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Nanobiophysics has emerged over the past two decades as one of the most innovative branches of nanoscience and remains a rapidly developing research area. It is a highly interdisciplinary field that integrates physics, biology, chemistry, materials science, nanotechnology, and medicine. The central aim of nanobiophysical studies is to elucidate the mechanisms underlying interactions between biomolecules and nanomaterials, to gain insight into biological processes in these systems at the molecular level, and to translate this understanding into medical and nanobiotechnological applications. These interactions involve complex processes such as adsorption, charge transfer, conformational changes, and the formation of biomolecular coronas on nanomaterial surfaces. Understanding how proteins, nucleic acids, and lipids bind to nanomaterials helps reveal how their nanoscale properties, such as size, shape, and surface chemistry, influence the biological activity of these biosystems. Advanced spectroscopic, microscopic, and computational methods are used to uncover these mechanisms at the molecular level. These tools enable researchers to understand how nanomaterials affect protein folding, DNA structure, enzyme activity, and membrane function. Such insights are essential for predicting nanomaterial behavior in biological environments and for designing safer, more efficient nanoplatforms for diagnostics, therapeutics, biosensing, and personalized medicine.

Nanobiotechnology has already found widespread use across many areas, including the development of advanced medical products and pharmaceuticals. By directly or indirectly interacting with biological systems, nanomaterials, as key products of nanobiotechnology, can significantly influence human health and quality of life. As nanotechnology

becomes increasingly embedded in everyday life, it becomes essential to understand both the beneficial and potentially harmful aspects of nanomaterial interactions with biosystems.

Studies on the toxicity of nanomaterials are crucial for evaluating their safety in biomedical and environmental applications. Due to their small size and high surface reactivity, nanomaterials can penetrate biological membranes and interact with cellular components, potentially causing oxidative stress, DNA damage, or inflammation. The extent of toxicity strongly depends on factors such as particle size, shape, surface charge, and concentration. Researchers use a combination of *in vitro* (cell culture) and *in vivo* (animal model) studies, along with computational simulation, to assess these effects and identify safe exposure limits. Understanding the mechanisms of nanomaterial toxicity is essential for developing rules and conditions that ensure both biosafety and biocompatible nanotechnology-produced products.

One of the important tasks in nanobiophysics is to ensure the biocompatibility of functionalized nanomaterials. While surface modification of nanomaterials is often used to improve stability, solubility, and targeting functionalization, these functional coatings can alter the nanomaterial's interaction with cells and biological molecules. In some cases, functionalized nanoparticles may induce oxidative stress, inflammation, or immune responses. Therefore, understanding how different functional groups influence biological pathways and long-term toxicity is essential for designing nanomaterials that are both effective and safe for biomedical use.

Many nanomaterials exhibit remarkable antibacterial properties, making them highly promising for biomedical applications such as wound healing and infection control. Metal and metal oxide nanoparticles, such as silver, zinc oxide, and copper oxide, as well as two-dimensional materials like MoS_2 and graphene derivatives, can effectively inhibit bacterial growth by generating reactive oxygen species, disrupting cell membranes, and interfering with metabolic pathways. Incorporating the nanomaterials into wound dressings enhances their antimicrobial activity, accelerates tissue regeneration, and reduces the risk of infection. Moreover, multifunctional nanocomposite dressings can provide controlled drug release and maintain a moist environment, further promoting faster and safer wound healing.

This special issue contains 8 full-text peer-reviewed articles based on the research results presented at the 9th International Conference "Nanobiophysics: Fundamental and Applied Aspects 2025" (Kharkiv, Ukraine). The Nanobiophysics conference series was jointly launched in 2009 by the B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine and the Institute of Physics of the National Academy of Sciences of Ukraine. Conferences are held every two years, alternately in Kharkiv and Kyiv. To discuss the urgent problems and new results achieved in nanobiophysics, the following sections were organized: nanobiohybrids formed by 1-D or 2-D nanomaterials with bioobjects, biomolecules on nanoparticles and nanostructured surfaces, physical aspects of biomolecular nanosystems, theoretical calculations and computer modeling of nanobiosystems, and applied aspects of nanobiophysics. Within the framework of the conference, a round table entitled "History of Biophysics in Kharkiv" was organized. The round table was dedicated to commemorating distinguished scientists who founded the scientific school of molecular biophysics in Kharkiv, which has achieved recognized standing both in Ukraine and internationally.

Two articles of this issue focused on the results of nanobiophysics study concerning DNA: one of them is dedicated to the quantum-chemical DFT study of Ag^+ complexes with DNA, and in the second one, the nanohybrids of DNA with carbon nanotube are considered employing Raman spectroscopy to determine the influence of biopolymer surrounding on the nanotubes.

DNA-metal interactions are important in both biological systems and DNA-based nanomaterials. These interactions influence the structural stability, electronic properties, and chemical reactivity of nucleic acids, thereby affecting gene regulation and enzymatic activity in living systems. In materials science, DNA assemblies offer the precise fabrication and functionalization of metallic nanostructures using DNA as a programmable scaffold or template. Metal-mediated DNA complexes are versatile nanoplatforms with tunable optical, electrical, and catalytic properties. In particular, complexes formed between DNA and Ag^+ ions are of considerable fundamental and practical interest. In such systems, silver ions can coordinate with nucleobases and form a one-dimensional metallic nanowire within the DNA double helix, leading to unique electronic and conductive characteristics. In the work of Y. Osokin and S. Perepelytsya, a quantum-chemical DFT study of Ag^+ complexes with DNA, focusing on Ag^+ binding to the nitrogen atoms in different positions of thymine, guanine, and 5-bromocytosine are presented. The results show that the stability of these complexes strongly depends on the nucleobase type and the position of the donor atom. These results are important for understanding the structural features of metallized DNA-Ag and its potential as a nanomaterial.

DNA-carbon nanotube hybrids represent one of the most versatile classes of bio-nanomaterials. These hybrids combine the molecular recognition properties of nucleic acids with the unique electronic and optical properties of single-wall carbon nanotubes (SWCNTs). Research in recent years has expanded from fundamental studies of DNA adsorption and chirality sorting of nanotubes toward applications in sensing, imaging, and bioelectronics. Despite impressive progress, several challenges remain, and understanding how DNA of different structural organizations adsorbed onto nanotubes affects the spectral properties of nanotubes

is one of them. In this issue, results of the Raman spectroscopy study of networking of carbon nanotubes wrapped with single- or double-stranded DNA or surrounded by N-methylpyrrolidone molecules in the region of D and G modes (V. A. Karachevtsev, N. V. Kurnosov, A. S. Linnik, O. S. Lytvyn) are presented. The spectra showed clear differences arising from the distinct interactions between SWCNT and their molecular surroundings. The observed peak shifts, broadening, and intensity changes are discussed in terms of bundling effects, charge transfer, stress on the surface of the nanotube induced by adsorbed molecules, and variations in the local dielectric environment.

MoS_2 quantum dots (QDs) are ultrasmall MoS_2 nanostructures that can be produced by liquid-phase exfoliation of bulk material. Using biological molecules during exfoliation facilitates the process as the biomolecules act as stabilizing and capping agents, preventing aggregation of the QDs. This biomolecule-assisted approach yields highly dispersed, biocompatible MoS_2 QDs with tunable optical properties, improved aqueous stability, and surface functionalities suitable for further conjugation. Such hybrids are promising for biosensors, bioimaging, antioxidant activity, photothermal therapy, and drug delivery, where their small size, low toxicity, and combined semiconductor and biomolecular properties offer distinct advantages. In the work of Kurnosov *et al.*, an optical spectroscopy study of MoS_2 nanostructures (QDs and nanosheets) obtained by ultrasound-assisted liquid phase exfoliation of bulk MoS_2 crystals in aqueous solutions of DNA/RNA nucleotides is performed. It was suggested that the MoS_2 interaction with nucleotides is essential for the emissive properties of exfoliated MoS_2 QDs. Observation of photoluminescence from MoS_2-nucleotide QD aqueous suspensions after long-term storage has demonstrated good stability of the MoS_2 QDs.

The structure of the complexes of the pristine nanostructure of MoS_2, containing surface point defects with two drug molecules (lamivudine and tegafur), as well as interaction energies between components were determined and analyzed by T. Piddubnyi, S. Stepanian, L. Adamowicz using the DFT method. These nanobiostructures are considered a potential nanoplatform for drug delivery. The possibility of forming a wide variety of complexes due to different tegafur and lamivudine conformers was analyzed. Complexes with a pristine surface are stabilized only by stacking interactions and have relatively low absolute values of interaction energies. Several complexes stabilized by coordination bonds with a strong interaction energy were proposed, taking into account the influence of the aqueous environment on these interaction energies.

The topic of drug binding to MoS_2 nanostructures is further developed in the article by V. A. Pashynska *et al.*, in which nanocomposites composed of MoS_2 and anticancer thio-derivatives of purine nucleobases [6-thiopurine (TP) and 2-thioadenine (TA)] were investigated using laser desorption/ionization (LDI) mass spectrometry and DFT calculations. The DFT results demonstrate the formation of stable non-covalent complexes between the drug molecules and MoS_2 nanosheets, with the drugs adsorbed on the surface in a stacking conformation, as well as covalent complexes involving drug binding at the edges of the nanostructure. These findings correlate well with the LDI data and indicate that the majority of the studied drug molecules retain their molecular integrity within the nanocomposite, which is essential for the anticancer efficacy of the proposed nanosystems. Nevertheless, the LDI mass spectra show that a fraction of TP and TA molecules undergo chemical transformations, such as covalent dimerization or oxidation, induced by the catalytic activity of MoS_2. These data should be taken into account under the development of MoS_2-based nanocomposites for biomedical applications as multifunctional drug delivery platforms.

The work by N. V. Tkach *et al.* presents the results of complex spectral studies of biologically active derivatives of indole: the amino acid tryptophan and 6H-indolo[2,3-b]quinoxaline (IQX) at room and low temperatures. The authors identified differences in the nature of the excited states of this compound, obtained an energy diagram of the first excited singlet and triplet states, and explained the role of the π-electron structure in the optical response of these structurally related molecules. DFT calculations of the HOMO-LUMO energy gap of the studied compounds showed good correlation with experimental data. The calculations also revealed spatial separation of the HOMO and LUMO orbitals in different parts of the structure of the IQX molecule.

Cell mechanical properties are essential for key cellular functions and arise from the integrated mechanics of the membrane, cytoskeleton, nucleus, and other organelles. During tumor progression toward a metastatic phenotype, these properties undergo significant changes that are critical for cancer dissemination. In the study of M. V. Olenchuk *et al.*, the mechanical properties of circulating metastatic tumor cells cultured under adhesive and non-adhesive conditions were quantified using micropipette aspiration. Comparative analysis across different cell lines and cultivation conditions provides insight into how mechanical stimuli regulate cellular biomechanics, contributing to a better understanding of the molecular and cellular biology of cancer.

Electrospinning has recently gained significant attention as a versatile method for producing polymer nanofibers that can incorporate biological molecules, drugs, and nanoparticles. Such nanofibers are increasingly important in nanobiotechnology and nanomedicine, particularly as wound dressings, due to their high porosity, sterility, and excellent capacity for controlled loading of active agents. Nanofiber matrix with incorporated antibiotics provides a creating of a delivery system capable of retaining antibiotics in the wound area for extended periods with a sus-

tained therapeutic dose to inhibit pathogenic bacteria. In the article of Plokhotnichenko *et al.*, the nanofiber mats were fabricated from polymethylmethacrylate with antibacterial antibiotics levofloxacin or chloramphenicol incurporated. In the work, a comparative analysis of the release kinetics for two different antibiotics from the mats and compare their antibacterial properties was conducted. These mats were characterized by the microscopic method, UV-visible absorption spectroscopy, and mass spectrometry. The drug release kinetics and the antibacterial properties of the drug-loaded mats against Gram-positive and Gram-negative bacteria were analyzed. The study found that both types of mats with different antibiotics demonstrated high efficacy against these bacteria.

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