

EFFECT OF THE SYNTHESIS METHOD ON THE STRUCTURAL PROPERTIES OF NANOCOMPOSITES FOR MEDICAL APPLICATIONS

Avramenko V.V.¹, Murlanova T.V.^{1,2}, Furtat I.M.¹, Meinusch R.², Vakuliuk P.V.¹, Smarsly B.², Pryshchepa O.³, Pomastowski P.³

¹ National University of Kyiv-Mohyla Academy, Ukraine, viktoria.avramenko@ukma.edu.ua

² Institute of Physical Chemistry, Justus Liebig University, Giessen, Germany.

³ Institute of Advanced Studies, Centre for Modern Interdisciplinary Technologies, Nicolaus Copernicus University in Torun, Torun, Poland

Antibiotic resistance represents one of the key threats to modern healthcare, necessitating the development of alternative approaches to the discovery and design of novel effective antimicrobial agents [1]. The application of nanotechnology enables the development of efficient delivery systems for biologically active substances [2]. The current challenge of limited efficacy of conventional antimicrobial agents against resistant bacterial strains and biofilms can be addressed through the development of advanced silica-based nanocomposite materials with immobilized antimicrobial agents, capable of enhancing the effectiveness against pathogens characterized by resistance to most commonly used antimicrobial agents.

The aim of the study was to synthesize silica-based nanocomposites with immobilized Tinidazole, a nitroimidazole derivative active against anaerobic bacteria and protozoa [3]. Given that the selection of an optimal synthesis strategy is critically important, two approaches were compared: the aqueous method, which involved adsorption of the substance from solution followed by vacuum drying, and the mechanochemical method, implemented through mechanical activation of the component mixture in a ball mill.

To evaluate the effect of the synthesis route on the structural properties of the resulting nanocomposites, the physicochemical characteristics obtained by both methods were compared. The N₂ adsorption–desorption isotherms of the initial silica and the resulting nanocomposites containing Tinidazole, synthesized by both the aqueous and mechanochemical methods, at different weight percentages correspond to type IV according to the IUPAC classification, exhibiting an H3 hysteresis loop [4]. This indicates that all samples possess a mesoporous structure.

Upon immobilization of Tinidazole, nanocomposites obtained by both the aqueous and mechanochemical methods demonstrate a decrease in specific surface area accompanied by an increase in pore volume compared to the initial silica (220 m²/g and 0.8 cm³/g, respectively), attributed to the adsorption of Tinidazole molecules onto the active sites of the carrier and the formation of a more loosely packed structure with a well-developed interparticle void network. For the aqueous method, the specific surface area decreased to 220, 180, and 130 m²/g at 4, 8, and 12% Tinidazole content, respectively, with pore volumes of 1.3, 1.2, and 1.2 cm³/g. For the mechanochemical method, the specific surface area values were 180, 170, and 145 m²/g at the same Tinidazole content, with pore volumes of 1.2, 1.2, and 1.4 cm³/g.

Analysis of the cumulative pore volume curves calculated using the NLDFT model reveals a distinct difference between the two routes: the aqueous method demonstrates a nonlinear behavior without a clear correlation between Tinidazole content and total pore volume, whereas the mechanochemical method exhibits a consistent and nearly proportional increase with increasing Tinidazole percentage. Compared to the initial silica, which exhibits a pore size distribution in the range of 3 – 10 nm, nanocomposites obtained by the aqueous method show a pronounced peak at approximately 25 nm, while those synthesized by the mechanochemical method reveal a peak shifted to approximately 40 nm, indicating a more pronounced restructuring of the porous structure with a predominance of larger pores.

Thus, the mechanochemical method demonstrates superior control over the structural properties of the resulting nanocomposites, providing a more consistent and reproducible porous structure compared to the aqueous method, which is critical for the reproducible preparation of silica-based drug delivery systems with predictable release characteristics.

1. Colilla M., Vallet–Regí M. Organically Modified Mesoporous Silica Nanoparticles against Bacterial Resistance. – *Chemistry of materials*. – 2023. – V.35.I.21. – P.8788–8805.
2. Ali A, Ali S.R., Hussain R., et al. Comparative study of silica and silica–decorated ZnO and ag nanocomposites for antimicrobial and photocatalytic applications. – *Scientific reports*. – 2025. – V.15.I.1. – P.5010.
3. Rams T.E., Sautter J.D., van Winkelhoff A.J. Comparative In Vitro Resistance of Human Periodontal Bacterial Pathogens to Tinidazole and Four Other Antibiotics. – *Antibiotics (Basel, Switzerland)*. – 2020. – V.9.I.2. – P.68.
4. Thommes M., Kaneko K., Neimark A.V., Olivier J.P., Rodriguez–Reinoso F., Rouquerol J., Sing K.S.W. Physisorption of gases, with special reference to the evaluation of surface area and pore size distribution (IUPAC Technical Report). – *Pure and Applied Chemistry*. – 2015. – V.87. – P.1051–1069.

POLYLACTIC ACID-COATED COPPER OXIDE-SILICA NANOPARTICLES AS A COST-EFFECTIVE ALTERNATIVE TO SILVER-BASED ANTIMICROBIAL MATERIALS

*Bespalko O.V.¹, Vakuliuk P.V.¹, Furtat I.M.¹, Pryshchepa O.², Smarsly B.⁴,
Kozakevych R.B.³, Pomastowski P.²*

¹National University of Kyiv-Mohyla Academy, o.bespalko@ukma.edu.ua

²Centre for Modern Interdisciplinary Technologies, Nicolaus Copernicus University in Torun,
Torun, Poland,

³Chuiko Institute of Surface Chemistry National Academy of Sciences of Ukraine,

⁴Institute of Physical Chemistry, Justus Liebig University, Giessen, Germany

The escalating threat of antimicrobial resistance (AMR) and the high cost of silver (Ag)-based nanomaterials have intensified the search for affordable, efficient, and sustainable alternatives [1, 2]. Copper oxide (CuO) has emerged as a promising candidate due to its low cost, broad-spectrum activity, and compatibility with inorganic supports [3, 4]. Recent studies have demonstrated that CuO-based composites can achieve antimicrobial efficacy through reactive oxygen species generation while offering significant economic advantages over silver—copper is priced at approximately \$3.50 per pound compared to \$400 per pound for silver [5]. Polylactic acid (PLA) functionalization offers a strategy to tailor surface chemistry and introduce biodegradability [6, 7], yet the impact of PLA on the antimicrobial performance of CuO-based systems relative to Ag-based counterparts remains poorly understood. In this work, we systematically evaluate the antimicrobial activity of fumed silica nanocomposites functionalized with either silver (SiO₂–Ag) or copper oxide (SiO₂–CuO), before and after PLA coating, to determine whether PLA-modified CuO can serve as a cost-effective alternative without compromising efficacy.

All materials were characterized by X-ray photoelectron spectroscopy (XPS) and nitrogen physisorption to confirm successful PLA attachment and preservation of the mesoporous architecture. XPS analysis of SiO₂–Ag–PLA and SiO₂–CuO–PLA showed characteristic ester-related C 1s components (C–O, O–C=O) and attenuation of inorganic signals, consistent with a conformal polymer overlayer of a few nanometres. Importantly, the Ag 3d and Cu 2p core-level spectra revealed no change in oxidation state after functionalization, indicating that the PLA deposition process does not alter the active metal phase. Physisorption measurements showed that both SiO₂–Ag and SiO₂–CuO possess Type IV isotherms with high surface areas (264 m²/g and 256 m²/g, respectively). After PLA coating, surface areas decreased moderately (to 187 m²/g for Ag and 172 m²/g for CuO), while the characteristic mesopore size distributions remained unchanged, confirming that the porous framework is retained. These findings are consistent with recent reports on PLA–silica composites, where polymer incorporation preserves the mesoporous architecture while enhancing functional properties [6, 8].