Development of a Multimodal Photoluminescent Carbon Nanosensor for Metal Ions in Water Using Artificial Neural Networks

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Abstract—The study presents a novel approach to the development of a photoluminescent multimodal carbon dots-based nanosensor for determining the concentration of Cu^{2+} , Ni^{2+} , Co^{2+} , Al^{3+} , Cr^{3+} and NO_3^- ions in water using machine learning methods. The results show that it is possible to determine the type and concentration of each of these ions in multicomponent aqueous media from the photoluminescence spectra of carbon dots. The mean absolute error of simultaneous determination of Cu^{2+} , Ni^{2+} , Co^{2+} , Al^{3+} , Cr^{3+} cations and NO_3^- anion concentration was 0.85, 0.97, 0.67, 0.81, 0.26, and 2.03 mM, respectively. The accuracy of the developed nanosensor fully meets the requirements for wastewater and process water composition control. The developed nanosensor can not only simultaneously determine the concentration of each of the 6 ions, but also provides real-time remote determination of ion concentrations.

Keywords: carbon dots; nanosensors; heavy metals cations; convolutional neural networks

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1. INTRODUCTION

The production and industrial use of fertilizers and pesticides, mining, metallurgy, and other human activities pollute the environment with heavy metals ions, which are not biodegradable and accumulate in surface and groundwater, soils, and living organisms. Therefore, the problem of quantifying metal ions in multicomponent media is extremely urgent.

Currently, there are multiple ways to determine the type and concentration of heavy metal ions in media, including amperometry [1], flow injection analysis [2], chromatography [3], atomic absorption spectroscopy [4] and other analytical methods. Optical spectroscopy techniques for example, photoluminescent, absorption and Raman spectroscopy [5–7] are also used for this purpose. While optical methods are less accurate than analytical methods, they don't require sampling or special sample preparation, making them express and remote. Special attention is paid to the creation of optical nanosensors due to the active development of materials science and nanotechnology.

Operating principles of optical nanosensors are based on nanoparticles' optical properties being

influenced by medium parameters or by the type and concentration of certain substances [8-14]. For example, the authors [11] proposed using silver nanoparticles modified with polyvinylpyrrolidone as optical sensors for Fe³⁺ ions. The operating principle of such sensor relies on measuring the absorption of light by nanoparticle during surface plasmon resonance in the presence of iron ions. Study [12] presents a liquid crystal sensor that was fabricated through immobilizing 3 μ g/mL bovine serum albumin solution on dimethyloctadecyl-[3-(trimethoxysilyl)propyl]ammonium chloride-coated glass slides. In order to estimate the concentration of heavy metal ions, brightness of polarized optical microscopy images of crystal on which a solution of the studied cation was deposited are used.

Carbon dots (CD) are a class of zero-dimensional carbon nanomaterials. CD are easy to synthesise, they exhibit low toxicity, time-stable optical properties, the ability to modify and functionalise their surface according to a specific task to be solved, they are the most biocompatible and nontoxic even among other carbon nanomaterials [15–23]. Unlike some other nanoparticle sensors, CD exhibit intense stable luminescence at room temperature: the luminescence quantum yield of these nanoparticles can reach more

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than 90% [19, 20], and the maximum of their photoluminescence (PL) locates from the UV to the IR region [21]. These properties enable creating photoluminescent nanosensors that are well dispersed in liquid media and allow tuning its sensitivity to certain properties of the medium by appropriate functionalization of the nanoparticle's surface or by doping them with different heteroatoms [24, 25].

There are a large number of studies showing the sensitivity of the CD PL to certain ions, revealing in a change in the CD PL spectrum characteristics in the presence of these ions [6, 10, 27-31]. This effect of the ions surrounding the nanoparticle on its PL is used to create a nanosensor to determine the type and concentration of ions. For example, the study [28] demonstrates the use of CD prepared via solvothermal method and doped with sulfur, nitrogen and oxygen atoms as a photoluminescent nanosensor of Cu^{2+} ions. Quenching of the nanoparticle's PL through static mechanism as a result of the interaction between surface functional groups and Cu²⁺ ions is an operating principle of such nanosensor. The linear dependence of the CD PL intensity on the concentration of Cu^{2+} ions ranging from 10 to 33.3 μ M provides a detection limit of Cu²⁺ 2 μ M in solution [28]. The authors [29] showed that CD prepared via hydrothermal synthesis and doped with boron and phosphorus atoms can be used as Cu^{2+} or Fe³⁺ sensor. The authors measured the concentrations of Cu²⁺ and Fe³⁺ cations in living cells with an accuracy of 0.18 and 0.27 μ M, respectively, using linear calibration dependences of the CD PL intensity on the concentration of the two studied ions, obtained separately for each ion. The authors attribute the causes of CD PL quenching in the presence of cations to NH₂ group protonation in a system with high acidity and the -OH group deprotonation in a system with high alkalinity. The publication [30] shows the possibility of using nitrogen-doped CD as a sensor for Cr⁴⁺ ions. Addition of Cr⁴⁺ ions in CD solution caused a decrease in the CD PL intensity. CD PL disappeared completely when Cr⁴⁺ concentration reached 0.6 mM. Such a high sensitivity of CD PL to Cr^{4+} ions provided ion detection limit of 0.26 μ M. The authors [31] developed CD-based nanosensors of Hg²⁺ and Ag⁺ ions with an ion detection limit of 4.8 and 1 nM, respectively. The PL intensity of CD synthesized from urine and diethylenetriamine decreased linearly under separate addition of Hg²⁺ and Ag⁺ ions in the concentration ranges $0.01-1 \ \mu M$ for Hg²⁺ and 0.001-1 μ M for Ag⁺ ions. Operating principle of the carbon nanosensor is based on the linear dependence of the magnitude of the CD PL static quenching on the ions' concentration. In [32], CD prepared by hydrothermal synthesis and doped with boron, nitrogen and sulfur atoms were studied. Photoluminescence in the red region of such CD showed selectivity to Fe^{3+} ions in water. The nanosensor developed by the authors enables detecting Fe^{3+} ions in the concentration range from 0.3 to 546 μ M with 90 nM accuracy.

All studies we are aware of referred to CD as unimodal optical nanosensors, i.e. sensors that detect one ion or two ions at most. However, currently, simultaneous detection of several ions is required with high accuracy in determining the concentration of each ion in real time. The incomplete clarity of the CD PL mechanisms, the lack of an analytical model describing the PL spectra, the significant dependence of CD PL on the synthesis method, precursors and conditions, the composition of surface functional groups and other factors do not allow solving the problem using classical (colorimetric, calibration curves, etc.) methods. Machine learning methods, primarily artificial neural networks (ANNs), are successfully used to solve inverse multiparameter problems [33–36].

ANNs are powerful algorithms for solving multiparametric inverse problems in various fields of Many authors have repeatedly human activity. demonstrated the success of the neural network approach in solving inverse problems of optical spectroscopy [6, 7, 33–36]. In the publication [33], multilayer perceptrons were used to analyze the manifestation of structural changes in proteins and lipids in Raman spectra of cancerous tissue which increased the accuracy of melanoma and brain cancer diagnosis. The paper [36] describes the use of generative-adversarial neural networks to generate Raman spectra of healthy and osteoporotic rabbit bones. It has been shown that increasing the volume of biomedical data requires ensuring that the distribution of the expanded dataset corresponds to the distribution of the original dataset and proving that the generated dataset is similar to the original one (but not identical). There are studies using ANN to solve multiparametric inverse problems of monitoring the state of natural and biological systems. In [37], the content of glutamine, glutamate, glucose, lactate and concentration of viable cells in the BHK-21 cell line were determined with perceptrons from the UV-VIS spectra of phenolic red. The authors of publications [38, 39] present the results of a successful neural network solution to problems of determining the concentration of carbon nanoagents in biological tissues using PL spectra of biological media injected with nanoagents.

This paper proposes a method for solving 6parametric optical spectroscopy inverse problem of determining the type and concentration of 6 ions in aqueous media from the excitation-emission matrices (EEM) of CD PL using convolutional neural networks (CNNs). The approbation of the developed carbon nanosensor was carried out on recycled water from the mining and metallurgical plant of the Trans-Baikal Territory of the Russian Federation was used.

2. MATERIALS AND METHODS 2.1. Research Objects

Ethylenediamine (Acros Organics, Belgium) and citric acid (Sigma Aldrich, United States) were used as precursors for the CD synthesis. Metal nitrates $Co(NO_3)_2$, $Cu(NO_3)_2$, $Ni(NO_3)_2$, $Al(NO_3)_3$, $Cr(NO_3)_3$ were classified as a "Reagent" (PanReac AppliChem, Spain, Germany). Bidistilled deionized water (Millipore Milli-Q water purification system) was used as a solvent. Carbon dots were prepared via hydrothermal synthesis. For this purpose, a mixture of precursors (citric acid and ethylenediamine, molar ratio 1 : 2) was placed in a Teflon container and then in a steel autoclave. Autoclave containing a mixture of precursors was placed in a muffle furnace with a temperature of 200°C for 3 h, to carry out CD hydrothermal synthesis. The resulting CD solution was passed through a membrane filter with a pore diameter of 0.22 μ m. The concentration of synthesized CD in water was estimated by gravimetric method, it was 28 g/L.

2.2. Characterization of Synthesized CD Aqueous Solution

CD concentration in the studied aqueous solutions was 5 mg/L. The pH value of the CD solution was 7.93. The sizes of nanoparticle aggregates and their Zeta-potentials in the studied CD solution were measured with Malvern Zetasizer NanoZS device and estimated as 11.3 ± 2.6 nm and -16.2 ± 1.3 mV, respectively. CD size obtained with transmission electron microscopy (TEM) (Fig. 1a) was 8.6 ± 1.6 nm.

The composition of the CD surface functional groups was studied using IR absorption spectroscopy (Bruker INVENIO R FTIR spectrometer) with a diamond console of attenuated total internal reflection (ATIR). Bands of valence vibrations ν_{OH} , ν_{CHx} , and ν_{NH} (2900–3600, 2800–3000, and 3300–3500 cm⁻¹, respectively) and bands of deformation vibrations δ_{OH} , δ_{CH_x} , and δ_{NH} (at 1645, 1370–1450, and 1580–1650 cm⁻¹, respectively) corresponding to them are observed in the obtained IR absorption spectra of CD evaporated from an aqueous solution (Fig. 1b). Intense bands with maxima in the region of 1539 and 1387 cm⁻¹ are probably caused by asymmetric and symmetrical vibrations ν_{NO_2} of nitro groups, respectively. Bands in the region of 1000–1300 cm⁻¹ correspond to ν_{COC} , δ_{CO} , δ_{CH} , δ_{NH} vibrations [40, 41].

2.3. Preparation of Aqueous Solutions of Carbon Dots with Metal Salts

To study metal cations affecting CD PL in water, initial aqueous solutions of salts with 6 mM concentration and CD aqueous solution with 5 mg/L concentration were prepared. Further these solutions were mixed so that the studied aqueous solutions contained CD with a fixed concentration of 5 mg/L and Cu²⁺, Ni²⁺, Co²⁺, Al³⁺, Cr³⁺ cations with a concentration varying from 0 to 6 with 1.5 mM increment. The concentration of NO₃⁻ anions directly depended on the concentration of cations and varied from 0 to 72 mM.

Thus, among the 3125 prepared samples there were 20 single-component solutions (containing one type of cation), 160 two-component solutions (containing any two types of cations), 640 three-component solutions (containing three types of cations simultaneously), 1280 four-component solutions (containing four types of cations simultaneously), and 1024 five-component solutions (containing five types of cations simultaneously). Aqueous solutions of CD with 5 mg/L concentration in the absence of ions were also studied.

3. PHOTOLUMINESCENCE SPECTROSCOPY OF AQUEOUS SOLUTIONS OF CARBON DOTS AND METAL SALTS

For all obtained solutions of CD and nitrates of metal salts, photoluminescence excitation-emission matrices were obtained on the Shimadzu RF-6000 spectrofluorimeter (Fig. 1). The signal was excited by radiation at 27 wavelengths: from 280 to 410 nm in steps of 5 nm. The spectra were recorded in the spectral range from 375 to 575 nm in increments of 1 nm. As examples, Fig. 2 shows the obtained excitation-emission photoluminescence matrices of an aqueous solution of CD with a concentration of 5 mg/L (Fig. 1a) and an aqueous solution of CD (5 mg/L) and salts of $Co(NO_3)_2 + Cr(NO_3)_3$ with concentrations of each salt of 6 mM (Fig. 2b).

As can be seen from the presented matrices, CD photoluminescence is excited with the highest intensity by radiation with a wavelength of 350 nm. The quantum yield of CD photoluminescence in water at a wavelength of 350 nm was measured using the reference dye [42]. It turned out to be $91.5 \pm 1.8\%$.



Fig. 1. (a) CD image obtained using TEM and (b) IR absorption spectra of CD evaporated from aqueous solution.



Fig. 2. Excitation-emission photoluminescence matrices of (a) an aqueous solution of CD with a concentration of 5 mg/L and (b) an aqueous solution of CD (5 mg/L) with salts of $Co(NO_3)_2 + Cr(NO_3)_3$ with concentrations of each salt of 6 mM.

3.1. The Effect of Ions Dissolved in Water on the Photoluminescence of Carbon Dots

Figure 3a shows the PL spectra of CD aqueous solutions in the presence of all the studied cations with a concentration of 6 mM. As can be seen from Fig. 3a, all the dissolved metal ions quench the CD PL to varying degrees. At the same time, the shape of the CD PL spectra does not change significantly when salts are added. Based on the data obtained it is possible to construct a series according to the degree of influence of the cations on the PL of the CD:

$$Cr^{3+} > Cu^{2+} > Co^{2+} > Al^{3+} > Ni^{2+}.$$

From Fig. 3b it follows that the degree of quenching carbon dots PL in water depends not only on the cation type but also on its concentration in the solution. This means that from the CD PL spectra it is possible not only to identify the type of dissolved ion, but also to determine its concentration in the solution. Thus, it is possible to develop a luminescent carbon nanosensor for heavy metal ions in water using the photoluminescence spectra of CD in multicomponent aqueous media. However, before solving the inverse 6-parametric problem of luminescence spectroscopy, i.e., learning how to determine the concentration of each ion from the PL spectra of CD in an aqueous solution containing 5 dissolved nitrates of heavy metals, it is necessary to understand whether the studied ions form complexes with CD as a result of their interaction in water. If complexes are formed as a result of the interaction of ions with the surface functional groups of the nanoparticles, then the CD will degrade over time as nanosensors.

3.2. Study of the Possibility of Complex Formation of Carbon Dots with Ions Dissolved in Water

In order to study the possible complex formation as a result of the interaction of CD with ions in water, kinetic curves of the decay of CD PL in the presence of each of the ions in solution were obtained. The registration was carried out by the system of highspeed analysis of the luminescence decay kinetics of substances Zolix OmniFluo 990 LPS. As an example, Fig. 4 shows the kinetic curve of PL decay of



Fig. 3. PL spectra of aqueous solutions of CD with a concentration of 5 mg/L: (a) without salts and with salts of Cu(NO₃)₂, Co(NO₃)₂, Ni(NO₃)₂, Al(NO₃)₃, Cr(NO₃)₃ with the same concentration of 6 mM; (b) with Cr(NO₃)₃ salt with different concentrations of Cr³⁺ from 0 to 6 mM. Excitation at 350 nm.

carbon dots in an aqueous solution in the absence and presence of cobalt ions.

The decaying part of all obtained kinetic curves was well approximated by two-exponential dependencies:

$$I(t) = \alpha_1 e^{-\frac{t}{\tau_1}} + \alpha_2 e^{-\frac{t}{\tau_2}},$$

where *I* is the intensity of PL, *t* is the time, α_1 , α_2 are the intensities of 1 and 2 types of photoluminophores, divided by characteristic photoluminescence lifetimes, τ_1 , τ_2 are the lifetimes of 1 and 2 types of photoluminophores.

Figure 5 shows the dependences of the lifetimes of the short-lived (a) and long-lived (b) components of the CD PL decay kinetics in solutions on the concentration of present cations in the concentration range from 0 to 6 mM. As can be seen from the obtained



Fig. 4. Kinetics of PL decay of CD solutions in the presence and absence of Co^{2+} ions.

PL decay kinetic curves, with an increase in the concentration of any of the studied ions, a decrease in the lifetime of CD PL is observed. Moreover, the degree of this decrease correlates quite satisfactorily with the degree of PL quenching. A decrease in the lifetime of CD PL means that the quenching of the photoluminescence of all the studied ions occurs according to a dynamic mechanism [42]. The dynamic type of the particle photoluminescence quenching, in turn, means that CD-ion complexes are not formed when ions interact with CD surface groups. Consequently, CD nanosensors of metal cations will not degrade over time in multicomponent aqueous solutions, i.e., they will be reusable.

4. APPLICATION OF MACHINE LEARNING METHODS FOR THE DEVELOPMENT OF A LUMINESCENT MULTIMODAL CARBON NANOSENSOR OF IONS

To develop a CD nanosensor capable of simultaneously determining the concentration of each of the Cu^{2+} , Ni^{2+} , Co^{2+} , Al^{3+} , Cr^{3+} , and NO_3^- ions in water using the CD luminescence spectra, i.e., to solve the inverse 6-parametric problem of luminescence spectroscopy, we used convolutional neural networks.

4.1. Initial Array of Spectral Data

As mentioned above, 3125 aqueous mixtures of the solutions of Cu^{2+} , Ni^{2+} , Co^{2+} , Al^{3+} , Cr^{3+} nitrates with cation concentration varying from 0 to 6 mM in concentration increment of 1.5 mM (while the concentration of NO_3^- anions varied in the range from 0 to 72 mM according to the changing cation concentrations) and CD with a fixed concentration of 5 mg/L were prepared. Of the 3125 samples prepared, there were 20 single-component solutions



Fig. 5. Dependences of the lifetime of the components of the CD PL decay kinetics on the concentration of cations present: (a) the first and (b) the second components.

(containing one type of cation), 160 two-component, 640 three-component, 1280 four-component, and 1024 five-component solutions (containing all five types of cations simultaneously).

The PL excitation-emission matrices of all the prepared CD and ions solutions were obtained (Fig. 2). The PL of the samples was excited by radiation at 27 wavelengths. Since the spectra were recorded in the spectral range from 375 to 575 nm in steps of 1 nm, the photoluminescence spectrum of each solution of CD and ions, when excited at one wavelength, contained 201 features. Each pattern fed to the input of the neural network was a tensor $[1 \times 27 \times 201]$, where the number of channels is in the first place, and the spatial dimensions of the image matrix (the number of excitation wavelengths and the number of PL features) are in the second place.

4.2. Preparation of the Spectral Dataset

To train the ANN, to prevent their overtraining, and to evaluate the results of use of the algorithms, the initial array of spectral data was randomly divided into training, validation and test sets in a ratio of 70 : 20 : 10, respectively. The training set was used directly to train the models; the validation set was used to ensure timely stopping of training (training was stopped if the mean squared error on the validation set did not decrease within 100 epochs); the test set was used to check the quality of the trained models on independent data. The spectral data in the sets did not overlap.

In order to avoid the influence of data splitting on the results of the ANN application, a five-fold crossvalidation was applied to the spectral sets. The initial data array was divided into training/validation/test sets 5 times. The results of using neural networks with five implementations of splitting into sets (within 5 folds) were averaged. In addition, to eliminate the influence of random initialization of the weights, for each of the 5 folds the ANN were trained 3 times, followed by averaging the results within each fold. Thus, the quality of the solution of the inverse problem of determining each of the six parameters by a network of a given configuration was evaluated on the basis of the results of 15 neural networks of this configuration. The statistical indicators of the solution of the problem for all the networks were averaged in each specific case.

The metrics used to evaluate the quality of the trained networks was the mean absolute error (MAE):

$$MAE = \frac{1}{N} \sum_{i=1}^{N} |y_i - \hat{y}_i|,$$

where N is the number of patterns, y_i is the real value of the target variable, \hat{y}_i is the prediction of the model.

4.3. Application of 2D Convolutional Neural Networks to Solve the Six-Parameter Inverse Problem of Photoluminescence Spectroscopy

The input patterns are the PL excitation-emission matrices, whose intensities in the neighbouring channels are strongly correlated, which was taken into account in the choice of the ANN architecture (Fig. 6). Two-dimensional convolutional networks (2D CNN) were chosen, which have proven themselves well for solving problems with data containing ordered correlated features, for example, images, optical spectra [6, 43]. The input to the neural network was provided by CD PL matrices representing a tensor of dimension $[1 \times 27 \times 201]$. The output of the convolutional layer with kernel size of 5, representing 3 activation maps, was connected to a fully connected layer (LeakyReLU activation function) (Fig. 6). The

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Fig. 6. 2D CNN architecture.

fully connected layer was connected to the network output (6 neurons, linear activation function).

The Adam gradient descent modification was used as the optimization algorithm, the learning rate was 0.001, the loss function was MSE, and the batch size was 64 examples. To prevent overtraining, L2 regularization with a regularization coefficient of 0.001 was applied. Training was performed on a 12th Generation Intel(R) Core(TM) i5-12400, 2.50 GHz CPU.

The application of 2D CNN to the obtained set of experimental spectral data provided the following mean absolute errors in determining the concentration of Cu²⁺, Ni²⁺, Co²⁺, Al³⁺, Cr³⁺, and NO₃⁻ ions on the test set: 0.99, 0.98, 0.9, 0.98, 0.24, and 2.78 mM, respectively (Fig. 7). The errors in determining the concentration of the ions on the training, validation and test data sets differ from each other within 10%, which indicates the stability of the solution of the studied inverse problem.

The results obtained show satisfactory accuracy for the determination of the concentration of selected ions in wastewater and process water [44–47], however, for the tasks of determining the concentration of ions in drinking water, the accuracy obtained is not sufficient: the concentration of heavy metal ions in water suitable for human consumption usually does not exceed 0.1 mM [48, 49].

5. APPROBATION OF THE DEVELOPED METHOD

To test the developed CD nanosensor of dissolved metal ions, recycled water from the mining and metallurgical plant of the Trans-Baikal Territory of the Russian Federation was used. The approbation consisted in a comparative analysis of the concentrations of metal cations present in circulating water, determined by an independent method—using X-ray fluorescence (XPF)—and two-dimensional convolutional neural networks (2D-CNN) trained on model aqueous solutions.

The Xenemetrix Genius IF LE X-ray photoluminescent energy dispersion spectrometer (X-ray source—X-ray tube, Rh anode, 50 kV, 50 W; detector-SDD LE silicon drift detector, resolution 125 ± 5 eV at 5.9 keV) was used to conduct a non-destructive qualitative and quantitative analysis of the technological aqueous medium composition. The operating voltage and current for the Rh tube were 16 kV and 10 mA, respectively. All XRF measurements were carried out three times in the air atmosphere with an accumulation time of 300 s each. The XRF spectrum of plant water is shown in Fig. 8.

CD were added to the studied circulating plant water so that the concentration of nanoparticles was 5 mg/L. A PL EEM of the plant technological aque-



Fig. 7. Mean absolute errors in determining ion concentration on test, training and validation datasets.



Fig. 8. XRF spectrum of technological plant water.



Fig. 9. PL excitation-emission matrix of technological plant water with the addition of CD with a concentration of 5 mg/L.

ous environment with CD was obtained (Fig. 9). The resulting matrix was fed to a convolutional neural network trained on the model solutions.

The concentrations of metal ions in the techno-

Table 1. The results of determining the ions concentration

 in plant process water with XRF and CNN

	XRF, mM	2D-CNN, mM
Cr^{3+}	1.96 ± 0.09	1.85
Co^{2+}	2.27 ± 0.07	2.31
Ni ²⁺	4.10 ± 0.10	4.02
Cu^{2+}	2.97 ± 0.01	3.00
Al^{3+}	0 ± 0	0

logical plant aqueous medium, obtained by XRF and using a neural network, are shown in Table 1.

A comparative analysis of metal ions concentrations in technological medium, determined by independent XRF and CNN methods, showed that the use of neural network approach ensures adequate operation of CD-based nanosensor determining qualitative and quantitative composition of technological aqueous media. It should be emphasized that the developed nanosensor can not only simultaneously determine the concentration of each ion, but also provides remote measurement of ion concentrations in real time.

6. CONCLUSIONS

As a result of the successful application of twodimensional convolutional neural networks to solve the inverse multiparameter problem of photoluminescent spectroscopy, a CD-based multimodal photoluminescent nanosensor was developed for the first time. It enables simultaneous measurement of the concentration of six ions: Cu²⁺, Ni²⁺, Co²⁺, Al³⁺, Cr³⁺, and NO₃⁻ in a multicomponent aqueous medium. The use of 2D-CNN provided simultaneous determination of the concentration of Cu²⁺, Ni²⁺, Co²⁺, Al³⁺, Cr³⁺, and NO₃⁻ ions with mean absolute errors of 0.85 \pm 0.01, 0.97 \pm 0.03, 0.67 \pm 0.06, 0.81 \pm 0.04, 0.26 \pm 0.01, and 2.03 \pm 0.09 mM, respectively.

A successful approbation of CD multimodal luminescent nanosensor was carried out in the process waters of a metallurgical plant. The accuracy of ion concentration determination with the nanosensor fully meets the requirements of process water and wastewater composition control. The developed CD nanosensor provides remote determination of ion concentrations in real time.

The approach proposed in this manuscript to solving inverse multiparameter problems of luminescent spectroscopy using artificial neural networks opens up broad prospects for creating a number of multimodal optical nanosensors based on various nanoparticles and nanocomplexes.

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CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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