

M. Mokliak¹, R. Ilnytskyi¹, L. Kaykan², Yu. Mazurenko^{2,3}, L. Turovska⁴,
M. Moiseienko³, V. Mokliak^{2,5}, V. Sheketa⁶

Neodymium Doped Copper Ferrite Nanocomposites as an Effective Magnetic Catalyst for the Organic Dyes Decomposition

¹Department of Applied Physics and Materials Science, Vasyl Stefanyk Carpathian National University, Ivano-Frankivsk, Ukraine; mariamoklyak@gmail.com

²Laboratory for Physics of Magnetic Films, G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, Kyiv, Ukraine; kaykan@nas.gov.ua, mazurenkoyus@nas.gov.ua, Mokliak_Volodymyr@nas.gov.ua

³Department of Medical Informatics, Medical and Biological Physics, Ivano-Frankivsk National Medical University, Ivano-Frankivsk, Ukraine; mmoiseyenko@ifnmu.edu.ua

⁴Department of Management and Business Administration, Faculty of Management,

Vasyl Stefanyk Carpathian National University, Ivano-Frankivsk, Ukraine; liliia.turovska@cnu.edu.ua

⁵Department of Physical and Mathematical Sciences, Ivano-Frankivsk National Technical University of Oil and Gas, Ivano-Frankivsk, Ukraine; volodymyr.mokliak@nung.edu.ua

⁶Department of Software Engineering, Ivano-Frankivsk National Technical University of Oil and Gas, Ivano-Frankivsk, Ukraine; vasyl.sheketa@nung.edu.ua

Neodymium-substituted copper ferrite nanoparticles with composition $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ ($x = 0.00\text{--}0.11$) were synthesized via the sol-gel autocombustion method and systematically analyzed for their structural, optical, and photocatalytic properties. X-ray diffraction combined with Rietveld refinement confirmed the formation of a dominant spinel ferrite phase with minor secondary phases, while Nd incorporation induced a reduction in crystallite size and an increase in lattice microstrain without disrupting the long-range spinel structure. Optical studies based on diffuse reflectance UV-Vis spectroscopy and Tauc analysis revealed direct allowed electronic transitions and a non-monotonic variation of the optical band gap (2.7–3.1 eV) as a function of Nd content, attributed to the combined effects of lattice distortion, defect states, and cation redistribution. Photocatalytic performance was evaluated through Congo Red degradation under light irradiation in the presence of H_2O_2 . Nd substitution significantly enhanced photocatalytic activity, with $\text{CuNd}_{0.09}\text{Fe}_{1.91}\text{O}_4$ showing the highest degradation efficiency (~96%), whereas the highest apparent rate constant (Langmuir-Hinshelwood model) was observed for $\text{CuNd}_{0.05}\text{Fe}_{1.95}\text{O}_4$. The results demonstrate that controlled Nd substitution effectively tunes the structural and electronic properties of CuFe_2O_4 , leading to improved photocatalytic performance and highlighting its potential for wastewater treatment applications.

Keywords: Spinel ferrites; Copper ferrite nanoparticles; Neodymium substitution; Nanocomposites; Water purification; Photocatalysis.

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Introduction

The increasing discharge of organic dyes from textile, paper, leather, and chemical industries poses a serious threat to aquatic ecosystems and human health due to their high toxicity [1], chemical stability, and resistance to conventional wastewater treatment processes [2–4]. Azo

dyes, such as Congo Red [5], are particularly problematic because of their complex aromatic structure and persistence in the environment. In this context, the development of efficient, low-cost, and recyclable photocatalysts for dye degradation has attracted considerable attention.

Spinel ferrites with the general formula MFe_2O_4

(M = divalent metal ion) have emerged as promising multifunctional materials owing to their chemical stability [6], tunable electronic structure [7], and magnetic properties, which enable facile separation and reuse [8]. Among them, copper ferrite (CuFe_2O_4) is of special interest due to its narrow band gap, visible-light absorption capability, and redox-active Cu and Fe cations [9, 10]. However, the photocatalytic efficiency of pristine CuFe_2O_4 is often limited by rapid electron–hole recombination and suboptimal charge carrier mobility, necessitating strategies to improve its performance.

Elemental substitution represents an effective approach to tailoring the structural electronic, and magnetic properties of spinel ferrites [7]. In particular, rare-earth ion substitution has been shown to significantly influence crystallite size, lattice strain, cation distribution, and defect density, thereby modifying optical absorption and charge carrier dynamics [11, 12]. Neodymium (Nd^{3+}), characterized by a large ionic radius and strong electronic polarization, can introduce localized lattice distortion and defect states when incorporated into the ferrite lattice [12]. These effects may enhance visible-light absorption, promote charge separation, and improve photocatalytic activity. Despite several reports on rare-earth-doped ferrites, systematic studies correlating Nd substitution, structural distortion, optical band structure, and photocatalytic performance in CuFe_2O_4 remain limited.

One way to improve photocatalytic activity is also the use of composite materials [13], which allows for effective modification of their electronic structure and band gap to change the behavior of optical absorption and charge carrier dynamics. In particular, the use of superparamagnetic catalytically active nanocomposites [14, 15] that are easily removed from the reaction medium under the influence of an external magnetic field. Furthermore, combining ferrite photocatalysts with hydrogen peroxide (H_2O_2) activate additional reactive oxygen species via photo-assisted Fenton-like processes, significantly enhancing degradation efficiency [16]. In such systems, the interaction between catalyst structure, electronic properties, and reaction kinetics plays a critical role in determining overall photocatalytic performance. Understanding these structure–property–activity relationships is essential for rational catalyst design.

In this work, Nd-substituted copper ferrite nanoparticles with composition $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ ($x = 0.00$ – 0.11) were synthesized using the sol–gel autocombustion method [12]. The effects of Nd incorporation on phase composition, crystallite size, lattice strain, and microstructure were systematically investigated using X-ray diffraction and electron microscopy. Optical properties were examined through diffuse reflectance UV–Vis spectroscopy, Tauc analysis, and differential optical methods to elucidate band gap evolution and defect-related absorption features [8, 16]. The photocatalytic activity of the synthesized ferrites was evaluated by Congo Red degradation under light irradiation in the presence of H_2O_2 , and the reaction kinetics were analyzed using the Langmuir–Hinshelwood model [8]. The study aims to establish clear correlations between Nd-induced structural and electronic modifications and the resulting photocatalytic performance, providing insights into the design of

efficient ferrite-based photocatalysts for wastewater treatment applications.

I. Materials and Methods

1.1. Synthesis of Nd-Substituted Copper Ferrite Nanoparticles

Nd-substituted copper ferrite nanoparticles with nominal composition $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ ($x = 0.00$ – 0.11) were synthesized using the sol–gel autocombustion method [17]. Analytical-grade iron(III) nitrate nonahydrate ($\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$), copper(II) nitrate trihydrate ($\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$), neodymium(III) nitrate hexahydrate ($\text{Nd}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$), and citric acid monohydrate ($\text{C}_6\text{H}_8\text{O}_7 \cdot \text{H}_2\text{O}$) were used as starting materials without further purification.

Stoichiometric amounts of the metal nitrates corresponding to the desired $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ compositions were dissolved separately in deionized water and then mixed under continuous magnetic stirring to obtain a homogeneous solution. Citric acid was added as a complexing agent and fuel, with the molar ratio of total metal cations to citric acid maintained at unity. The pH of the resulting solution was adjusted to approximately 7 by dropwise addition of a 25% aqueous ammonia solution, promoting effective chelation and gel formation [12].

The mixed solution was heated at moderate temperature under constant stirring until a viscous gel was formed. Further heating led to spontaneous autocombustion, yielding a voluminous, fine powder. The samples were labeled as F0 ($x = 0.00$) and N1, N3, N5, N7, N9, N11 corresponding to $x = 0.01, 0.03, 0.05, 0.07, 0.09, \text{ and } 0.11$, respectively. The obtained powders were subsequently used for structural, microstructural, and optical characterization.

1.2. Structural and Microstructural Characterization

Phase composition and crystal structure of the samples were examined by powder X-ray diffraction using an Empyrean diffractometer (Malvern Panalytical, UK) configured in the Bragg–Brentano reflection mode and employing $\text{Cu K}\alpha$ radiation with a wavelength of 1.5406 \AA . XRD data were collected over the angular range of $2\theta = 20^\circ$ – 90° using a step increment of 0.033° .

The morphology and chemical composition of the powder samples were examined using scanning electron microscopy (SEM) with a Tescan Vega-3 LMU microscope (TESCAN Brno, s.r.o., Czech Republic) equipped with a Bruker Nano XFlash 410M energy-dispersive X-ray spectrometry (EDX) detector.

For SEM observations, the powder samples were mounted on aluminum stubs using double-sided conductive carbon tape. The measurements were performed in high-vacuum mode ($\leq 0.018 \text{ Pa}$) using a motorized stage at an accelerating voltage of 15 keV .

EDX analysis was carried out on selected representative areas of the samples with lateral dimensions on the order of several micrometers, corresponding to the SEM observation regions, at a magnification of approximately $5000\times$ and an accelerating voltage of 15 keV . This approach ensured averaging over multiple

particles and minimized the influence of local compositional fluctuations.

Data acquisition and processing were performed using the ESPRIT 1.9 software package (Bruker Nano GmbH, Berlin, Germany).

1.3. Optical and Photocatalytic Studies

Optical absorption measurements were carried out using a UV/VIS SPECORD 210 PLUS double-beam UV–Vis spectrophotometer (Analytik Jena AG, Germany), operating in the wavelength range from 185 to 1200 nm. The double-beam configuration enabled simultaneous acquisition of sample and reference signals, ensuring high measurement stability and accurate baseline correction. Instrument control, data acquisition, and processing were performed using ASpect UV software with the 21 CFR Part 11 Compliance module (Analytik Jena AG, Germany).

Photocatalytic degradation experiments were performed using $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ nanoparticles as the catalyst in the presence of hydrogen peroxide. The catalyst loading was fixed at 0.5 g L^{-1} for all experiments. Hydrogen peroxide (H_2O_2) was added to the reaction mixture at a concentration of 250 mmol L^{-1} to promote the generation of reactive oxygen species.

Congo Red (CR) was used as the model organic dye. The working dye concentration was 10 mg L^{-1} for all $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ –CR systems. All photocatalytic tests were carried out under identical conditions to ensure reliable comparison of degradation efficiency across different Nd-substituted samples.

II. Results and discussion

2.1. Structural and Morphological Studies

Figure 1(a) displays the X-ray diffraction (XRD) patterns of the synthesized $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ nanoparticle series. All compositions exhibit well-defined diffraction peaks that can be indexed to a cubic spinel structure with space group $\text{Fd}3\text{m}$ [18].

Figure 1 demonstrates that all $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ samples are dominated by a spinel-type diffraction pattern, where the main reflections indexed as (111), (220), (311), (400), (422), (511), and (440) are well reproduced by the Rietveld fits (Y_{calc}) and the difference curves ($Y_{\text{obs}} - Y_{\text{calc}}$) remain close to the baseline, indicating an overall reliable description of the diffraction profiles across the series. The refinement indicates that the primary crystalline phase is the CuFe_2O_4 spinel, while minor secondary phases (CuFeO_2 and CuO) are also present.

Quantitatively (Table 1), the spinel fraction increases from 81.81% (CuFe_2O_4) to ~85–87% at low Nd contents ($x = 0.01$ – 0.05), suggesting improved formation of the ferrite phase, whereas at higher substitution levels the spinel fraction slightly decreases to ~86.56–86.57% ($x = 0.09$ – 0.11), which may reflect a solubility limit and strain-driven segregation into CuO and CuFeO_2 [19]. In parallel, the lattice parameter a varies only slightly (8.3784–8.3820 Å) with a small expansion at intermediate x ($x = 0.03$ – 0.07), consistent with Nd-related local lattice distortion without large peak shifts at these low substitution levels. The microstructural parameters evolve

more strongly: the crystallite size decreases from 37.6 nm to ~25–31 nm (minimum at $x = 0.09$, ~25.26 nm), while the microstrain increases from 0.003151 to ~0.00399–0.003996 and then saturates, indicating enhanced lattice defect density and suppressed crystallite growth in the Nd-substituted samples.

The preserved spinel peak set together with modest changes in a but pronounced changes in size and strain supports the conclusion that Nd addition primarily affects the structure through microstructural disorder and local distortions while retaining the long-range spinel framework. These trends provide a structural basis for the optical behavior, since increased strain/disorder and reduced crystallite size modify the absorption edge and contribute to the non-monotonic $E_g(x)$ dependence [20].

Figure 2 shows FESEM images of $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ samples ($x = 0.00, 0.03, 0.07, \text{ and } 0.11$), revealing an agglomerated microstructure composed of irregularly shaped particles for all compositions. Such agglomeration, typical for chemically synthesized ferrites, arises from magnetic dipole–dipole interactions and partial sintering during combustion [21]. The undoped CuFe_2O_4 sample consists of relatively larger agglomerates with plate-like and fractured features, while Nd-substituted samples exhibit more fragmented aggregates composed of finer structural units, indicating suppression of crystallite growth. This trend is consistent with XRD results showing reduced crystallite size and increased microstrain upon Nd incorporation. At the highest Nd content ($x = 0.11$), the microstructure remains highly agglomerated but becomes more compact, which may be related to increased defect density and partial formation of secondary phases. FESEM observations confirm that Nd substitution primarily induces nanoscale structural refinement within agglomerated particles, supporting the structure–property relationships discussed in the optical analysis section.

2.2. Optical Studies

In spinel ferrites, the optical band gap is determined by electronic transitions involving O 2p states in the valence band and transition-metal 3d states [22] in the conduction band, and is highly sensitive to cation substitution, lattice strain, and nanoscale structural disorder. In $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ ferrites, partial replacement of Fe^{3+} by Nd^{3+} introduces local lattice distortion due to the large ionic radius of Nd^{3+} , alters cation distribution within octahedral sites, and modifies the degree of p–d orbital hybridization, all of which directly affect the optical absorption edge [23, 24].

Diffuse reflectance UV–Vis spectroscopy was used to quantify these effects through determination of the optical band gap energy E_g . The absorption behavior was analyzed using the Tauc relation [8],

$$(ahv)^n = A(hv - E_g),$$

where α is the absorption coefficient, $h\nu$ is the photon energy, A is a proportionality constant, and n depends on the nature of the electronic transition.

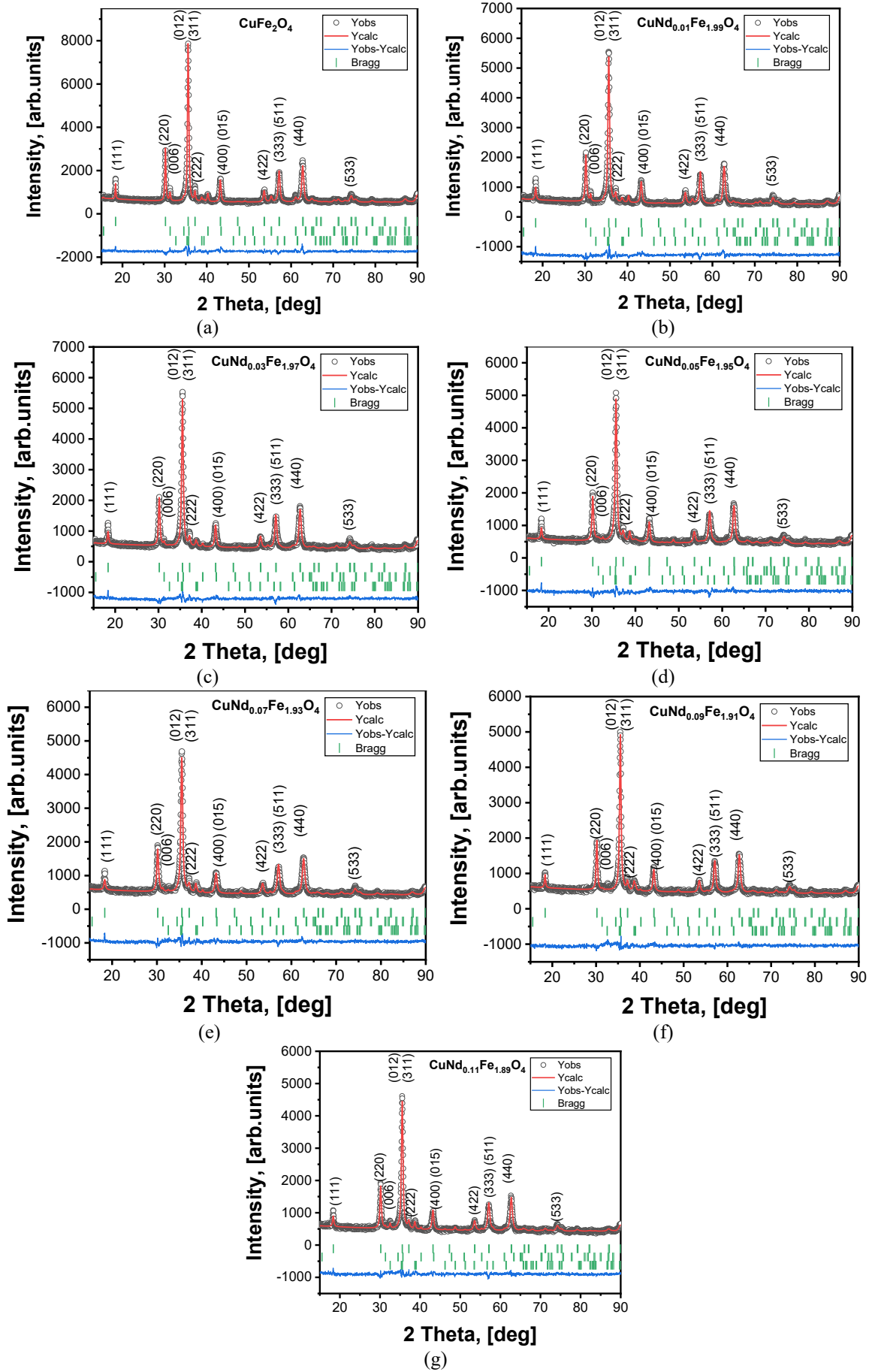


Fig. 1. Rietveld refinement profile of XRD data of as prepared $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ samples. The dots correspond to the experimental data and the solid line is for the Rietveld refinement fit. The lower curve is the difference between the observed and calculated at each step.

Table 1.

Phase Composition and Structural Parameters of $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ Nanoparticles

Sample	CuFe ₂ O ₄			CuFeO ₂ , %	CuO, %	Lattice strain
	Phase, %	a, Å	Crystallite size, nm			
CuFe ₂ O ₄	81.81	8.3798	37.6	14.28	3.91	0.00315
CuNd _{0.01} Fe _{1.99} O ₄	85.54	8.3784	31.53	10.66	3.81	0.00381
CuNd _{0.03} Fe _{1.97} O ₄	87.49	8.3812	30.45	7.19	5.32	0.00388
CuNd _{0.05} Fe _{1.95} O ₄	87.47	8.382	27.06	6.67	6.27	0.00396
CuNd _{0.07} Fe _{1.93} O ₄	86.75	8.382	26.54	6.19	7.05	0.00399
CuNd _{0.09} Fe _{1.91} O ₄	86.57	8.3805	25.26	5.8	7.63	0.00400
CuNd _{0.11} Fe _{1.89} O ₄	86.56	8.3799	26.09	6.49	6.94	0.00399

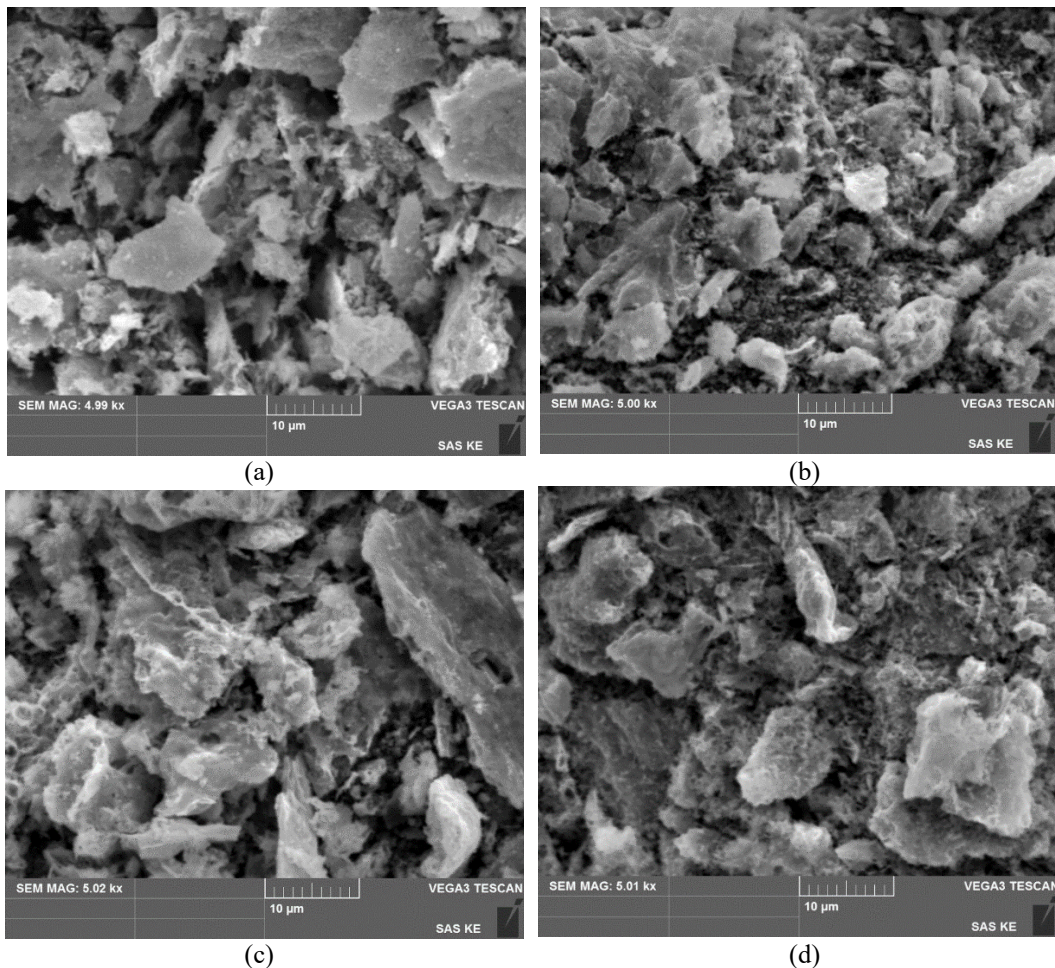


Fig. 2. FESEM images for 0.00 (a), 0.03 (b), 0.07 (c) and 0.11 (d) of $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ samples.

Figure 3 shows the Tauc plots for $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ ferrites, confirming that the dominant optical absorption edge can be treated as a direct allowed transition for all compositions, and reveals a non-monotonic dependence of the optical band gap E_g on Nd content. The undoped CuFe_2O_4 sample exhibits $E_g = 2.86$ eV, consistent with nanoscale copper ferrites, while low Nd^{3+} substitution ($x = 0.01\text{--}0.05$) leads to a slight band-gap reduction (2.76–2.82 eV) due to defect-related band tailing caused by lattice distortion from the larger Nd^{3+} ionic radius. As summarized in Table 1, low-Nd-substitution compositional range is characterized by a pronounced reduction in crystallite size (from ~37.6 to ~30 nm) and increasing microstrain. At intermediate Nd contents

($x \approx 0.07\text{--}0.10$), the crystallite size reaches a minimum (~26–27 nm) and microstrain reaches its maximum, accompanied by slight lattice expansion, resulting in a sharp increase of E_g up to ~3.10 eV. This behavior reflects the combined influence of size reduction, enhanced lattice strain, and modified cation distribution, which alters O 2p–Fe 3d hybridization and widens the band gap [25]. At higher Nd concentrations, the emergence of secondary phases (CuO and CuFeO_2) and increased structural disorder counteract these effects, leading to a subsequent decrease in E_g .

For comparative purposes across the series, E_g was operationally extracted from the high-energy linear region assuming direct allowed transition; additional sub-band

features observed in differential analysis reflect defect-related states and do not contradict the comparative E_g definition. Figure 4 illustrates the optical absorption behavior of the CuFe_2O_4 sample analyzed using both the conventional Tauc method and a differential approach [26, 27]. In Figure 4a, the Tauc plot $(\alpha h\nu)^2$ versus $h\nu$ exhibits several quasi-linear regions rather than a single well-defined absorption edge. Extrapolation of these regions yields apparent transition energies at approximately 1.57 eV, 2.14 eV, and 2.99 eV, suggesting that more than one absorption mechanism contributes to the optical

response and that CuFe_2O_4 cannot be fully described by a single direct band-to-band transition.

To further resolve these features, Figure 4b shows the first derivative $d(\ln(\alpha h\nu))/d(h\nu)$. Distinct maxima occur at about 1.57 eV, 2.14 eV, 2.35 eV, and 2.65 eV, indicating multiple absorption-related features. The lowest-energy feature (~ 1.57 eV) may be associated with defect- or disorder-induced localized states typical for nanoscale ferrites, while the features in the 2.1–2.7 eV range can be attributed to additional electronic transitions and defect-assisted absorption involving O 2p and transition-metal 3d

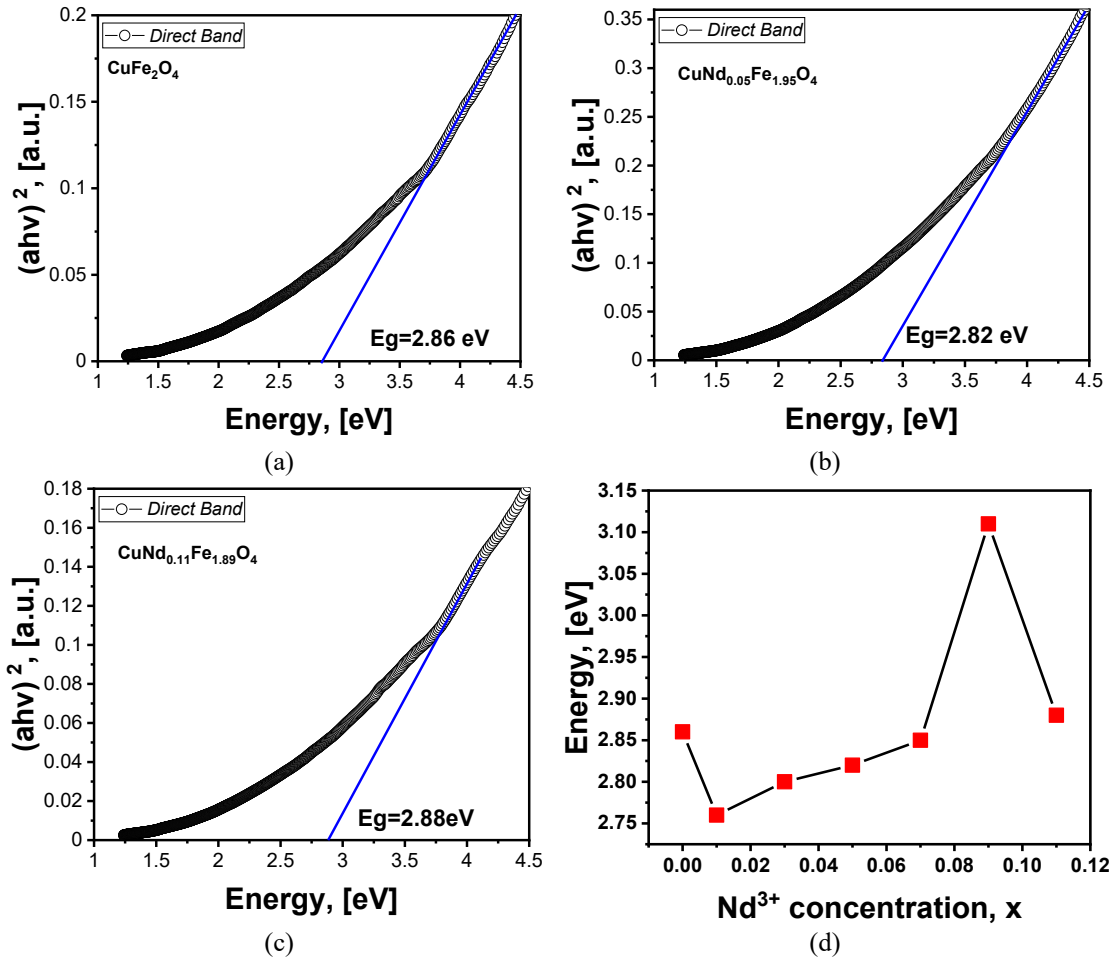


Fig. 3. Tauc plot for determining the optical band gap (E_g) for $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ samples with direct allowed transitions.

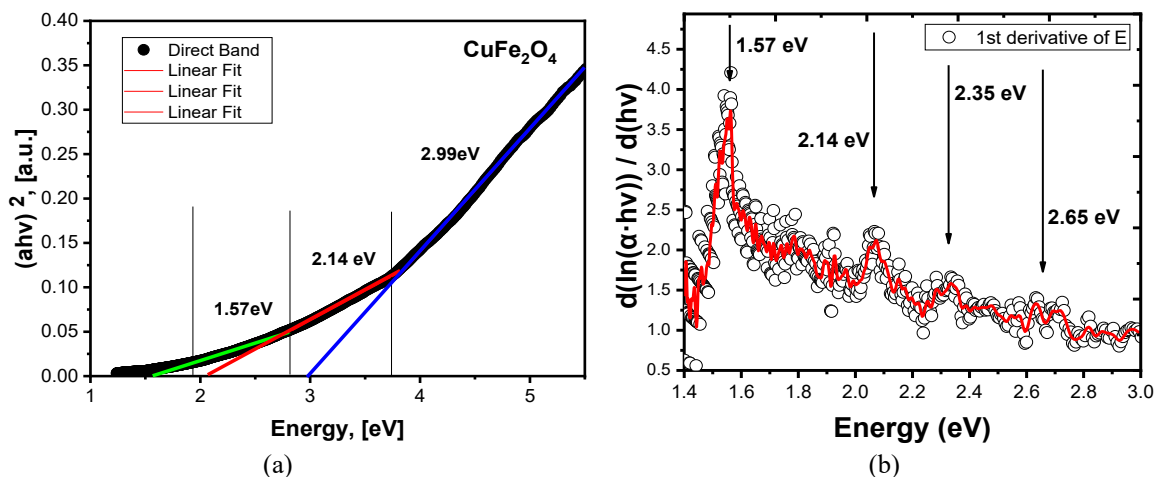


Fig. 4. Differential plot for CuFe_2O_4 sample.

states.

The highest-energy transition near ~ 2.99 eV, extracted from the high-energy linear region of the Tauc plot, represents the apparent high-energy absorption edge, which is slightly higher than the effective E_g extracted in Figure 3 due to the influence of sub-band absorption and band tailing on the Tauc analysis. The coexistence of lower-energy features highlights the influence of defect states, cation disorder, and lattice imperfections on the optical response of ferrite nanoparticles [28].

The combined Tauc and differential analyses indicate a multi-feature absorption behavior where band-edge transitions coexist with sub-band absorption, explaining the broad absorption edge observed in UV-Vis spectra.

2.3. Photocatalytic Studies

Figure 5 presents the time-dependent UV-Vis absorption spectra of Congo Red in the presence of $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ photocatalysts under light irradiation. For all samples, the characteristic absorption band of Congo Red in the visible region progressively decreases with irradiation time, indicating continuous degradation of the dye molecules. No noticeable shift in the absorption maximum is observed, suggesting that the degradation proceeds primarily through destruction of the chromophoric structure [29] rather than simple molecular transformation.

The undoped CuFe_2O_4 sample (Figure 5a) exhibits a

gradual decrease in absorbance, reflecting moderate photocatalytic activity. Upon Nd substitution, a more pronounced reduction in absorbance intensity is observed, particularly for $\text{CuNd}_{0.03}\text{Fe}_{1.97}\text{O}_4$ and $\text{CuNd}_{0.07}\text{Fe}_{1.93}\text{O}_4$ (Figure 5b, c), indicating enhanced photocatalytic efficiency. This improvement is consistent with the structural and optical modifications induced by Nd incorporation [30], such as reduced crystallite size, increased lattice strain, and altered electronic structure, which can facilitate charge carrier generation and separation.

Figure 6a compares the photocatalytic performance of pure and Nd-substituted copper ferrites through the normalized concentration ratio C/C_0 as a function of irradiation time. All samples exhibit a continuous decrease in C/C_0 after light exposure, confirming effective photocatalytic degradation of Congo Red. The undoped CuFe_2O_4 (F0) shows a moderate degradation rate, reaching a removal efficiency of about 78.2% after 180 min. Nd substitution leads to a clear enhancement in photocatalytic activity, with faster decay of C/C_0 observed for most doped compositions. In particular, samples with intermediate Nd contents (N5 and N9) display the most pronounced degradation behavior, consistent with the stronger absorbance decay observed in Figure 5.

The reaction kinetics were analyzed using a Langmuir-Hinshelwood model [7], as shown in Figure 6b, where linear relationships between $\ln(C_0/C)$ and



Fig. 5. Time-dependent UV-Vis absorption spectra of (a) CuFe_2O_4 , (b) $\text{CuNd}_{0.03}\text{Fe}_{1.97}\text{O}_4$, (c) $\text{CuNd}_{0.07}\text{Fe}_{1.93}\text{O}_4$, and (d) $\text{CuNd}_{0.11}\text{Fe}_{1.89}\text{O}_4$ nanoparticles. The decrease in absorbance intensity over time indicates the photocatalytic degradation efficiency of the samples under light irradiation.

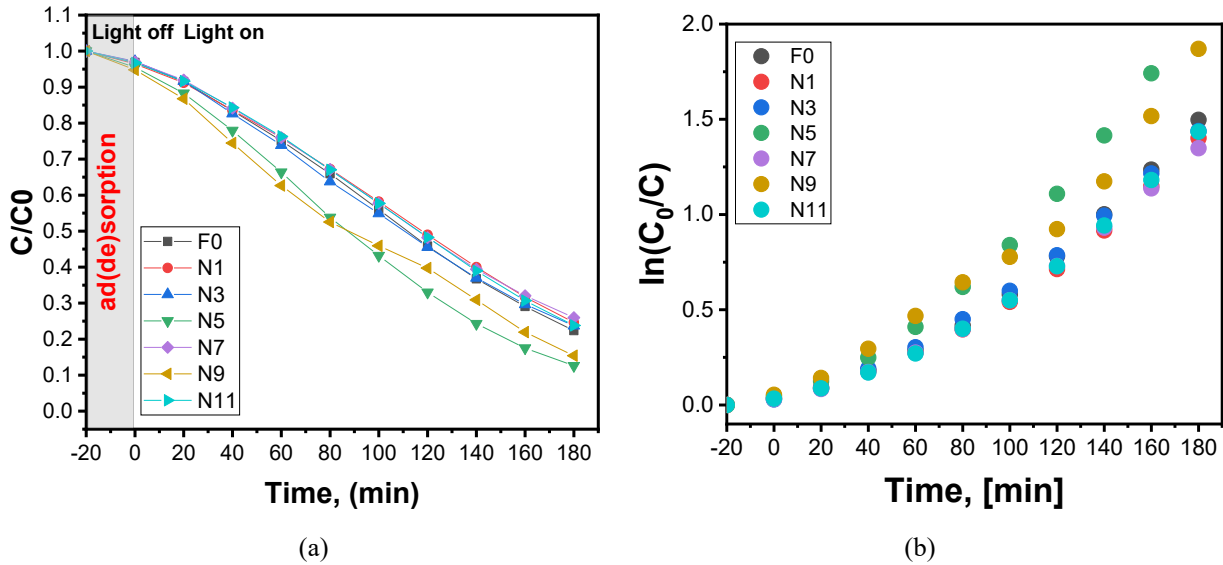


Fig. 6. Photocatalytic performance and kinetic study of Congo Red degradation: (a) Variation of C/C_0 as a function of irradiation time; (b) Pseudo-first-order kinetic plots of $\ln(C_0/C)$ versus time for the pure (F0) and Neodymium-substituted (N1–N11) copper ferrite samples.

Table 2. Langmuir–Hinshelwood kinetic parameters for Congo Red photocatalytic degradation over $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ samples, where k_{L-H} is the apparent pseudo-first-order rate constant, R^2 is the linear fit coefficient, t is the irradiation time, and K_{max} is the maximum degradation efficiency.

Sample	$k_{L-H} \times 10^{-2}, \text{min}^{-1}$	R^2	t, min	$K_{max}, \%$
CuFe_2O_4	0.00932	0.96	180	78.20
$\text{CuNd}_{0.01}\text{Fe}_{1.99}\text{O}_4$	0.00867	0.96	180	80.66
$\text{CuNd}_{0.03}\text{Fe}_{1.97}\text{O}_4$	0.00870	0.96	180	81.28
$\text{CuNd}_{0.05}\text{Fe}_{1.95}\text{O}_4$	0.01260	0.96	180	84.71
$\text{CuNd}_{0.07}\text{Fe}_{1.93}\text{O}_4$	0.00816	0.97	180	88.31
$\text{CuNd}_{0.09}\text{Fe}_{1.91}\text{O}_4$	0.01185	0.97	180	95.93
$\text{CuNd}_{0.11}\text{Fe}_{1.89}\text{O}_4$	0.00906	0.97	180	88.51

irradiation time are obtained for all samples. The high correlation coefficients ($R^2 \approx 0.96\text{--}0.97$) listed in Table 2 confirm that the photocatalytic degradation of Congo Red follows pseudo-first-order kinetics over the investigated time range. The apparent rate constants (k_{L-H}) further quantify the effect of Nd substitution. Compared to CuFe_2O_4 ($k = 0.00932 \times 10^{-2} \text{ min}^{-1}$), a noticeable increase in the rate constant is observed for $\text{CuNd}_{0.05}\text{Fe}_{1.95}\text{O}_4$ ($0.01260 \times 10^{-2} \text{ min}^{-1}$) and $\text{CuNd}_{0.09}\text{Fe}_{1.91}\text{O}_4$ ($0.01185 \times 10^{-2} \text{ min}^{-1}$), which also show high degradation efficiencies of 84.7% and 95.9%, respectively.

The non-monotonic dependence of both the kinetic constant and maximum degradation efficiency on Nd content reflects the competing effects of structural and electronic modifications induced by Nd incorporation [31]. As discussed in the structural and optical sections, moderate Nd substitution reduces crystallite size, increases lattice strain, and modifies the band structure, which can enhance charge carrier generation and suppress electron–hole recombination. These factors collectively improve photocatalytic efficiency for intermediate Nd concentrations. At higher Nd content (N11), although substantial degradation ($\approx 88.5\%$) is still achieved, the slight decrease in k_{L-H} suggests that excessive structural disorder and the presence of secondary phases may introduce recombination centers, partially counteracting

the beneficial effects.

The results demonstrate that Nd substitution effectively tunes the photocatalytic activity of CuFe_2O_4 , with $\text{CuNd}_{0.09}\text{Fe}_{1.91}\text{O}_4$ exhibiting the optimal balance between structural disorder and electronic efficiency, leading to the highest Congo Red degradation rate under the studied conditions.

Conclusions

Nd-substituted copper ferrite nanoparticles with composition $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ ($x = 0.00\text{--}0.11$) were successfully synthesized via the sol–gel autocombustion method, and their structural, optical, and photocatalytic properties were systematically investigated. X-ray diffraction and Rietveld refinement confirmed the formation of a dominant spinel ferrite phase for all compositions, with minor amounts of CuO and CuFeO_2 as secondary phases. Nd incorporation did not disrupt the long-range spinel structure but induced significant microstructural changes, including a pronounced reduction in crystallite size and an increase in lattice microstrain, reaching a maximum at intermediate Nd contents.

Optical studies based on diffuse reflectance UV–Vis

spectroscopy and Tauc analysis revealed direct allowed electronic transitions for all samples and a non-monotonic dependence of the optical band gap on Nd concentration. The band gap varied within the range of approximately 2.7–3.1 eV and was governed by the interaction between crystallite size reduction, lattice strain, defect-related band tailing, and modified O 2p–Fe 3d hybridization. Differential optical analysis further demonstrated that the optical response of CuFe_2O_4 consists of multiple absorption contributions, highlighting the role of defect- and disorder-related sub-band states.

Photocatalytic performance was evaluated through the degradation of Congo Red under light irradiation in the presence of H_2O_2 . Nd substitution significantly enhanced the photocatalytic activity compared to undoped CuFe_2O_4 . The degradation process followed the Langmuir–Hinshelwood pseudo-first-order kinetic model with high correlation coefficients. Among the investigated compositions, $\text{CuNd}_{0.09}\text{Fe}_{1.91}\text{O}_4$ exhibited the highest photocatalytic efficiency (~96%), whereas the highest apparent rate constant was observed for $\text{CuNd}_{0.05}\text{Fe}_{1.95}\text{O}_4$. This behavior is attributed to the optimal balance between structural disorder, electronic structure modification, and suppression of charge carrier recombination. At higher Nd contents, excessive disorder and secondary phase formation partially reduced the photocatalytic performance.

The results demonstrate that controlled Nd substitution is an effective strategy for tuning the structure and electronic properties of CuFe_2O_4 , leading to substantially improved photocatalytic efficiency. These findings highlight the potential of Nd-substituted copper ferrites as efficient and magnetically recoverable photocatalysts for the degradation of organic pollutants in

wastewater treatment applications.

Data Availability Statement:

Data is contained within the article.

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Mokliak Mariia – PhD Student, Department of Applied Physics and Materials Science;

Kaykan Larysa – Doctor of Physical and Mathematical Sciences, Senior Researcher, Leading Research Scientist at the Laboratory for Physics of Magnetic Films;

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Turovska Liliia – Candidate of Chemical Sciences (Ph.D), Vice-Rector for Research and International Affairs;

Moiseienko Mykola – Doctor of Biological Sciences, Professor, Head of the Department of Medical Informatics, Medical and Biological Physics;

Mokliak Volodymyr – Doctor of Physical and Mathematical Sciences, Professor of the Department of Physical and Mathematical Sciences, Head of Laboratory for Physics of Magnetic Films;

Sheketa Vasyl – Doctor of Technical Sciences, Professor, Professor of the Department of Software Engineering.

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М. Мокляк¹, Л. Кайкан², Ю. Мазуренко^{2,3}, Л. Туровська⁴, М. Мойсеєнко³,
В. Мокляк^{2,5}, В. Шекета⁶

Наноккомпозити на основі мідного фериту заміщеного неодимом, як ефективний магнітний каталізатор для деградації органічних барвників

¹Кафедра прикладної фізики та матеріалознавства, Карпатський національний університет імені Василя Стефаника, Івано-Франківськ, Україна, mariamoklyak@gmail.com

²Лабораторія фізики магнітних плівок, Інститут металофізики імені Г.В. Курдюмова НАН України, Київ, Україна; kavkan@nas.gov.ua, mazurenkoyus@nas.gov.ua, Mokliak_Volodymyr@nas.gov.ua

³Кафедра медичної інформатики, медичної та біологічної фізики, Івано-Франківський національний медичний університет, Івано-Франківськ, Україна, mmoisevenko@ifnmu.edu.ua;

⁴Кафедра менеджменту та бізнес-адміністрування, факультет менеджменту, Карпатський національний університет імені Василя Стефаника, Івано-Франківськ, Україна; lilia.turovska@cnu.edu.ua

⁵Кафедра фізико-математичних наук, Івано-Франківський національний технічний університет нафти і газу, Івано-Франківськ, Україна; volodymyr.mokliak@nung.edu.ua

⁶Кафедра інженерії програмного забезпечення, Івано-Франківський національний технічний університет нафти і газу, Івано-Франківськ, Україна; vasyl.sheketa@nung.edu.ua

Неодим-заміщені наночастинки мідного фериту складу $\text{CuNd}_x\text{Fe}_{2-x}\text{O}_4$ ($x = 0.00\text{--}0.11$) були синтезовані методом золь-гель автогоріння та досліджено їхні структурні, оптичні й фотокаталітичні властивості. Рентгенівська дифракція в поєднанні з уточненням Рітвельда підтвердила утворення домінуючої фази шпінельного фериту з незначними вторинними фазами, тоді як включення Nd викликало зменшення розміру кристалітів та збільшення мікродеформації ґратки без руйнування далекого порядку шпінельної структури. Оптичні дослідження на основі UV–Vis спектроскопії та аналізу Така виявили прямі дозволені електронні переходи й немонотонну зміну ширини оптичної забороненої зони (2.7–3.1 eV) зі зростанням вмісту Nd, що зумовлено сукупною дією спотворення ґратки, дефектних станів і перерозподілу катіонів. Фотокаталітичну ефективність оцінювали за деградацією барвника Конго червоний під дією світлового опромінення у присутності H_2O_2 . Заміщення Nd значно підвищило фотокаталітичну активність, зразок $\text{CuNd}_{0.09}\text{Fe}_{1.91}\text{O}_4$ показав найвищу ефективність деградації (~96%), тоді як найвища видима константа швидкості (модель Ленгмюра-Хіншелвуда) спостерігалася для $\text{CuNd}_{0.05}\text{Fe}_{1.95}\text{O}_4$. Результати показують, що контрольоване заміщення Nd ефективно змінює структурні та електронні властивості CuFe_2O_4 , що призводить до покращення фотокаталітичної активності та підкреслює його потенціал для застосування в очищенні води.

Ключові слова: шпінельні ферити; наночастинки мідного фериту; заміщення неодимом; наноккомпозити; очищення води; фотокаталіз.