

## Electronic Supplementary Information (ESI)

# Nanoscale zeolitic imidazolate framework-8 as a selective adsorbent for theophylline over caffeine and diprophylline

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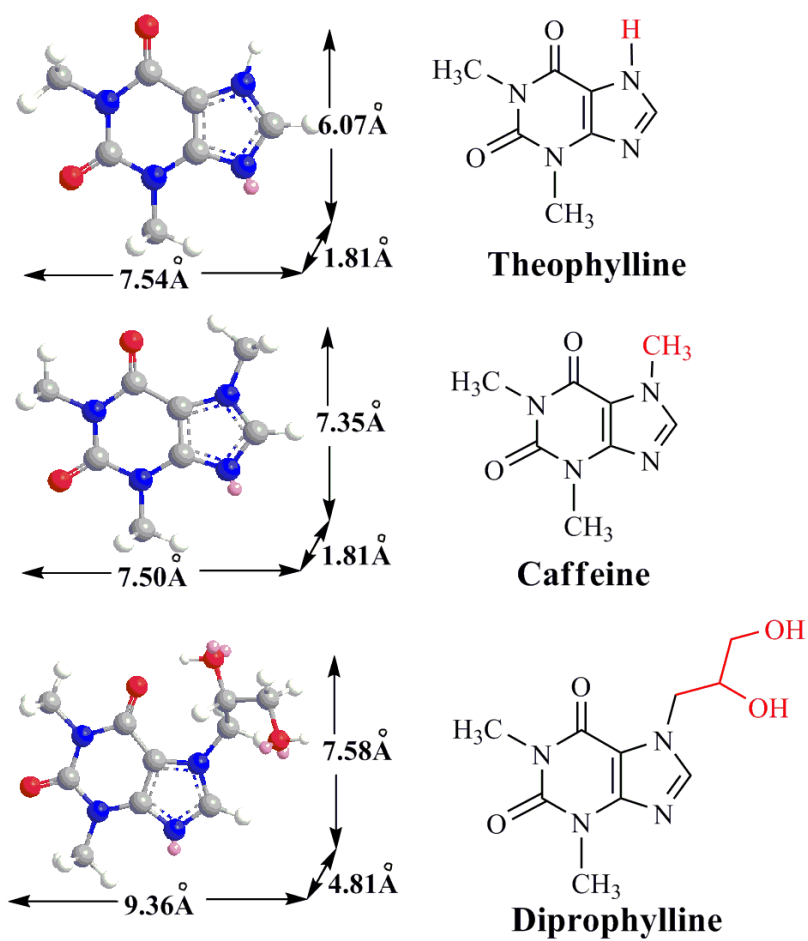


Fig.S1 Structure of xanthine-based pharmaceutical analogs simulated with ChemBioOffice 2008 (Cambridge Soft Corporation). Molecular kinetic diameters were approximated using the minimum cross-sectional area.

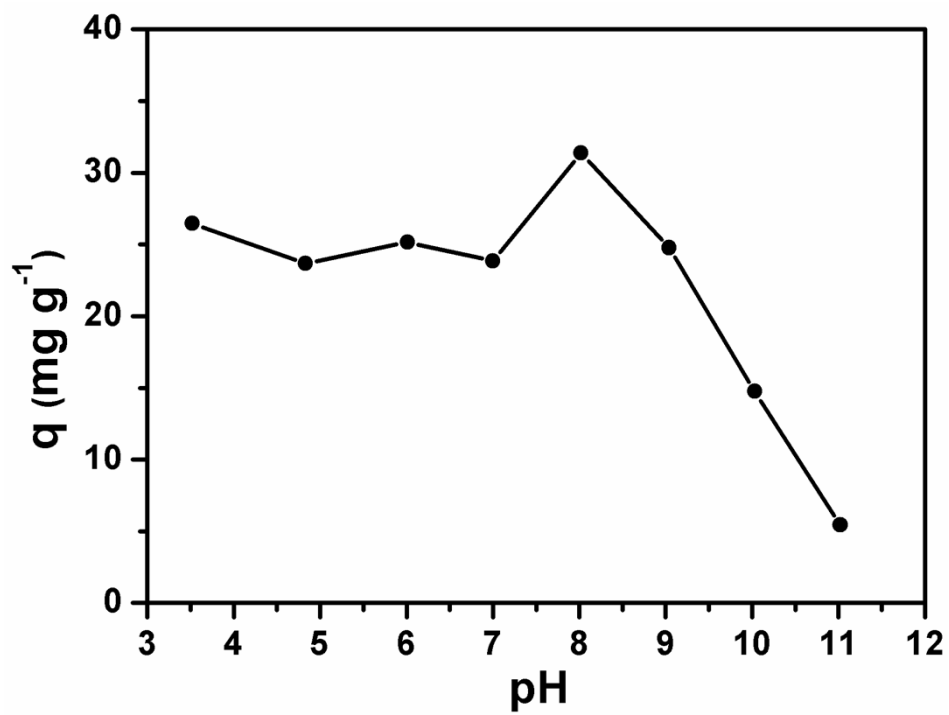


Fig. S2 Effect of pH on the adsorption of TPE ( $100 \text{ mg L}^{-1}$ ) on ZIF-8 ( $10.0 \text{ mg}$ ) containing  $0.01\text{M NaCl}$ .

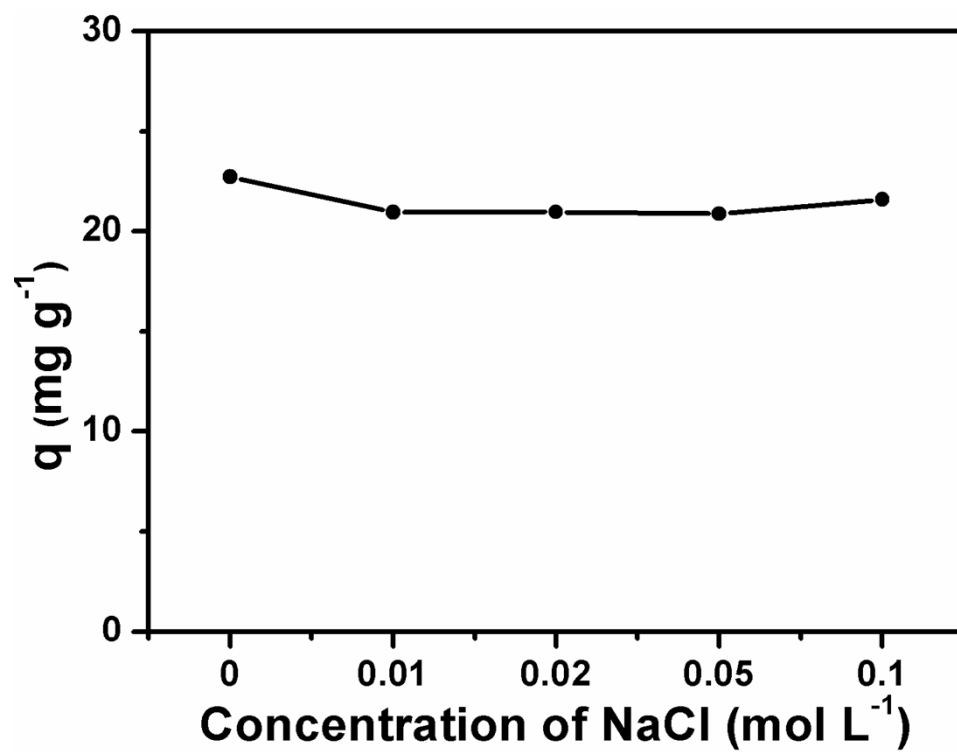


Fig.S3 Effect of the concentration of NaCl on the adsorption of TPE ( $100 \text{ mg L}^{-1}$ ) on ZIF-8 ( $10 \text{ mg L}^{-1}$ ). Other conditions: temperature,  $25^\circ\text{C}$ ; a tris-HCl buffer of pH 8.0.

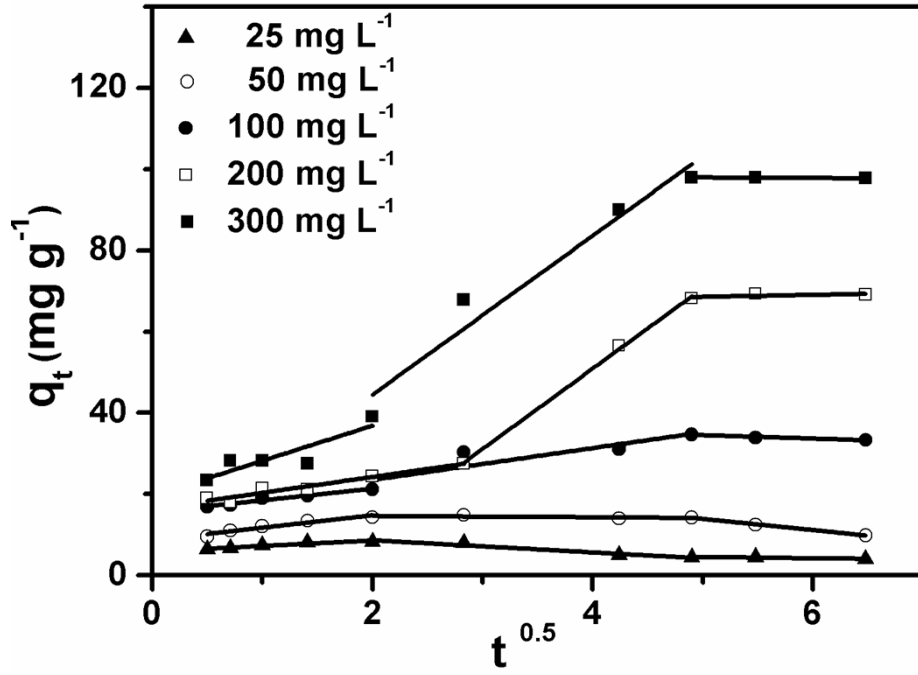


Fig. S4 Intraparticle diffusion plots for the adsorption of TPE on ZIF-8 (10 mg) with different initial concentrations of TPE at 25°C and pH 8.0.

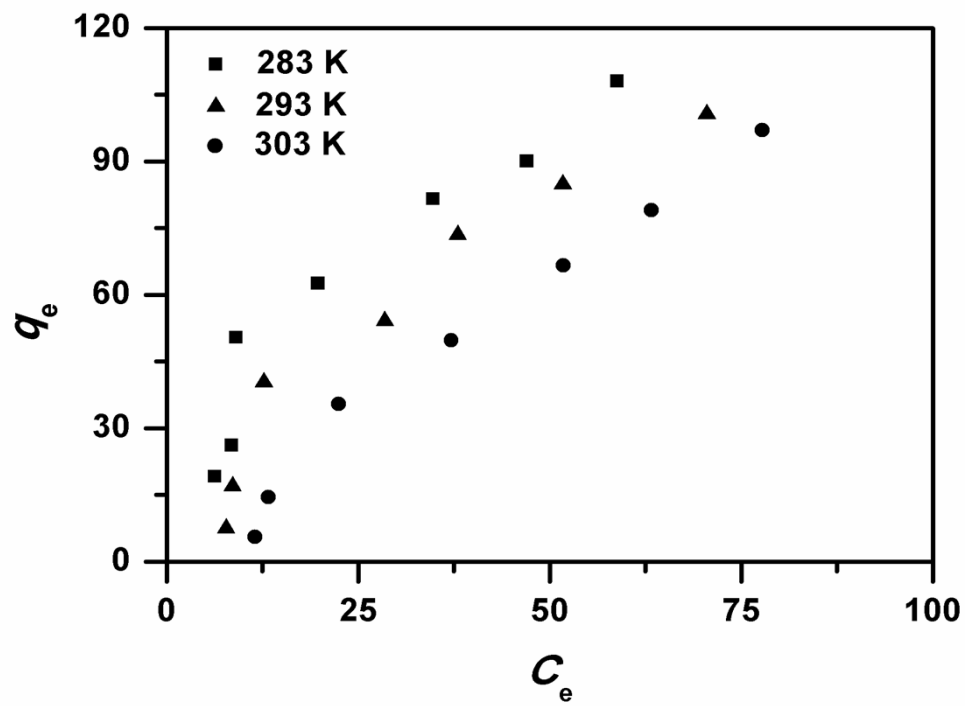


Fig.S5 Adsorption isotherms of TPE onto ZIF-8 at different temperatures.

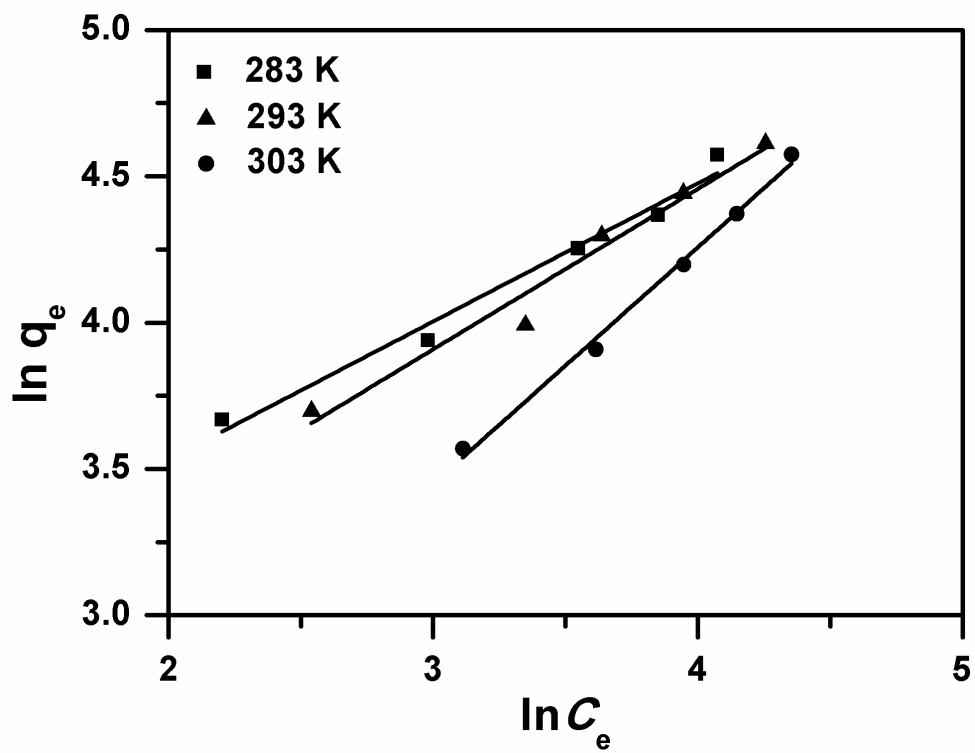


Fig.S6 Linearized Freundlich isotherms for TPE adsorption by the ZIF-8 at different temperatures.

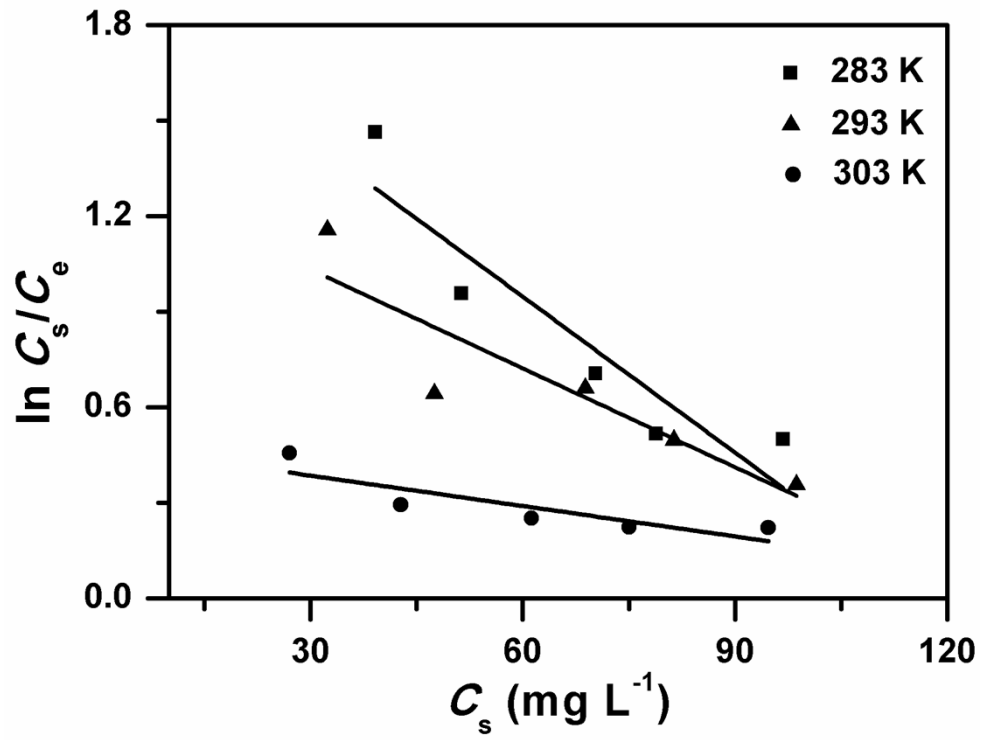


Fig.S7 Plots of  $\ln C_s/C_e$  vs.  $C_s$  at various temperatures.



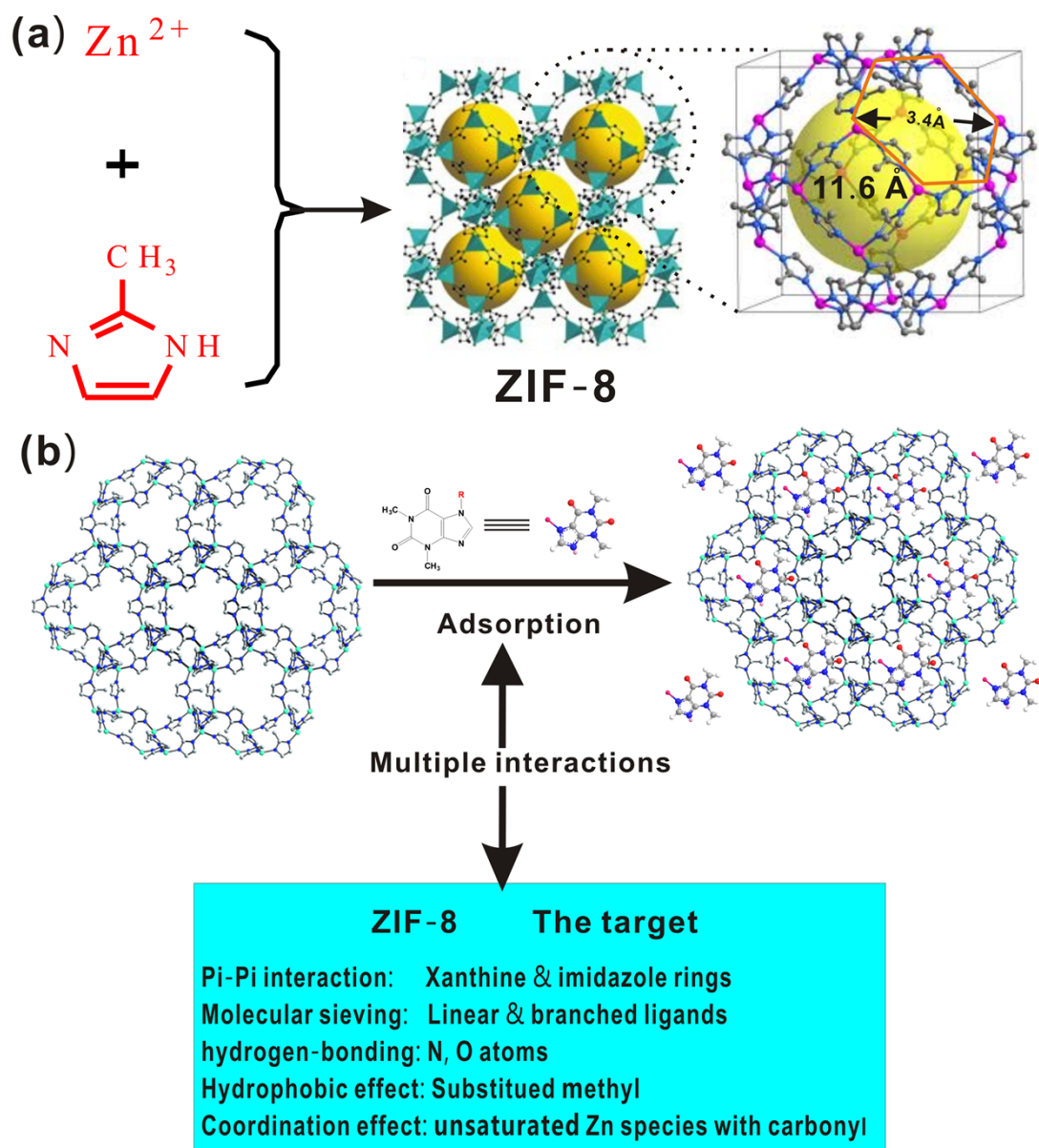


Fig. S8 (a) ZIF-8 composed of zinc (II) and 2-methylimidazole featured with larger cavities (11.6 Å) and small apertures (3.4Å), this figure is a combination of figures from Ref.S1 and in Ref.S2 with little modification. Copyright by 2006 National Academy of Sciences and Copyright 2008 by American Association for the Advancement of Science and with their permissions and (b) Potential part embedding process occurred between the guest molecules and ZIF-8 nanocrystal. This figure is little modified of a figure from Ref.S3. Copyright 2010 by The Royal Society of Chemistry and with permission.

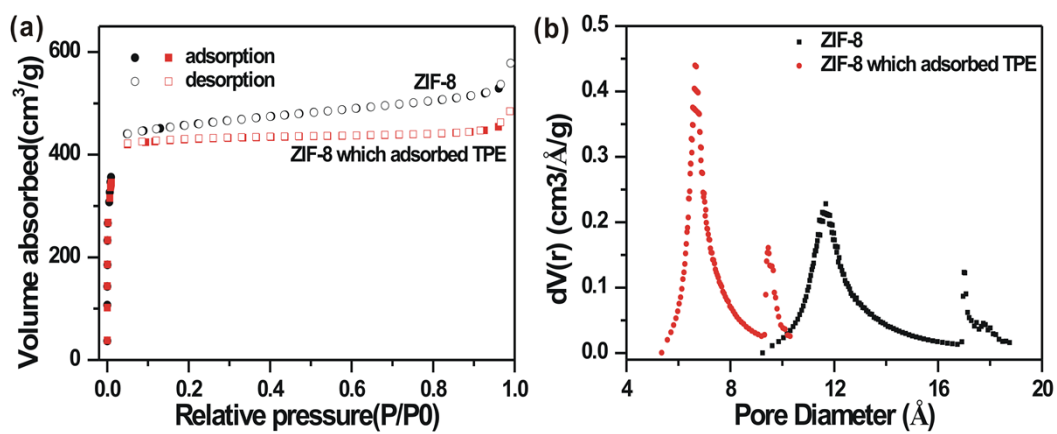


Fig.S9: (a) Nitrogen-sorption-isotherm of the ZIF-8, ZIF-8 which adsorbed TPE. (b) the corresponding pore size distributions calculated by the Horvath–Kawazoe method.

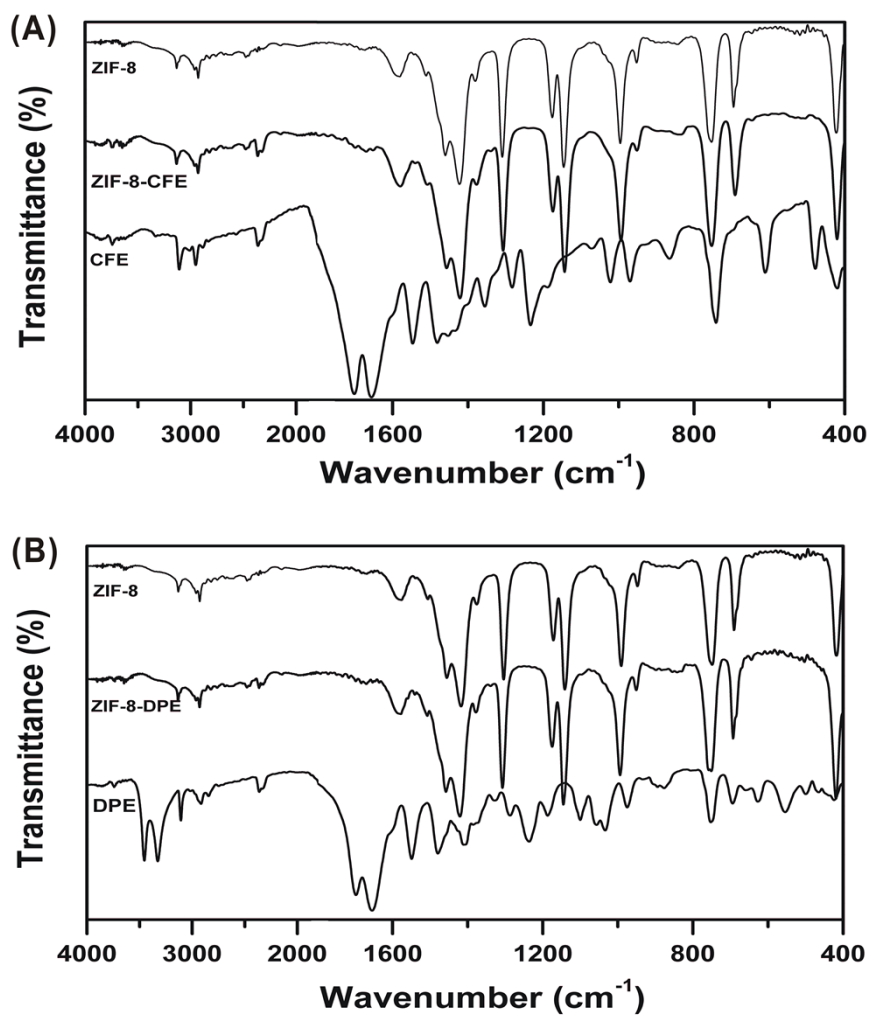


Fig.S10 FT-IR spectra for before and adsorption of CFE (A) and DPE (B) on ZIF-8

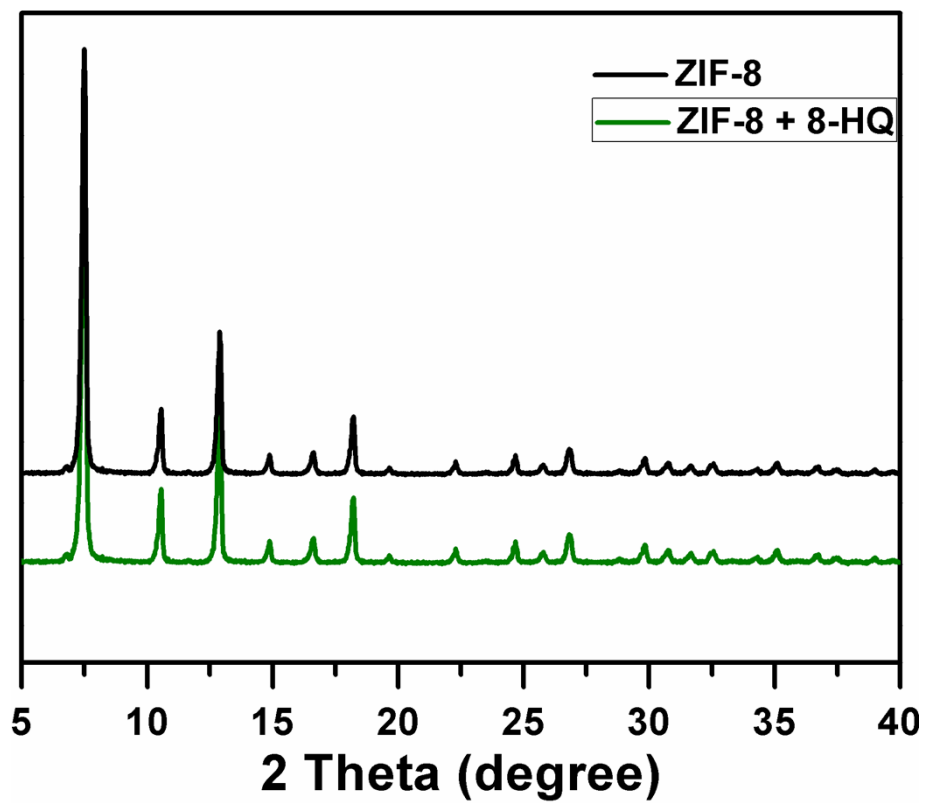


Fig.S11 XRD spectra of sole ZIF-8 and ZIF-8 after adsorption of 8-hydroxyquinoline (8-HQ)

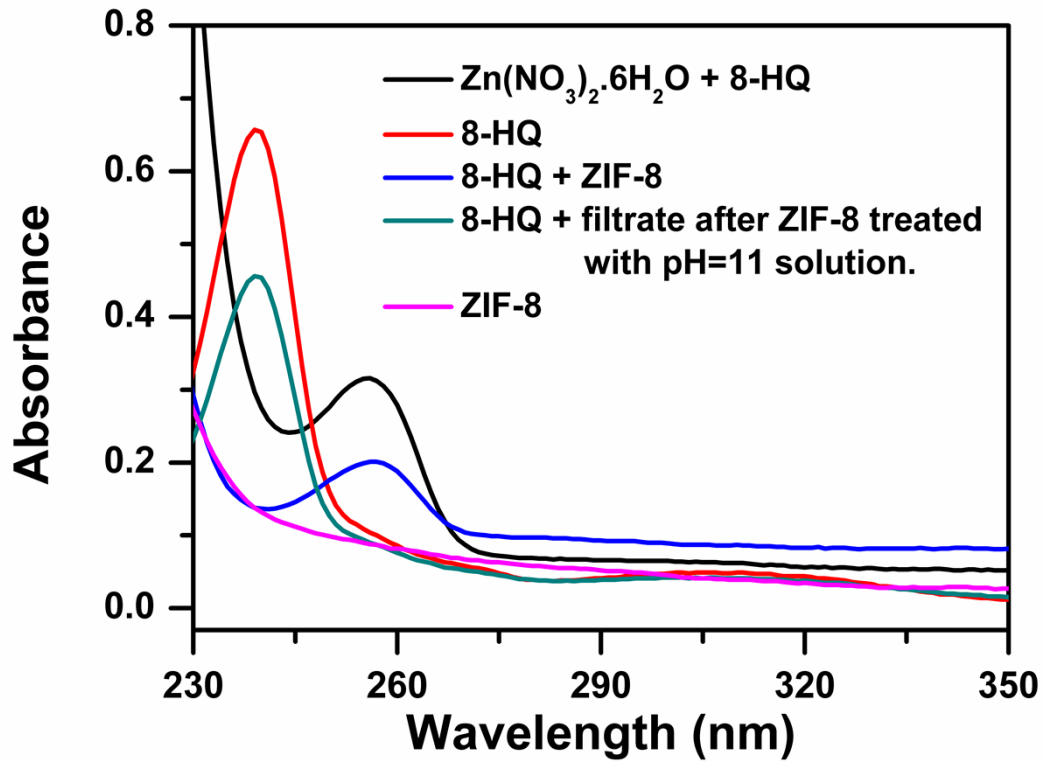


Fig.S12 UV-vis spectra for interaction of ZIF-8 and 8-hydroxyquinoline (8-HQ)

Table S1 Freundlich Parameters for TPE on ZIF-8.

Temperature(K)	Freundlich adsorption isotherm model		
	$K_F$	n	$R^2$
283.15	13.308	2.120	0.9802
293.15	9.612	1.823	0.9711
303.15	2.779	1.236	0.9943

Table S2 The structure parameters of ZIF-8 and ZIF-8 adsorbed of TPE

Sample	$S_{\text{BET}}(\text{m}^2\text{g}^{-1})$	Pore diameter(Å)	Pore volume( $\text{cm}^3\text{g}^{-1}$ )
ZIF-8	2205	11.6, 17	0.89
ZIF-8 adsorbed of TPE	1880	6.7, 9.4	0.74

Table S3 Effect of desorption solvent on desorption of TPE, DPE and CFE on ZIF-8

Desorption solvent	TPE (%)	DPE (%)	CFE (%)
4 mL pH=11 tris	42.5	4.2	16.4
2 mLacetonitrile and 2 mL pH=11tris	46.1	2.8	12.9
4 mL acetonitrile	30.4	13.3	10.5
4 mL 0.1%ammonia	48.3	3.8	15.3
4 mL 0.1M NaOH	52.9	3.1	12.4



Table S4 The reusability of spent ZIF-8

Reuse Cycle	adsorption capacity (mg/g)		
	TPE	DPE	CFE
1 <sup>st</sup> run	9.97	2.73	6.11
2 <sup>nd</sup> run	10.01	2.67	6.18
3 <sup>rd</sup> run	9.77	2.93	6.39
4 <sup>th</sup> run	9.96	2.65	6.35
5 <sup>th</sup> run	10.01	2.66	6.38
RSD	1.00	4.00	2.00

## References

(Ref.S1) Park, K. S.; Ni, Z.; Côté, A. P.; Choi, J. Y.; Huang, R.; Uribe-Romo, F. J.; Chae, H. K.; O’Keeffe, M.; Yaghi, O. M., Exceptional chemical and thermal stability of zeolitic imidazolate frameworks. *Proceedings of the National Academy of Sciences* 2006, 103 (27), 10186-10191.

(Ref.S2) Banerjee, R.; Phan, A.; Wang, B.; Knobler, C.; Furukawa, H.; O’Keeffe, M.; Yaghi, O. M., High-Throughput Synthesis of Zeolitic Imidazolate Frameworks and Application to CO<sub>2</sub> Capture. *Science* 2008, 319 (5865), 939-943.

(Ref. S3) Demessence, A.; Boissiere, C.; Grosso, D.; Horcajada, P.; Serre, C.; Ferey, G.; Soler-Illia, G. J. A. A.; Sanchez, C., Adsorption properties in high optical quality nanoZIF-8 thin films with tunable thickness. *Journal of Materials Chemistry* 2010, 20 (36), 7676-7681.