Electronic Supplementary Information

Triazatriangulenium-based porous organic polymers for carbon dioxide capture

Xin-Ming Hu,^{a,b} Qi Chen,^a Zhu-Yin Sui,^a Zhi-Qiang Zhao,^a Nicolas

Bovet,^b Bo W. Laursen,*^b Bao-Hang Han*^a

^a CAS Key Laboratory of Nanosystem and Hierarchical Fabrication,

National Center for Nanoscience and Technology, Beijing 100190, China

Email: <u>hanbh@nanoctr.cn</u>

^b Nano-Science Center and Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 København Ø, Denmark E-mail: <u>bwl@nano.ku.dk</u>

Cl	F	В	S	Ο	Ν	С	Polymer
0	9.01	1.28	11.40	0	4.98	69.75	TATA-1 ^a
0.99	6.18	1.21	12.71	2.32	4.76	71.83	TAPOP-1
0	6.95	0.99	0	0	7.69	80.22	TATA- 2^a
1 26	7 54	0.96	0	0.93	8 09	81.22	ΤΑΡΟΡ-2
	6.18 6.95	1.21 0.99	12.71 0	2.32 0	4.76 7.69	71.83 80.22	TAPOP-1 TATA-2 ^{<i>a</i>}

Table S1. Chemical composition (wt%) of TAPOPs determined by XPS analysis.

^{*a*} Theoretical value for TATA monomers.

POPs	Monomer Structures	$\frac{S_{\rm BET}}{(\rm m^2~g^{-1})}$	CO_2 Uptake (wt %) ^a	Q _{st} (kJ mol ⁻¹)	Ref.
TAPOP-2		930	13.6	34.7	This work
CPOP-1		2220	21.2	27	S1
CPOP-5		1050	11.8	31.5	S2
CPOP-6		980	11.5	30	S2
MFCMP-1		840	16.2	30	S3

Table S2. Textural property and CO_2 uptake of carbazole-based POPs with similar structure.

^{*a*} at 273 K and 1.0 bar.

References:

S1 Q. Chen, M. Luo, P. Hammershøj, D. Zhou, Y. Han, B. W. Laursen, C.-G. Yan and B.-H. Han, Microporous polycarbazole with high specific surface area for gas storage and separation. *J. Am. Chem. Soc.*, 2012, **134** (14), 6084–6087.



Figure S1. Mass spectra of the reaction mixtures of Ph₃TATA in FeCl₃-CHCl₃ (a) and FeCl₃-CH₂Cl₂-CF₃COOH (b) system after a certain time interval.



Figure S2. SEM images of (a) TAPOP-1 and (b) TAPOP-2.



Figure S3. XRD patterns of TAPOPs.



Figure S4. TGA curves of TAPOPs.



Figure S5. Normalized absorption (a) and emission (b) spectra of TATA monomers and TAPOPs.



Figure S6. Emission images of the TATA monomers and TAPOPs. (a) TATA-1, (b) TAPOP-1, (c) TATA-2, (d) TAPOP-2.



Figure S7. CO₂ and N₂ adsorption isotherms of TAPOPs at 273 K.



¹H NMR spectrum of TATA-1



¹³C NMR spectrum of TATA-1



¹⁹F NMR spectrum of TATA-1



Mass spectrum of TATA-1



¹³C NMR spectrum of TATA-2



¹⁹F NMR spectrum of TATA-2



Mass spectra of TATA-2



¹³C NMR spectrum of Cl-Ph₃TATA



¹⁹F NMR spectrum of Cl-Ph₃TATA



Mass spectrum of Cl-Ph₃TATA

- S2 Q. Chen, D.-P. Liu, M. Luo, L.-J. Feng, Y.-C. Zhao and B.-H. Han, Nitrogencontaining microporous conjugated polymers via carbazole-based oxidative coupling polymerization: Preparation, porosity, and gas uptake. *Small*, 2014, **10** (2), 308–315.
- S3 Y. Zhang, A. Sigen, Y. Zou, X. Luo, Z. Li, H. Xia, X. Liu and Y. Mu, Gas uptake, molecular sensing and organocatalytic performances of a multifunctional carbazole-based conjugated microporous polymer. *J. Mater. Chem. A*, 2014, 2 (33), 13422–13430.