commun.*, 2014, **50**, 7933.
6. L. Pan, Q. Chen, J.-H. Zhu, J.-G. Yu, Y.-J. He and B.-H. Han, *Polym. Chem.*, 2015, **6**, 2478.
7. C. F. Martín, E. Stöckel, R. Clowes, D. J. Adams, A. I. Cooper, J. J. Pis, F. Rubiera and C. Pevida, *J. Mater. Chem.*, 2011, **21**, 5475.
8. J. Q. Wang, W. H. Sng, G. S. Yi and Y. G. Zhang, *Chem. Commun.*, 2015, **51**, 12076.
9. H. Y. Li, B. Meng, S. M. Mahurin, S.-H. Chai, K. M. Nelson, D. C. Baker, H. L. Liu and S. Dai, *J. Mater. Chem. A*, 2015, **3**, 20913.
10. A. Dani, V. Crocellà, C. Magistris, V. Santoro, J. Y. Yuan and S. Bordiga, *J. Mater. Chem. A*, 2017, **5**, 372.
11. R. Dawson, D. J. Adams and A. I. Cooper, *Chem. Sci.*, 2011, **2**, 1173.
12. T. Ben, C. Y. Pei, D. L. Zhang, J. Xu, F. Deng, X. F. Jing and S. L. Qiu, *Energy Environ. Sci.*, 2011, **4**, 3991.
13. M. Saleh, S. Bin Baek, H. M. Lee and K. S. Kim, *J. Phys. Chem. C*, 2015, **119**, 5395.
14. Q. Chen, M. Luo, P. Hammershøj, D. Zhou, Y. Han, B. W. Laursen, C.-G. Yan, and B.-H. Han, *J. Am. Chem. Soc.*, 2012, **134**, 6084.