

Supporting information

Enhanced adsorptive removal of anionic and cationic dyes from single or mixed dye solutions using MOF PCN-222

Haichao Li,^a Xinyu Cao,^a Chuang Zhang,^a Qing Yu,^a Zijian Zhao,^a Xuedun Niu,^b Xiaodong Sun,^b Yunling Liu,^b Li Ma,^{*ac} Zhengqiang Li^{*a}

^a Key Laboratory for Molecular Enzymology, Engineering of Ministry of Education, School of Life Sciences, Jilin University, 2699 Qianjin Street, Changchun 130012, Jilin Province, PR China.

^b State Key Laboratory of Inorganic Synthesis & Preparative Chemistry, College of Chemistry, Jilin University, 2699 Qianjin Street, Changchun 130012, Jilin Province, PR China.

^c Department of Physics, Georgia Southern University, Statesboro, GA 30460, USA.

Corresponding Author

Zhengqiang Li, E-mail: lzq@jlu.edu.cn

Li Ma, E-mail: lma@georgiasouthern.edu

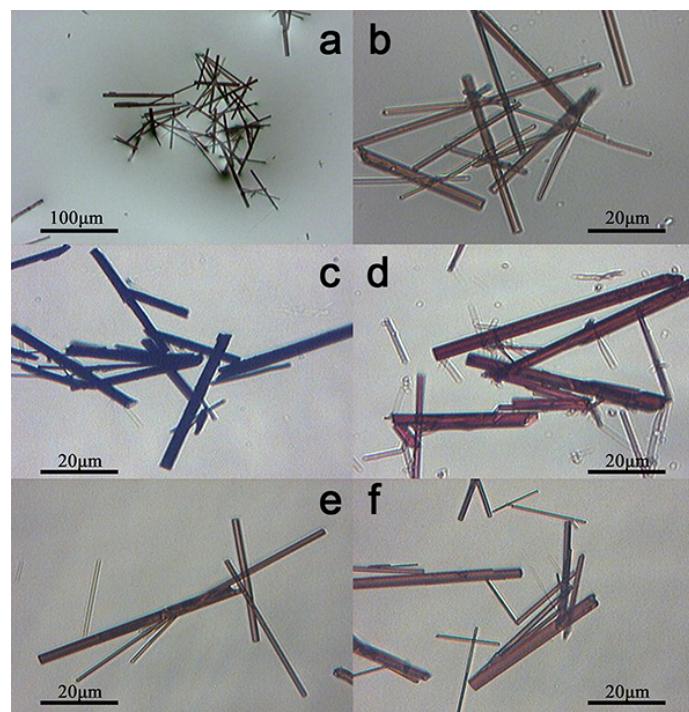


Fig. S1 Optical microscopy images of PCN-222 before adsorption under magnification of (a) low magnification and (b) high magnification , (c) after adsorbing MB, (d) after adsorbing MO, (e) after 8 reuse cycles of MB adsorption/removal, and (f) after 8 reuse cycles of MO adsorption/removal.

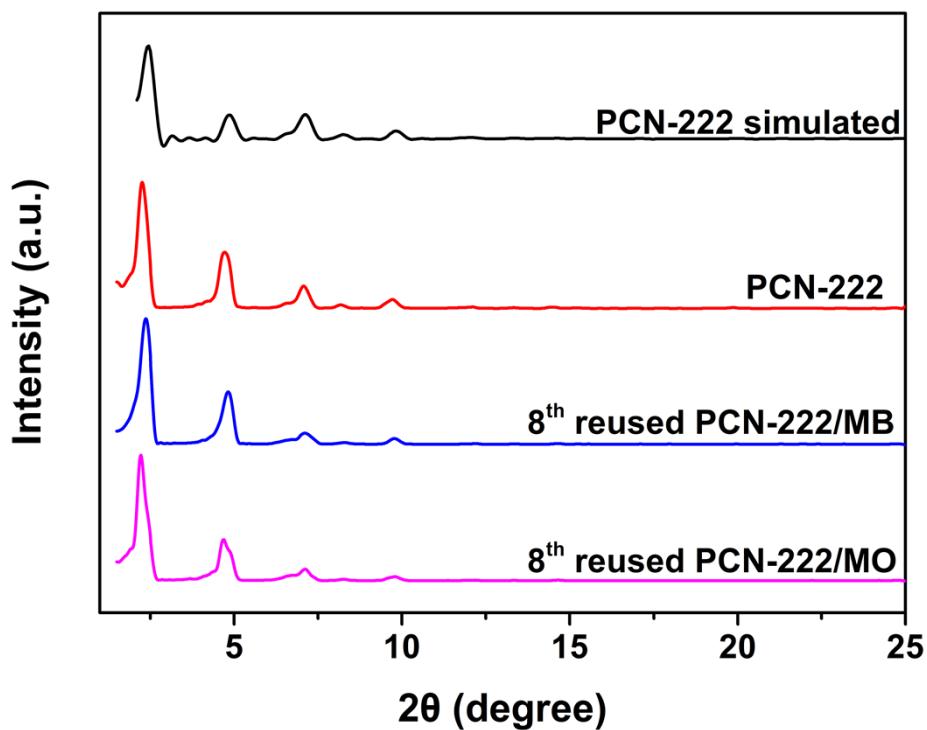


Fig. S2 Powder XRD patterns of PCN-222 as prepared (red line) and after reused for 8 cycles with MB (blue line) and with MO (purple line) and simulated (black line) .

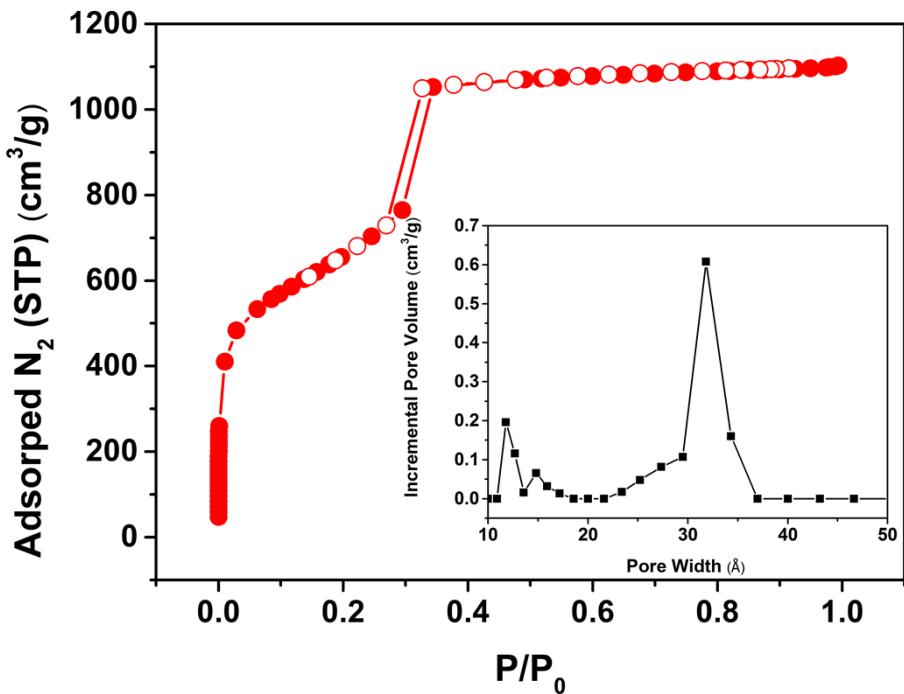


Fig. S3 N_2 adsorption (open red dots)/desorption (solid red dots) isotherms and the corresponding pore size distribution (inset) of PCN-222 as synthesized based on the density functional theory (DFT) method.

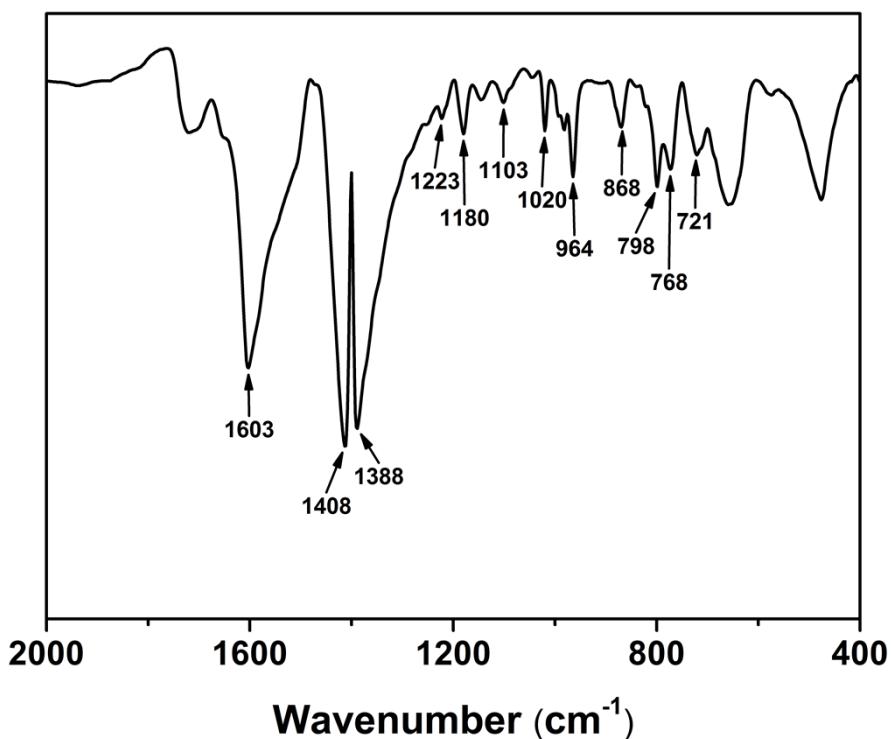


Fig. S4 FT-IR spectrum of PCN-222 powder.

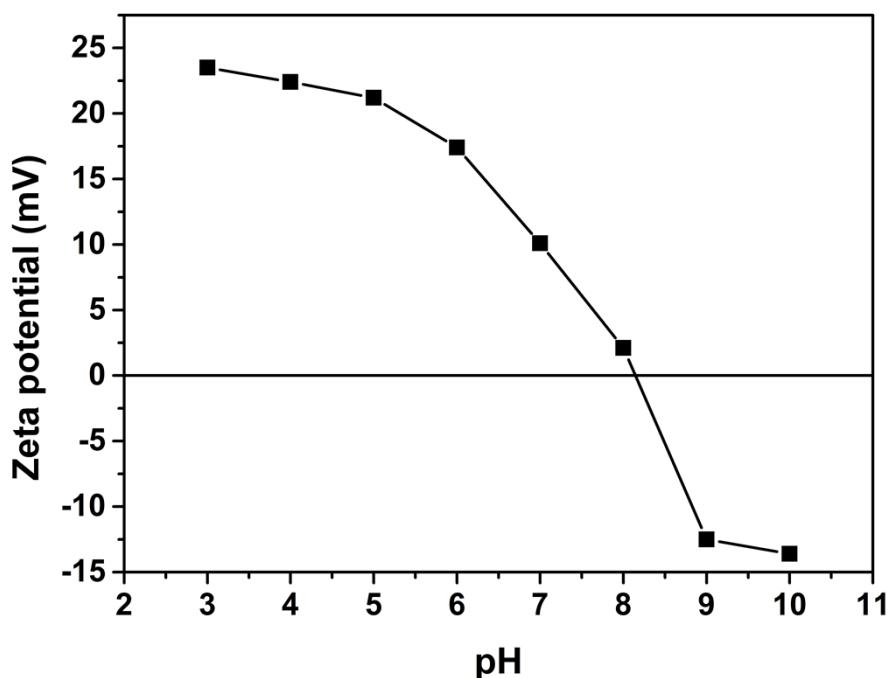


Fig. S5 Effect of initial pH on Zeta potential of PCN-222.

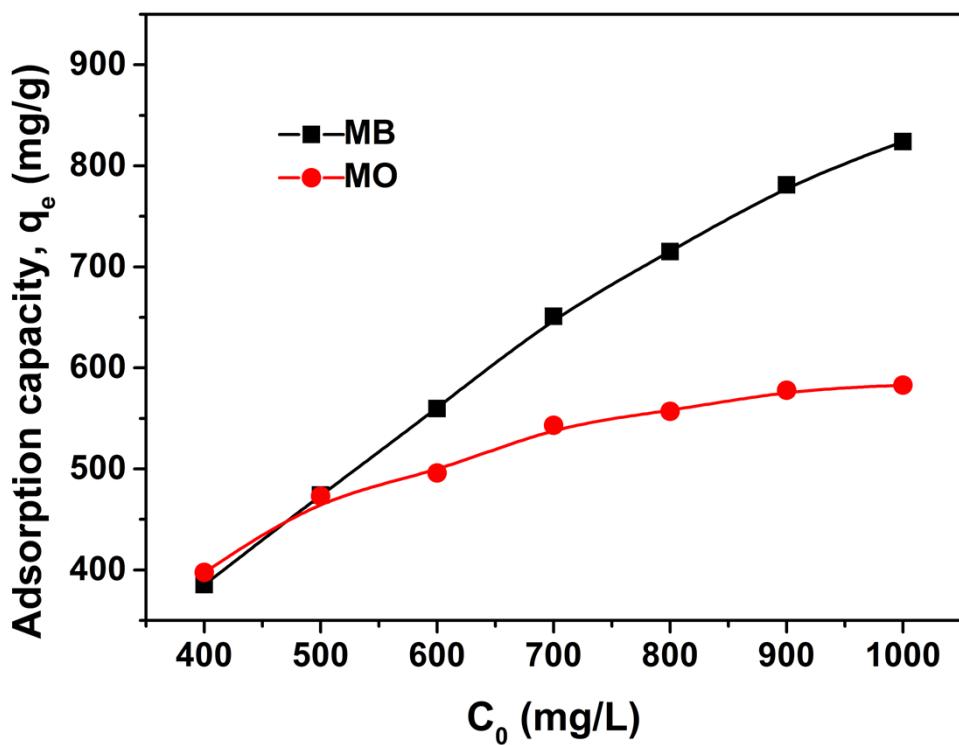


Fig. S6 Experimental adsorption capacities of MB (black solid squares) and MO (red solid circles) as a function of initial concentration at pH 9 and 5 respectively and room temperature.

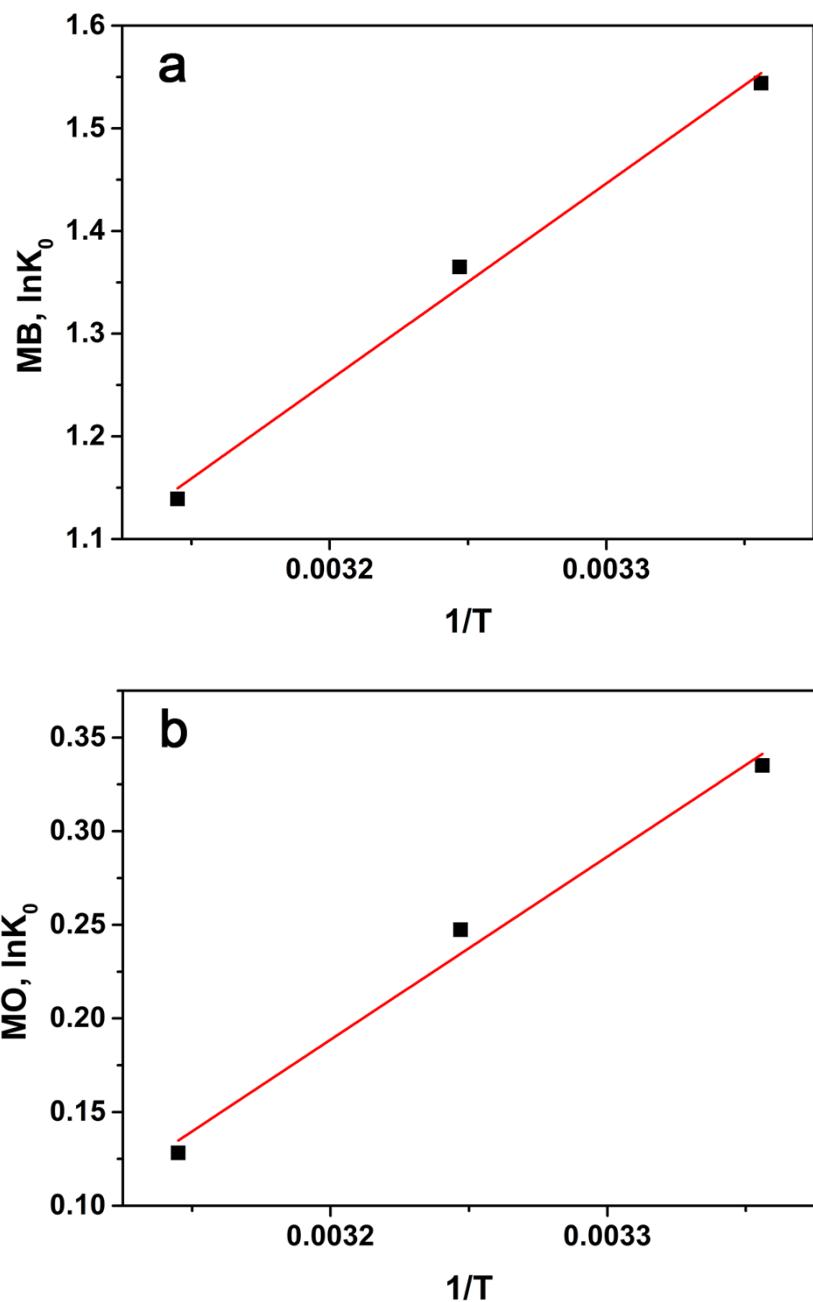


Fig. S7 Van't Hoff plot of (a) MB and (b) MO adsorption onto PCN-222.

1 **Table S1.** FT-IR fingerprint bands of the organic linker of PCN-222.

Modes	FT-IR (cm⁻¹)		Descriptions
	This work	Reference	
v₂₅	721	721	γ(C-H, N-H, OH)
v₂₈	768	768	breath (pyr) + γ(C-H, N-H, OH)
v₃₀	798	798	Porph γ(C-H, N-H)
v₃₄	868	868	δ(C-N-C) + Phenyl γ(C-H)
v₃₅	964	964	breath (pyr + phenyl)
v₃₉	1020	1020	def (phenyl)
v₄₁	1103	1103	Pyr δ(C-H)
v₄₄	1180	1176	phenyl δ(C-H) + δ(O-H)
v₄₅	1223	1223	phenyl (breath + δ(C-H + O-H))
v₅₀	1388	1385	ν(C _α + C _β)
v₅₂	1408	1402	phenyl δ(C-H)
v₅₉	1603	1605	def (phenyl)

3 **Table S2.**

4 The adsorption amounts of eight cationic and anionic dyes at pH 6 (Test with a column).

Dye	Structure	Maximum adsorption wavelength (nm)	Maximum adsorption capacity (mg/g) at pH 6
MB		664	601
MG		617	2880
RhB		554	200
MO		464	572
IC		610	497
AF		547	1472
AO		372	748
FD		490	301