Electronic Supplementary Information

Surfactant-FreeGreenSynthesisofFe3O4Nanoparticlescappedwith3,4-Dihydroxyphenethylcarbamodithioate:StableRecyclableMagneticNanoparticlesforRapidandEfficientRemoval of Hg(II)Ions from Water

Sada Venkateswarlu and Minyoung Yoon*

Department of Nanochemistry, College of Bionano, Gachon University, Sungnam, 13120, Republic of Korea

*Corresponding author. Tel.: 82-31-750-8721.

E-mail address: myyoon@gachon.ac.kr

Pseudo-first-order kinetics study

The linear form of pseudo-first-order kinetic model is described by the equation

$$\log(q_e - q_t) = \log q_e - \left(\frac{k_1}{2.303}\right)t \tag{1}$$

Where k_l (min⁻¹) is a pseudo-first-order rate constant of adsorption, where q_e (mg/g) and q_t (mg/g) are the amount of the Hg(II) adsorbed at equilibrium and at time t, respectively. The pseudo-first-order kinetic constant was determined from slope of the plot of log($q_e - q_t$) vs t.



Figure S1. Pseudo first-order adsorption kinetics of Hg(II) on DHPCT@Fe₃O₄ MNPs.

Table S1. Kinetic parameters of pseudo-first-order and pseudo-second-order models for the adsorption of Hg(II) on the DHPCT@Fe₃O₄ MNPs.

Pseudo-first-order				Pseudo-second-order		
$q_{\rm e,exp}$ (mg/g)	k_1 (g/mg min ⁻¹)	$q_{\rm e,}$ cal (mg/g)	<i>R</i> ²	$k_2 \ (g/mg \min^{-1})$	$q_{\rm e,}$ cal (mg/g)	<i>R</i> ²
19.463	0.0290	11.384	0.905	0.0039	21.186	0.999

Isotherm type	Constant	Value
Langmuir	$q_{\rm m} ({\rm mg/g})$	52.10
	<i>b</i> (L/mg)	1.654
	R^2	0.999
Freundlich	$k_{\rm f}$ (mg/g)	16.707
	n	3.503
	R^2	0.981

Table S2. Langmuir and Freundlich isotherm constants for Hg(II) adsorption

Selective adsorption experiment

The selectivity of the adsorbent material for various metal ions is an important parameter related to the application potential of adsorption processes. Stock solutions for selectivity experiments were prepared using nitrate, sulfate and chloride metal salts (Pb(NO₃)₂, Ni(NO₃)₂·6H₂O, CuSO₄, Co(NO₃)₂·6H₂O, and ZnCl₂) dissolving in deionized Millipore water. The DHPCT@Fe₃O₄ composite (2.5 mg) was placed in a 100 ml Erlenmeyer flask with of a metal ions (Pb(II), Ni(II), Cu(II), Co(II), Zn(II) and Hg(II)) mixture solution (25.0 ml, concentration: 60 mg/L, pH: 7). The mixture solution was ultrasonicated for 10 min and shaken in an incubator for 1 hour at 303 K. After adsorbing with the mixed metal ions, the magnetic nano-adsorbent was separated from the solution by external magnet. The concentrations of the mixed metal ions were determined using atomic absorption spectroscopy (AAS).

Biogenic synthesis of Fe₃O₄ to show reproducibility

To study the effect of watermelon rind extract concentration and the reproducibility in Fe_3O_4 nanoparticles, the watermelon rind extract solutions with a different concentration were prepared by dilution of original extract solution with distilled water. The volume ratio of watermelon rind extract and water was (20:20, 30:10 and 40:0) with a total solution volume of 40 ml. Due to the dilution effect of the extract solution by the addition of water, the concentration of polyphenols in extract will be decreased resulting in the incomplete formation of Fe_3O_4 MNPs. However, 40 ml of

pure watermelon rind extract is suitable for the formation of Fe_3O_4 MNPs. With the use of the pure watermelon rind extract derived from different watermelon, we have always found an agglomerated Fe_3O_4 MNPs with a similar nanoparticle size and a magnetic property. Therefore, we expect the Fe_3O_4 MNP synthesis using watermelon rind extract can be generally applied to the most of watermelons.