Research Article
doi.org/10.1002/slct.202203316
Chemistry Europe
European Chemical Societies Publishing

Determination of Chromium in Contaminated Water Samples Using Chemically Modified Nanoadsorbent: A Computational and Experimental Study

Shelja Tiwari,[a] Amit Lochab,[a] Kajal Jindal,[b] and Reena Saxena*[a]

In the reported work, a solid phase extraction method for speciation of chromium species in contaminated industrial and river water samples has been studied by using both experimental and computational methods. Multiwalled carbon nanotubes (MWCNTs) functionalized with tris(2-aminoethyl)amine (TREN) was used as a solid phase extractant for the hyphenated preconcentration of chromium species. The characterization of the immobilized MWCNTs was done by FTIR and SEM analysis. This hyphenated system significantly improves the overall analytical performance by reducing sample consumption and sampling time. The computational results supported the experimental findings. The negative adsorption energy (−2.71 eV) suggested that the interaction process between chromium and modified nanoadsorbent is spontaneous. The system showed a limit of detection of 0.07 $\mu g L^{-1}$ at optimized condition with an RSD value of 1.2%. Adsorption capacity was measured using Lagergren's equation which showed that adsorption kinetics follows pseudo second-order. The suggested method was applied to contaminated real water samples by performing spike recovery tests. The validation of the reported system was done by analysing NIST Standard Reference Material Trace Elements in Natural Water 1640a.

Introduction

Carbon nanotubes have gained a lot of attention in the last few years owing to their extraordinary chemical, mechanical and optical properties.[1] These CNTs have also been classified as a great sorbent material for sorption of metal ions and organic pollutants. CNTs are of two types-single-walled (SWCNTs) and multiwalled (MWCNTs). MWCNTs are gathering major interest because of their application as metal adsorbents in environmental remediation.[2] The surface of MWCNTs possesses unsaturated atoms which provides in high chemical activity and also results in easy binding with other atoms. The large surface area and presence of π-π electrostatic interactions facilitates the adsorption of metal ions.[3] Chemically modified MWCNTs can be used as solid phase extractant in metal extraction studies as the modification provides better selectivity and sensitivity. The chemical modification of MWCNTs can be done by a two-step process. In the first step, MWCNTs are oxidised to introduce carboxylate functionality and in the next step various chelating agents can be introduced via amide, ester, acyl linkage.[4] The presented method discusses use of chemically modified MWCNTs for preconcentrative speciation and determination of chromium species in industrial and real water samples.

The metal ions on the basis of their requirement are categorized as essential, non-essential and toxic metal ions. The toxicity exhibited by a metal ion is governed by the oxidation state it exists in. Chromium is one of the metal ions whose one oxidation state (+3) is essential for humans and other oxidation state (+6) is a known carcinogen. Cr(III) is required for proper functioning of pancreas and glucose metabolism. Cr(VI) is known to exhibit carcinogenic activity owing to its high solubility and mobility as it can easily penetrate through the cell membrane.[5] The maximum allowed amount of total chromium in drinking water established by WHO is 0.05 $mg L^{-1}$.[6] The day by day increasing industrial activities are introducing chromium species to environmental bodies, thus it is crucial to determine the chromium concentration in environmental samples.[7] Speciation analysis provides information about the individual concentrations of the different chemical forms of an element present in a sample. Due to antagonistic behaviour of the two most stable of chromium these studies are very significant. So far, many singular spectro-analytical methods have been described for determination of chromium in various matrices. Flame atomic absorption spectrometry (FAAS) is one of the most popular methods used for direct determination of chromium species in many environmental and biological samples. The direct use of FAAS for chromium determination faces many challenges such as interferences from matrix ions, lack of sensitivity due to low concentrations etc. The most popular method used to overcome these disadvantages involves hyphenation of FAAS to a flow injection (FI) preconcentration system. The hyphenated FI-FAAS system using a solid phase extractant for preconcentration of analyte ion provides many advantages over singular detection methods. This system is automated, fast, sensitive, and introduction of a preconcentration step allows selective sorption of metal ions at suitable conditions.[8]

[a] *Dr. S. Tiwari, A. Lochab, Prof. R. Saxena*
Department of Chemistry
Kirori Mal College, University of Delhi
Delhi 110007, India
E-mail: rsaxena@kmc.du.ac.in
[b] *Dr. K. Jindal*
Department of Physics
Kirori Mal College, University of Delhi
Delhi 110007, India

Supporting information for this article is available on the WWW under https://doi.org/10.1002/slct.202203316