Carbon-based optical multimodal nanosensor of heavy metal ions in liquid media

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Nowadays, the problem of controlling the amount of heavy metal ions in liquid natural media is an urgent task in the field of ecology. As an optical sensor for determining the composition of multicomponent media, carbon dots (CD) represent a promising alternative to other nanomaterials due to their stable optical properties, low toxicity, a huge variety of available synthesis methods.

However, the problem of identification and determination of the concentration of heavy metal ions in liquid media by CD fluorescence and absorption spectra using conventional spectroscopic methods is complicated by the nonlinear nature of the CD fluorescence and complex chemical composition of liquid media. In this study, the solution of the indicated inverse problem of optical spectroscopy with an optical nanosensor is implemented using the model of artificial neural networks.

The problem was solved using three sets of optical spectroscopy data: 1) fluorescence spectra of aqueous suspensions of CD in the presence of the studied ions under 345 nm wavelength excitation (FL345); 2) optical absorption spectra (OA); 3) dataset, comprising both FL345 and OA spectra stacked together (FL345+OA). 1000 aqueous suspensions of CD were experimentally obtained in the presence of Cr^{3+}, Cu^{2+}, Ni^{2+} cations, their concentrations ranging from 0 to 4.95 mM.

The application of multilayer perceptrons to the datasets provided the root mean squared errors in determining the ion concentration as low as: 1.11 mM for Cu^{2+}, 1.55 mM for Ni^{2+}, 0.48 mM for Cr^{3+}. The results of the study are discussed in more detail in the report.

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