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## **Electronic Supporting Information (ESI)**

## Flexible and Mechanically-stable MIL-101(Cr)@PFs for Efficient Benzene Vapor and CO<sub>2</sub> Adsorption Zhenyu Zhou<sup>a</sup>, Baihua Cheng<sup>a</sup>, Chen Ma<sup>a</sup>, Feng Xu<sup>b</sup>, Jing XIAO<sup>b\*\*</sup>, Qinbin Xi<sup>b</sup>, Zhong LI<sup>a\*</sup> a. School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou, 510640, China

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Fig. S1 Pictures of 50MIL-101(Cr)@PFs(a) and its flexibility performance(b);67MIL-

101(Cr)@PFs(c) and its flexibility performance (d).

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Fig. S2 PXRD pattern of MIL-101(Cr)@PFs

Table S1	Textural	properties	of MIL-101(Cr)	and MIL-101(Cr)@PFs
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Samples	BET surface area (m <sup>2</sup> /g)	Langmuir surface area
		$(m^{2}/g)$
25MIL-101(Cr)@PFs	812	1188
40 MIL-101(Cr)@PFs	1256	1703
50 MIL-101(Cr)@PFs	1630	2318
67 MIL-101(Cr)@PFs	2174	2974
MIL-101(Cr)	3347	4687



Fig. S3 Pore size distribution of MIL-101(Cr) and 50MIL-101(Cr)@PFs



Fig. S4 SEM pictures of (a) MIL-101(Cr), (b) virgin pulp fibers, (c) 50MIL-101(Cr)@PFs



Fig.S5 TGA Curves of MIL-101(Cr)@PFs, MIL-101(Cr) and virgin pulp fiber

		at 298 K		
Samples	Benzene vapor	The percentages of	CO <sub>2</sub> uptake at	The percentages of
	uptake when	benzene vapor	1 bar	CO <sub>2</sub> uptake on
	$P \approx 25 \text{ mbar}$	uptake on MIL-	(mmol/g)	MIL-101(Cr)@PFs
	(mmol/g)	101(Cr)@PFs to		to MIL-101(Cr)
		MIL-101(Cr)		
25MIL-	4.1	24.8%	0.80	24.7%
101(Cr)@PFs				
40MIL-	6.47	39.1%	1.25	38.6%
101(Cr)@PFs				
50MIL-	8.06	48.7%	1.56	48.1%
101(Cr)@PFs				
67MIL-	10.29	62.2%	2.13	65.7%
101(Cr)@PFs				
MIL-101(Cr)	16.54	100%	3.24	100%

**Table S2** Benzene and CO2 adsorption capacities of MIL-101(Cr) and MIL-101(Cr)@PFsat 298 K

Table S3 CO<sub>2</sub> uptakes of some MOFs and conventional adsorbents at 1 bar.

Adsorbent	Adsorption	Temperature	Reference
	capacity (mmol/g)	(K)	
MCM-41	0.67	298	1
Zeolite-13X	~1.70	298	2
ZSM-5	~1.50	303	3
Activated carbon	2.0	298	4
ZIF-68	1.69	298	5
UIO-66	1.79	298	6
MOF-5	2.10	296	7
MIL-100(Cr)	~2.23	298	8
67MIL-101(Cr)@Fs	2.13	298	This work
MIL-101(Cr)	3.24	298	This work

101(Cr)@PFs					
	MIL-	67MIL-	50MIL-	40MIL-	25MIL-
	101(Cr)	101(Cr)@PFs	101(Cr)@PFs	101(Cr)@PFs	101(Cr)@PFs
q	17.296	10.404	8.518	7.056	5.091
b	0.0140	0.0347	0.0344	0.0434	0.0566
c	2.424	2.033	2.070	1.914	1.626
R <sup>2</sup>	0.9826	0.9857	0.9865	0.9754	0.9747

Table S4 Fitting parameters of L-F model for benzene adsorption on MIL-101(Cr) and MIL-

 Table S5 Fitting parameters of L-F model for CO2 adsorption on MIL-101(Cr) and MIL 

 101(Cr) and MIL 

101(Cr)@PFs					
	MIL-	67MIL-	50MIL-	40MIL-	25MIL-
	101(Cr)	101(Cr)@PFs	101(Cr)@PFs	101(Cr)@PFs	101(Cr)@PFs
q	16.798	15.684	6.738	4.556	5.270
b	0.237	0.157	0.304	0.377	0.180
c	0.613	0.773	0.836	0.953	0.865
R <sup>2</sup>	0.9997	0.9999	0.9999	0.9999	0.9999



Fig.S6 CO<sub>2</sub> isotherms of 50MIL-101(Cr)@PFs at 298 K(regeneration for five times).

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**Fig.S7** Cycling adsorption/desorption runs of 50MIL-101(Cr)@PFs with the average value and standard error of desorption efficiency of 99.52% and 0.156%.

## REFERENCE

- 1. J. Zhou, H. Zhao, J. Li, Y. Zhu, J. Hu, H. Liu and Y. Hu, *Solid State Sciences*, 2013, 24, 107-114.
- 2. J. McEwen, J.-D. Hayman and A. O. Yazaydin, *Chemical Physics*, 2013, 412, 72-76.
- 3. Y. Li, H. Yi, X. Tang, F. Li and Q. Yuan, *Chemical Engineering Journal*, 2013, **229**, 50-56.
- 4. R.-L. Tseng, F.-C. Wu and R.-S. Juang, *Separation and Purification Technology*, 2015, **140**, 53-60.
- 5. R. Banerjee, H. Furukawa, D. Britt, C. Knobler, M. O'Keeffe and O. M. Yaghi, *Journal* of the American Chemical Society, 2009, **131**, 3875-3877.
- Z. Hu, M. Khurana, Y. H. Seah, M. Zhang, Z. Guo and D. Zhao, *Chem. Eng. Sci.*, 2015, 124, 61-69.
- 7. Z. Zhao, Z. Li and Y. Lin, Industrial & Engineering Chemistry Research, 2009, 48, 10015-10020.
- 8. L. Li, J. Yang, J. Li, Y. Chen and J. Li, *Microporous Mesoporous Mat.*, 2014, **198**, 236-246.