Biomolecules and their complexes with nanostructures

Over the past two decades, molecules executing the important role in biology begun to be exploited in material science to build the programmed nanoscale architectures. The inherent molecular recognition properties of some biomolecules in combination with nanostructures promotes a fabrication of the miniature and sensitive sensors, a wide spectrum of intermolecular interactions among biomolecules allows a versatile functionalization of nanomaterials that extends their scope. On other hand, nanomaterials represent a great alternative for the development of the next generation of tools for biomedical applications, ranging from bioanalysis, antibacterial and wound repair, bioimaging, drug delivery, and cancer therapy to tissue engineering and medical devices. Carbon nanomaterials which include fullerenes, nanotubes, graphene family materials, diamonds are the most popular objects in this field due to their intriguing physical, chemical, electronic, and optical properties.

The rapid development of nanoscience and nanotechnology including in this research area biological molecules motivates the acquisition necessity of fundamental knowledge about new nanobiohybrids. All these have initiated appearance of such new branches of science as nanobiophysics. Nanobiophysics research focuses on manipulating single biomolecules, on the development of interfaces between single biomolecules and single nanoparticles, on studying the physical properties of new nanobiostructures, on the bio-diagnostics and the development of biological sensing devices, and on the application of nanobiophysics results in medicine.

Low temperatures are often used in biomolecule research when detailed information on the structural, energy, and spectroscopy characteristics of small building blocks of complex biomolecules is needed to elucidate the basic mechanisms of their biological function at the molecular level. Low temperatures allow to combine the experimental data with the quantum-mechanical and *ab-initio* calculations and, as a result, to obtain the general characteristics of biomolecules concerning their structures and intermolecular interactions.

This special issue introduces the field of nanobiophysics through 8 original articles and 1 review. Three articles concentrate our attention on some physical properties of the most important biomolecule as DNA including its components: nucleobase and nucleoside. In these investigations low temperatures play a key role. As most biological processes occur in an aqueous environment a special article is devoted to the simulation of intermolecular properties of water molecules embedded in an argon crystal fragment. In two articles the physical properties of nanomaterials that are relevant in nanomedicine are considered: in the first one the interaction between two carbon nanomaterials are analyzed and in the other one the magnetic properties of two nanoparticles are studied.

This special issue includes the review that is focused on the conformation and spectral analysis of nucleosides at low temperatures. The nucleosides were trapped in matrices formed by solidified inert gases at temperatures close to liquid helium. Many years of exploitation of this technique in combining with different spectroscopic detection equipment's and quantum-physical calculations proved that this method is a powerful research tool. Another paper proposed a hypothesis about the formation possibility of biological molecules in space at low temperatures.

The review paper by A. Yu. Ivanov and S. G. Stepanian is focused on the application of various action spectroscopy and absorption spectroscopy methods for studying the structure of biological molecules in an isolated state at low temperatures. The main attention is paid to recent results achieved in the study of the nucleosides which are the structural units of DNA and RNA. The authors compare results obtained by different spectroscopic and theoretical methods. The analysis of studies carried out for both neutral and ionized molecules is presented. It is shown that modern methods of low-temperature spectroscopy make it possible to successfully determine the conformational landscape of complex biomolecules.

The paper by L. N. Christophorov *et al.* presents an approach that allows obtaining kinetic equations that enable describing the behavior in time of slow processes occurring against the background of faster ones. The authors demonstrated how the physical processes in biosystems can be described using averaged (coarse-grained) kinetic and dynamic equations. The general approach is illustrated by examples concerning the transport of electrons and excitations, as well as the dynamics of transient conformational processes. In particular, the authors analyzed one-electron and two-electron donor-acceptor transfer between redox centers, as well as the transfer of triplet excitation between pigments in the pigment-protein complex.

Another method that is successfully used in studies of the structure of biological molecules is the isolation of the molecules and their complexes in low-temperature crystals (matrices) of inert gases in combination with IR spectroscopy. A. Vasylieva *et al.* studied water clusters of different sizes embedded in argon fcc crystal fragments. The simulation of the systems was performed using the quantum mechanical method DFT/M06-2X. The argon matrix effects on the structural, energy, and spectral peculiarities of individual water clusters are determined.

The possible role of hydrogen peroxide molecules that are products of cell radiolysis, in blocking DNA activity in cancer cells during irradiation with heavy ions is investigated by S. N. Volkov. The author used the quantum-mechanical approach based on the density functional method taking into account the aqueous medium to study the competitive interactions of water and hydrogen peroxide molecules with DNA nucleic bases. Estimation of the characteristic parameters allows showing the possibility to block the genetic activity of DNA by hydrogen peroxide in biological cells after their irradiation with ion beams. It was also noted that the torsion oscillations around the O-O bond in peroxide molecule can be observed well in DNA vibrational spectra at the condition of low temperatures.

The interaction of DNA with metal ions which play an important role in conformation dynamic structure of DNA, its electronic and thermodynamic properties were analyzed by D. Gryn *et al.* using spectral methods. Studying the dependence of fluorescence and phosphorescence spectra of the DNA at 77 K on the relative concentration of the Ni^{2+} ions the authors try to estimate the average of triplet exciton path length. They also showed that the presence of nickel (cobalt) ions does not affect on the DNA photostability under UV light irradiation. The obtained results can be applied to nanomedicine for developing new drugs for photodynamic therapy.

Detail analysis of the noncovalent interaction between semiconducting single-walled carbon nanotubes (SWNTs) and graphene oxide (GO) using Raman spectroscopy was carried out by N. V. Kurnosov and V. A. Karachevtsev. In their paper it was shown that introducing of biological globules (enzyme glucose oxidase) in the SWNTs-GO composite film allows to weaken a mechanical stress of GO on the nanotubes. The obtained new information provides a better understanding of the physical mechanisms of the interaction among components of hybrid 3D nanostructures formed by low-dimensional carbon nanostructures including biological macromolecules.

The magnetic properties of Fe3O4 and ZnFe2O4 nanoparticles are studied by K. Yu. Sova *et al.* exploiting the spectroscopy of the ferromagnetic resonance. It was concluded that the magnetic properties of nanoparticles depend significantly on the synthesis method, in turn, analyzing the FMR spectra can determine the efficiency of drug delivery to organs and tissues. The results obtained are important in the control of the state of complex magnetic nanoparticles with chemotherapeutic drugs in the form of biologically active magnetic fluids. In addition, the nanoparticles studied can be useful for the medicine to treat cancer by developing of the hyperthermia technique.

The paper by S. A. Krasnokutski studies the possibility of formation of biological molecules in space by the He droplet isolation technique. In this method, liquid helium serves as an ideal chemical inert third body, that absorbs the reaction energy but does not provide any catalytic or inhibitor influence on the reaction. The obtained results indicate the formation of organic and biological molecules in space due to the condensation of atomic carbon together with other species, which are abundant in the interstellar medium.

Applied aspect of nanobioscience is presented in the article of D. O. Harbuz *et al.* in which the elaboration of a new express method for melatonin determination in the human body using a point-contact sensor for detection of the breath gas is described. The authors claim that the proposed method is accurate enough to be used for medical purposes in real-time.

To summarize, this issue is written by experts in different fields of biophysics, material science, physics, and bioengineering and demonstrates the great progress achieved in recent years in nanoscience and nanobiotechnology. We hope the articles presented in the issue will be useful to researchers working in the area of nanobiophysics, material science, biology, medicine, and chemistry.

We would like to thank all the authors for accepting the invitation to contribute to this issue.

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