

Silica–silver core–shell nanoparticles incorporated with cellulose filter paper as an effective colorimetric probe for mercury ion detection in aqueous media: Experimental and computational evaluations

Abstract

This study investigates the facile and rapid detection of mercury ions using silica–silver core–shell nanoparticles (SiO₂–AgNPs) incorporating a paper-based colorimetric sensor strip. A strong surface plasmon resonance peak at $\lambda = 430$ nm was observed for the resultant SiO₂–AgNPs. The attachment of the AgNPs to the surface of SiO₂ and the deposition of the AgNPs on the paper strip were confirmed using an electron microscope. The sensing of the SiO₂–AgNPs toward the mercuric ion (Hg²⁺) in an aqueous solution indicated a rapid response in terms of a color change from yellowish-brown to colorless with a response time of 5–10 s. The prepared SiO₂–AgNPs deposited on the paper strip exhibited high selectivity toward Hg²⁺ compared with other metal ions. The limit of detection for this assay was 1.13 nM, with an excellent correlation value of $R^2 = 0.9936$. In addition, the complexation mode of the SiO₂–AgNPs with Hg²⁺ was also elucidated via theoretical calculations using the density functional theory approach. This approach also provides insight into the complexation structure in terms of the electronic alteration of the SiO₂–AgNPs prior to and following their interaction with Hg²⁺. Overall, the study demonstrates that SiO₂–AgNP-based sensor materials can be utilized for the selective recognition of Hg²⁺ in aqueous solutions.

Keywords

Colorimetric sensor; DFT; Mercury detection; Silica–silver; SPR