



Metal oxide based carbon nanocomposite as sensing platform for electrochemical detection of cadmium- computational and experimental approach

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ABSTRACT

Cadmium is detected using an electrochemical sensor prepared by fabricating ITO substrate with metal oxide based carbon nanocomposite (SnO₂, MnO₂, MWCNTs and ionic liquid (IL)). The computational studies showed that the interaction of metal oxide based nanocomposites with cadmium is thermodynamically favorable (adsorption energy of -1.37 and -8.71 eV for SnO₂ adsorbed cadmium and MnO₂ adsorbed cadmium respectively). Metal oxide shows good conductivity and provide structural stability to the redox process at the surface. The fabricated sensor, SnO₂/MWCNTs/IL/ITO and MnO₂/MWCNTs/IL/ITO showed good sensitivity towards cadmium by having linearity range of 20–200 and 300–2000 ppb with a limit of detection 3.61 and 41.34 ppb respectively. The sensor showed good reproducibility and repeatability at optimized conditions. The recovery response to check the stability and resistance to interfering ions showed good results which is credited to the chemical stability and selective sites of SnO₂/MWCNTs/IL and MnO₂/MWCNTs/IL nanocomposite. The sensor showed good performance in real water samples analysis by showing efficient recovery through spike recovery test with a confidence interval above 95 %.

1. Introduction

Cadmium is considered as one of the toxic elements that comes in the category of heavy metals. It is being widely used in several industries in electroplating, alloys, batteries, pigments and solar cells etc. The untreated disposal of such materials can increase the concentration of cadmium in our environment which can further enter our food chain. The maximum permissible limit for cadmium in drinking water as set by World Health Organization (WHO) is 3 ppb above which it is harmful. The long term exposure of such toxic heavy metals can produce harmful effects on cardiovascular, nervous, respiratory, reproductive and skeletal systems. It is classified as carcinogenic by several health agencies and can cause a well-known disease 'Itai-Itai' [1].

The main anthropogenic sources of releasing cadmium in our environment includes burning of fossils, refining, smelting and use of phosphate fertilizers. Cadmium is accumulated in our body through food chain from various plants and animals. Natural processes like volcanic

eruptions abrasion of soil and rocks also the major factors for increasing the concentration of cadmium in the environment. The Comprehensive Environmental Response, Compensation, and Liability Act has prioritized cadmium at number 7 from a list of 275 hazardous materials list permanently. Also, International Agency for Research on Cancer, a body of WHO have categorized cadmium and cadmium containing compounds as human carcinogens (group-1) [2].

Cadmium enters our body either through gastro-intestinal or respiratory tract which is then absorbed in our blood through albumin and erythrocytes and finally accumulates in our liver and kidney. However, the excretion of cadmium out of our body is generally through urine at much lower rate. Its adverse effects are not only confined to humans, as it imposes serious health concerns on aquatic, and other terrestrial animals also. So, the determination of cadmium in the environment becomes very crucial. Use of computational chemistry have evolved a lot in last few years as it helps in reducing time and cost effectively. Here the analytical capability of the sensor can be verified using the

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