Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2015

Supporting Information

Purification of Phenol-contaminated Water by Adsorption with Quaternized poly(dimethylaminopropyl methacrylamide)-grafted PVBC Microspheres

Juntao Gu,^a Shaojun Yuan,^{a,*} Yu Zheng,^a Wei Jiang,^a Bin Liang,^a Simo O Pehkonen,^b

> ^a Multi-phases Mass Transfer & Reaction Engineering Lab, College of Chemical Engineering, Sichuan University, Chengdu 610065, China
> ^b Department of Environmental Sciences, University of Eastern Finland, 70211 Kuopio, Finland

^{*}To whom all correspondence should be addressed Tel: +86-28-85990133, Fax: +86-28-85460556 E-mail: <u>yuanshaojun@gmail.com</u> (S.J. Yuan)

Adsorbents	Equilibrium time (h)	Initial phenol concentration (ppm)	Sorption capacity ^a (mmol·g ⁻¹)	Refs
Activated Carbon		· · · /		
Granular activated carbon	96	100	2.53 (pH = 5.5)	10
Activated carbon fibers	24	140	1.09 (pH not given)	65
Vetiver roots activated carbon	Not given	20-100	1.54 (pH = 4.0-5.0)	11
Coconut shell-based activated carbon	48	100-500	2.18 (pH = 7.0)	66
Polymeric adsorbent				
Hypercrosslinked polymer HJ-Z01	7	200-1000	1.81 (pH = 6.0)	14
Aminated polymeric resin (MN-150)	72	200-1000	2.46 (pH = 6.5-7.5)	67
Aminated polystyrene (NDA103)	24	15-200	1.43 (pH not given)	29
N-butylimidazolium-grafted resins (MCl)	1	50-1000	0.99 (pH = 11.0)	68
Fly ash	2	100	1.52 (pH = 8.0)	15
nitrogen-functionalized magnetic ordered carbon (N- Fe/OMC)	4	25	1.97 (pH =7.0)	72
Sewage sludge	24	100	1.0 (pH = 6.0 - 7.0)	20
chitosan–calcium alginate blended beads	4	100	1.15 (pH =7.0)	12
Red clay	4	50	0.74 (pH = 6.0)	19
PVBC-g-QPDMAPMA microspheres	1	200	2.23 (pH=6.5)	This stu

Table S1 Comparison sorption of phenol on the different adsorbents

^a The sorption capacity refers to the equilibrium adsorption capacity of sorbents for phenol.



Figure S1. (a) The UV spectrum profiles as a function of the concentration of aqueous phenol solution and (b) the calibration curves of the aqueous phenol solution at a concentration of 0.48, 1.44, 2.40, 3.84 and 4.80 mg·L⁻¹



Figure S2. Representative optical images and SEM images at different magnifications (×50 and ×500) of (a-c) the pristine PVBC, (d-f) the PVBC-*g*-PDMAPMA2 and (g-i) the PVBC-*g*-QPDMAPMA2 microspheres.



Figure S3. The ATR-FTIR spectra of the surfaces of (a) the cross-linked PVBC microspheres, (b) the PVBC-*g*-PDMAPMA1 microspheres from 2 h of ATRP reaction, and (c) the PVBC-*g*-PDMAPMA2 microspheres from 6 h of ATRP reaction.



Figure S4. ATR-FTIR spectra of the surfaces of (a) the PVBC-*g*-QPDMAPMA1 and (b) the PVBC-*g*-QPDMAPMA2 microspheres.



Figure S5. Freundlich-fitted adsorption isotherms of phenol on the PVBC-g-QPDMAPMA2 microspheres at 298.15, 308.15, 318.15, and 328.15 K. Experimental conditions: $C_0 = 1.05 - 5.31 \text{ mmol} \cdot \text{L}^{-1}$ (i.e. 100 - 500 mg $\cdot \text{L}^{-1}$), T = 298.15 K, m = 0.1 g, v = 100 mL, t = 24 h, and initial pH =6.5.



Figure S6. Temkin-fitted adsorption isotherms of phenol on the PVBC-g-QPDMAPMA2 microspheres at 298.15, 308.15, 318.15, and 328.15 K. Experimental conditions: $C_0 = 1.05 - 5.31 \text{ mmol} \cdot \text{L}^{-1}$ (i.e. 100 - 500 mg $\cdot \text{L}^{-1}$), T = 298.15 K, m = 0.1 g, v = 100 mL, t = 24 h, and initial pH =6.5.



Figure S7. Van't Hoff plot for the adsorption of phenol on the quaternized PVBC-g-QPDMAPMA2 microspheres.



Figure S8. (a) The proposed adsorption mechanism of phenol on the quanterinzed PVBC-g-QPDMAPMA microspheres via electrostatic interactions and hydrogen bonding, and (b) the regeneration of the microsphere adsorbents by the ion exchange process in a $0.1 \text{ mol} \cdot \text{L}^{-1}$ NaOH solution.



Figure S9. The wide scan, O 1s, C 1s and N 1s core-level XPS spectra of the quaternized PVBC-g-QPDMAPMA2 microsphere surface after the adsorption of phenol at a 2.13 mmol·L⁻¹ (i.e. 200 mg·L⁻¹) phenol solution at 25 °C and 150 rpm for 24 h.