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SUPPLEMENTARY MATERIAL TO

New thiamine-functionalized silica microparticles as a sorbent for the removal of lead, mercury and cadmium ions from aqueous media

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ADSORPTION ISOTHERMS

In adsorption studies, the interaction between adsorbate and adsorbent is described by adsorption isotherms,[1] which are critical in optimizing the use of adsorbents. When the adsorbent is in contact with a surrounding solution of a certain composition, adsorption occurs and after a sufficient time, the adsorbent and the surrounding fluid attain equilibrium.[2] The Langmuir and Freundlich adsorption models were fitted to the data obtained from the adsorption isotherm. The Langmuir equation (1) was the simplest theoretical model for monolayer adsorption and the Langmuir model was developed to represent adsorption on an adsorbent. The ideal Langmuir model generally gives an appropriate representation of the behavior of a system at low sorbate concentrations. On the other hand, the Freundlich equation (2) is an empirical approach for adsorbents with very uneven adsorbing surfaces. This model is applicable for an adsorption of a single solute system within a fixed range of concentrations.[3] The equations of the above two types of sorption isotherms are expressed as follows:

$$q_e = \frac{Q_m k_L c_e}{1 + k_L c_e} \quad (1)$$

$$\ln q_e = \ln K_F + \frac{1}{n} \ln c_e \quad (2)$$

where q_e is equilibrium uptake capacity of M3APS, c_e is the concentration of metal ions in the supernatant after sorption, n and K_F are empirical constants of

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the Freundlich equation, and Q_m and k_L are Langmuir constants related to the capacity and energy of the adsorption, respectively.

RECOVERY AND REUSE

Many of adsorbents can be reused several times for practical applications. The adsorption and desorption processes were repeated 5 times to examine uptake capacity of M3APS. The desorption study was realized with acidic solutions. First, M3APS was loaded with metal ions under optimum conditions. Then, the metal ions were desorbed using 0.1 mol L^{-1} HNO_3 and the results are given in Table S-I. Table S-I shows that the regeneration procedure and desorption efficiency were generally high and M3APS could be used 5 times without significant loss of its adsorption capacities.

TABLE S-I. Adsorption and desorption capacity of M3APS

Cycle	Pb(II)		Hg(II)		Cd(II)	
	Adsorption mg g^{-1}	Desorption %	Adsorption mg g^{-1}	Desorption %	Adsorption mg g^{-1}	Desorption %
1	39.4	98.1	30.9	97.2	9.5	94.5
2	38.9	97.3	30.2	96.5	8.3	93.4
3	38.2	96.1	29.7	96.1	7.6	92.6
4	37.2	95.1	28.8	95.2	7.1	92.1
5	36.6	94.9	27.4	94.4	6.6	91.8

THE GIBBS ENERGY CHANGE

The Gibbs energy change of the adsorption was calculated using the following equation:

$$\Delta G = -RT \ln K_L \quad (3)$$

where ΔG is the Gibbs energy change (kJ mol^{-1}), R is the ideal gas constant (8.314 mol^{-1} K^{-1}), T is the solution temperature (K), and K_L is the Langmuir constant (L mol^{-1}).[4–6] The values of ΔG for adsorption of Pb(II), Hg(II) and Cd(II) were –25.3, –21.6 and –16.5 kJ mol^{-1}, respectively. The negative values for the Gibbs free energy show that the adsorption process of Pb(II), Hg(II) and Cd(II) on M3APS is spontaneous in nature and demonstrate the feasibility of the process.

COMPARISON WITH SOME OF OTHER ADSORBENTS

A comparison of the proposed systems with other systems is given in Table S-II. Some parameters obtained were comparable to those presented by other described in the literature. As could be seen from the data in Table S-II, the proposed method using M3APS has relatively high adsorption capacities and high pH values in comparison with other methods that used modified silica gels as adsorbents.

TABLE S-II. Comparative data from recent studies for the adsorption of metal ions

System	Studied metal	pH	Adsorption capacity mg g^{-1}	Ref.
Modified almond shell	Pb(II), Cd(II)	5	7.00–9.00	6
Urea functional hydrogel	Pb(II), Cd(II)	5	26.0	7
P(VIM/AAc/HEMA) hydrogels	Pb(II)	4.5	30.38	8
1,3,4-Trithiane	Hg(II), Sb(III), Cd(II), Pb(II)	5	9.50–35.5	9
Dithizone-modified silica gel	Cu(II), Pb(II), Ni(II), Fe(III), Cd(II), Zn(II) Co(II)	1–6	2.06–8.28	10
Resacetophenone-modified silica gel	Cu(II), Pb(II), Ni(II), Fe(III), Cd(II), Zn(II) Co(II)	5.5–7.5	6.5–15.2	11
Gallic acid-modified silica gel	Pb(II), Cu(II), Cd(II), Ni(II)	3–7	4.62–15.38	12
Silica gel phase functionalized by choline	Pb(II), Hg(II), Cd(II), Cu(II), Ni(II), Co(II)	7	11.7–60.1	13
Pyrazol-3-ylimine-modified silica gel	Pb(II), Cd(II), Cu(II), Zn(II)	2–8	0.96–74.89	14
Vitamin B1-modified 3-aminopropyl silica gel	Pb(II), Hg(II), Cd(II)	5	9.54–39.4	This work

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