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Comparison studies of adsorption properties for Hg(II) and Au(III) on polystyrene-supported bis-8-oxyquinoline-terminated open-chain crown ether

Changmei Sun, Chunxue Li, Chunhua Wang, Rongjun Qu *, Yuzhong Niu, Hongbo Geng

School of Chemistry and Materials Science, Ludong University, Yantai 264025, China

HIGHLIGHTS

- Differences between adsorption properties for Hg and Au ions on PS-DB were studied.
- DFT method was successfully used to verify adsorption natures for Hg and Au ions.
- Adsorption kinetics of the two metal ions were comprehensively compared.

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ABSTRACT

Differences between adsorption properties for Hg(II) and Au(III) on polystyrene-supported bis-8-oxyquinoline-terminated open-chain crown ether (PS-DB) were studied by scanning electron microscope (SEM), X-ray diffraction (XRD) and the density functional theory (DFT) method. The comparison studies included kinetics, equilibriums and thermodynamics of the adsorption process. Pseudo-first-order and pseudo-second-order kinetic models were applied to test the experimental data. The pseudo-second-order kinetic model provided a better correlation with the experimental data for Hg(II) in comparison with the pseudo-first-order model. While for Au(III), the conclusion was the reverse. Both the adsorption rate and adsorption amount at equilibrium for Hg(II) were greater than those for Au(III) ions, which was probably caused by the differences in form and volume between the two kinds of absorbed ions. Langmuir, Freundlich and Tempkin isotherm models were applied in the adsorption isotherm study. The results showed that the Langmuir and Tempkin isotherm models were more applicable in describing the processes. The thermodynamic parameters for the adsorption process such as free energy of adsorption (ΔG), enthalpy of adsorption (ΔH) and entropy of adsorption (ΔS) were calculated. The density functional theory (DFT) method was used to investigate the coordination geometries and the interactions between the metal ions with PS-DB. These results showed that the adsorption for Hg(II) was physisorption while that for Au(III) was chemisorption, which was also consistent with the data obtained from the Dubinin–Radushkevich (D–R) isotherm model and ΔH values.

1. Introduction

In recent years, the presence of heavy metal ions in industrial effluents, water supplies and mine waters has become an important environmental problem due to their more stringent discharge norms, increased usage and the cumulative adverse characteristics of their high toxicity [1]. Among these contaminants, mercury is very pervasive with its high toxicity, which is readily accumulated by organisms [2]. It can be released into the environment from anthropogenic activities that include agriculture, battery production, fossil fuel burning, mining and metallurgical processes, paint and chlor-alkali industries and wood pulping [3]. Besides heavy metals, precious metals, such as gold, are also widely used in many fields such as catalysts, electrical and electronic industries, corrosion resistant materials and jewelry, because of their specific physical and chemical properties. Because of the value and scarcity of precious metals, it is an economic necessity to treat their aqueous waste solutions in order to try to recover them.

Various techniques, such as adsorption, solvent extraction and polymeric membranes, are currently being used to remove and recover metal ions from the environment [4–7]. One of the most promising methods is the use of chelating adsorption. Chelating adsorbents are generally efficient in the removal and recovery of metal ions because of their physical and chemical stabilities. For the synthesis of a successful adsorbent, it is essential to choose or design efficient functional groups having high affinity ability towards metal ions. Recently, we designed a novel functional group

* Corresponding author. Tel.: +86 535 6699201.
E-mail address: rongjunqu@sohu.com (R. Qu).

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