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2

Nonlinear mechanism of magnetic field impact on charge transport in macromolecules

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Charge transport accompanies redox processes in respiration, and involves electron transport chain in Krebbs cycle. Some stages of this transport occur in polypeptide macromolecules which support the formation of bound nonlinear electron states in the form of solitons formed due to relatively strong electron-lattice interaction in hydrogen-bonded polypeptide chains [1]. As an external magnetic field can affect the dynamics of solitons, we study the influence of an external time oscillating magnetic field on the dynamics of solitons. It is shown that the soliton properties depend on the amplitude and the frequency of the magnetic field, as well as on the orientation of the magnetic field with respect to the molecular chain axis. It is shown that in a perpendicular magnetic field the soliton dynamics is a superposition of the free electron plane wave in the plane perpendicular to the molecular chain, and of the soliton propagation along the chain. The latter is described by the modified Nonlinear Schrödinger equation with an extra term depending on the magnetic field. This equation is solved using nonlinear perturbation theory [2,3]. It is shown that the soliton velocity and phase are oscillating in time at the main frequency of the external field frequency, as well as at its higher harmonic multiple.
Such complex effects of external time-depending magnetic fields on the dynamics of solitons in polypeptides affects the charge transport in the redox processes of biological systems and could explain the physical mechanism of the therapeutic effects of oscillating magnetic fields.

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[2] L. Brizhik. Chaos, Sol. Fractals 187 (2024) 115459
[3] L. Brizhik. Low Temp. Phys. 51 (2025) 655

3

Multifunctional nanodispersed X-ray phosphors in a drug delivery system in X-ray photodynamic therapy

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A promising approach that can provide minimally invasive treatment, in particular, of malignant tumours located both in soft tissues and in hard-to-reach areas of the body (e.g., in the cranial cavity), is the implementation of the principles of the latest scientific and practical interdisciplinary direction – X-ray excited photodynamic therapy (XE-PDT), in which X-rays are used to activate the photosensitive component by transferring energy from phosphors. The concept of XE-PDT is actively developing worldwide, and the implementation of its results in clinical practice can provide solutions to many modern medical and biological problems, such as drug resistance, low selectivity and safety of cytotoxic drugs.

Thus, the development of functional, highly efficient, biocompatible, nanoscale phosphors that are sensitive to biologically safe, highly penetrating ‘soft’ X-ray radiation with specified luminescence spectral characteristics for the implementation of the XE-PDT method is a pressing task.

Based on the focus of the work, nanodispersed phosphors based on lanthanum fluoride (or phosphate) and hydroxyapatite activated by REE ions (terbium) ions (LaF3:Tb3+, LaPO4:Tb3+ and HA:Tb3+), obtained by co-precipitation from aqueous solutions. These phosphors are characterised by high quantum yield, significant Stokes shift, low toxicity and high biocompatibility, high chemical stability, and clear emission bands.

A comprehensive study and comparison of physicochemical characteristics was conducted, and nanostructure synthesis technologies were optimised. It was established that the X-ray luminescence spectra show bands characteristic of optical transitions in Tb3+-activated phosphors, and their spectral position under the synthesis conditions used depends little on the chemical composition of the nanocrystalline matrices. It was found that high amorphisation and defectiveness of the crystal structure of the samples have little effect on the position of Tb3+ energy levels in their forbidden zone. However, they significantly affect the intensity of X-ray luminescence, in particular due to scattering on defects in the crystal structure. In addition, water molecules on the surface of the phosphor, in the composition of crystal hydrates, as well as surface hydroxyl groups can be centres of luminescence quenching.

Morphological features were noted: LaF3:Tb3+ is characterised by spherical nanoparticles (Dav =11.17±3.09 nm), LaPO4:Tb3+ exhibits slight anisotropy in crystallite growth (Lav=19.92±4.55 nm), while HA:Tb3+ crystallites are characterised by significant anisotropy in growth and a rod-like shape (Lav=54.28±11.87 nm).

The results of XRD studies indicate the formation of single-phase crystals, for which the angular position, shape, width and intensity ratio of the reflections practically do not differ from the diffractograms of the corresponding terbium-doped nanostructure samples. The features of the diffractograms include: 1 – broadening of diffraction reflections, 2 – presence of a diffuse halo in the diffraction angle range of 15–40 degrees for all test samples. The first indicates the nanocrystalline nature of the particles, while the second is associated with partial amorphisation of the phases.

It has been shown that in an NSS medium at physiological pH values of 6–7, the ζ-potential values for the synthesized samples indicate acceptable colloidal stability of the suspensions. For LaF3:Tb3+ (ζ = 28 mV, pH = 2) and LaPO4:Tb3+ (ζ = 23 mV, pH = 3) samples are characterised by colloidal stability in an acidic environment. For HA:Tb3+, colloidal stability increases in an alkaline environment (ζ = −27 mV at pH 11).

A significant difference in the quantitative distribution of basic and acidic active centres on the surface is shown: there are both strong basic (electron-donating orbitals F−, oxygen in PO4−, OH−) and weak acidic (electron-accepting orbitals La3+, Ca2+, Tb3+) Lewis centres.

The physicochemical characteristics of HA:Tb3+ nanoparticles functionalised with citrate groups (HA:Tb3+/Citr) were synthesised and studied. Functionalization contributes to increased colloidal stability in a wide pH range (5–11), creates additional active centers (carboxyl groups −COOH), and increases the biocompatibility of nanoparticles, which is important for materials used in medical and biological applications. In vitro biocompatibility studies conducted in collaboration with specialists from the O.O. Bogomolets Institute of Physiology of NAS of Ukraine confirmed the biocompatibility of the developed material.

Based on HA:Tb3+/Citr, a targeted delivery model was created and studied, which can be applied within the concepts of photopharmacology and photodynamic therapy. The study used a photosensitive complex compound of ruthenium-bipyridine-nicotine complex [Ru(bpy)2(Nic)2]Cl2 (RuBiNicotine), which was immobilised on the surface of HA:Tb3+/Citr nanoparticles. When irradiated with light in the wavelength range of 405 nm, 473 nm or 532 nm (for synthesised samples, X-ray-induced luminescence is recorded at 487, 542, 582 and 620 nm), it photolyzes with the release of nicotine. A quantitative determination of the released nicotine was carried out for samples under UV irradiation and X-ray irradiation. As a result of X-ray irradiation, 4.17% of nicotine was released, and under UV irradiation, 98.26% was released.

The research results may be useful for application in the fields of photopharmacology and photodynamic therapy in the development of targeted drug delivery systems and local therapy for diseases.

4

Quantum-chemical modeling of mono- and biligand complexes of silver ions with some DNA nucleotide bases

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One of the promising objects for the creation of new functional materials is the metallized DNA molecule. Such a system is a unique combination of the biopolymer matrix of DNA and the properties of metal ions, in particular Ag⁺. The presence of intercalated Ag⁺ ions in the DNA structure provides the possibility of forming one-dimensional nanostructures in the form of nanowires [1]. At the same time, for the correct modeling of such systems, a necessary procedure is a step-by-step optimization, the initial stage of which is the quantum-chemical modeling of complexes of DNA nucleotide bases with Ag⁺ ions in the form of L–Ag⁺ and L–Ag⁺–L, where L is the ligands of the studied nitrogenous bases. In our case, the anions of thymine (T[–]) and guanine (G[–]), and the molecular forms guanine (G), cytosine (C), 5-bromocytosine (C-Br) and adenine (A).
Calculations were performed within the framework of density functional theory (DFT) in the Gaussian 03 software package. Argentum atoms were described by the Def2-TZVP ECP basis set. The 6-311++G(d, p) basis set was used to describe the nucleotide base atoms. The PCM and SMD models were used as solvation models. The empirical correction for the dispersion interaction GD3 was used. Calculations of the effective charge of the central atom were made using the natural orbital theory (NBO). The criterion for comparing the stability of the complexes was the energy effect of complex formation. Calculations of the energy effects of Gibbs energy, enthalpy and zero-order energy for the [Ag⁺–L] complexes were performed according to the equation:
<pre>
L + Ag⁺ = [Ag⁺–L] + ΔE₁
ΔE₁ = E(Ag⁺–L) – (E(L) + E(Ag⁺))
</pre>

For the [L–Ag⁺–L] complexes, the energy effects of formation were calculated according to the equation:
<pre>
L + [Ag⁺–L] = [L–Ag⁺–L] + ΔE₂
ΔE₂ = E(L–Ag⁺–L) – (E(L) + E(Ag⁺–L))
</pre>

It was shown that electroneutral Ag⁺ complexes with the N3 atom of thymine and the N1 atom of guanine demonstrated the highest thermodynamic stability. Positively charged complexes gave lower thermodynamic stability. Among them, Ag⁺ complexes with the N1 atom of adenine were found to be the least stable, which explains the experimentally observed “jumping out” of adenine from the double helix in the metallized Ag-DNA molecule [1]. A comparison of the computational approaches used in [2] shows that the B3LYP functional in combination with the SMD solvation model provides the most suitable description of the [Ag⁺–L] complexes, since it systematically gives lower formation energies than B3LYP/PCM and predicts the Ag-N bond lengths more consistently than M06-2X. Therefore, optimization was performed for the [L–Ag⁺–L] complexes using this method.

 Kondo, J., Tada, Y., Dairaku, T., Hattori, Y., Saneyoshi, H., Ono, A., Tanaka, Y. (2017). A metallo-DNA nanowire with uninterrupted one-dimensional silver array. Nature chemistry, 9(10), 956–960. Ye. Osokin, S. Perepelytsya. (2026). Stability of Ag-DNA Nucleotide Base Complexes: A Quantum-Chemical Study. Low Temperature Physics, 2026, Vol. 52.

5

Bionanomaterials for drug delivery: computational and experimental study of MoS2-based nanocomposites with anticancer drugs

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The development of effective new bionanomaterials for targeted drug delivery is one of the most pressing applied problems of modern nanoscience and nanotechnologies for biomedical applications. The contributions of computational biophysics, as well as combined experimental and theoretical nanobiophysical research, to the study of intermolecular interactions between nanocarriers and therapeutic molecules in the drug delivery nanobiosystems are difficult to overestimate. Among the variety of nanomaterials that have recently been proposed for use in drug delivery, 2D MoS2 nanosheets have caught our attention, due to the unique physicochemical properties of MoS2 that offer the possibility of utilizing this nanomaterial as a multifunctional drug delivery platform for anticancer drug delivery combined with photothermal therapy of tumors.

This report presents the results of our computational and mass spectrometry experimental characterization of nanobiocomposites of MoS2 nanosheets with a representative of set of anticancer drugs based on derivatives of DNA nitrogen bases 6-thiopurine (TP), 2-thioadenine (TA), 5-fluorouracil (FU), or with widely used anticancer medication doxorubicin (DOX).

Ab initio DFT/M06-2X computational modelling of nanobiohybrids of MoS2 nanosheet with a molecule of the mentioned anticancer drugs was performed to examine the possible structures of the MoS2-based drug delivery nanobiocomplexes. In particular, the structures of the covalent and noncovalent complexes of MoS2 particles with the drug molecules were determined, and the energies of such complexes were calculated. Based on the modelling results, the biologically significant peculiarities of the anticancer agents interactions with MoS2 nanosheets are discussed, and the nanomaterials applicability for drug delivery is estimated.

For the experimental study, binary nanocomposites (MoS2 + drug) for each anticancer agent were obtained via ultrasound treatment and examined by laser desorption/ionization (LDI) mass spectrometry. Analysis of the mass spectra obtained demonstrates the presence of peaks of intact molecular ions of the anticancer drugs in the spectra of the majority of the studied nanocomposites. It testifies to the preservation of the drug’s molecular structure within the nanocomposites with MoS2, which is crucial for maintaining the drugs’ therapeutic activity. At the same time, we revealed spectral confirmations of some chemical transformations (oxidation processes) of sulfur-containing anticancer drugs (TP, TA) induced by catalytically active MoS2. We believe that such chemical transformations of drug molecules can reduce their therapeutic activity, which is mostly related to the thio-groups of TP and TA.

We suppose that the current study results should be considered in the development and application of MoS2-based bionanomaterials.

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Protein-ligand docking with machine learning

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Computational prediction of small-molecule binding to protein targets has been central to drug discovery for decades, yet conventional physics-based docking methods have largely reached a performance plateau. Machine learning (ML)-based alternatives offer a promising shift, though concerns about prediction quality, chemical plausibility of generated poses, and the lack of rigorous evaluation standards have slowed their practical adoption.

This work presents an ML-based docking method and evaluates it across several practically relevant scenarios: binding sites containing non-protein entities such as metal ions, cofactors, and ordered water molecules, and docking into ligand-free (apo) protein conformations. To ensure unbiased assessment, the model was trained and tested on a large, structurally diverse benchmark derived from experimentally determined three-dimensional structures, with cluster-based data partitioning to minimize information leakage. Performance was compared against several widely used conventional docking programs.

In the general evaluation setting, the proposed method reduced positional error by 29–38% relative to conventional approaches while maintaining low computational cost. In binding pockets containing ions and conserved water molecules, median pose deviations decreased by 0.7-0.8 Å compared to the best classical alternative. Under the most challenging apo protein conditions, the method achieved a median improvement of approximately 2.1 Å over the leading conventional tool.

These results demonstrate that the ML-based approach consistently outperforms established techniques in accuracy, generalizes to complex binding environments and conformational uncertainty, and produces chemically and geometrically valid poses suitable for integration into modern drug discovery pipelines.

7

Mechanical properties of circulating tumor cells as markers of metastatic activity

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During the transformation of a tumor cell into a metastatic cell, a number of radical transformations occur, in which changes in mechanical properties play a key role, in particular, the loss of epithelial intercellular contacts, cytoskeletal reorganization, cell shape change, and a series of events that include the crossing of barriers. So, the mechanical properties of the cell membrane change significantly and are crucial at each stage of the metastatic cascade. Therefore, the study of the mechanical properties of tumor cell membranes may open new avenues for diagnostics, as well as antitumor and antimetastatic therapy.

The micropipette aspiration method was used to determine the mechanical characteristics of the cells. This method allows non-invasive measurement of the integral macroscopic elastic characteristics of cells during their suction into the micropipette capillary due to the reduced pressure in it. The work shows that cells grown in a deadhesive manner have a more homogeneous population compared to adhesive ones, and are also characterized by a smaller range of surface elastic modulus values. LLC cells are characterized by a lower surface elastic modulus than LLC/R9 cells, which correlates with the metastatic activity of the cells. The mechanical parameters of cells obtained in the work can be useful as specific markers for establishing the metastatic potential of tumor cells, for diagnosing metastatic cells, for developing new strategies and antitumor (antimetastatic) therapy.

1. M.V. Olenchuk, O.P. Gnatyuk, S.V. Romanenko, P.V. Belan, D.L. Kolesnik, G.I. Solyanik, G.I. Dovbeshko “Mechanical properties of the membrane of circulating metastatic tumor cells as a diagnostic marker” was accepted into the journal “Low Temperature Physics” in 2026.

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Physicochemical properties and neurotoxicity of hazardous carbon smoke nanoparticles with heavy metals

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Now in Ukraine with huge artillery shelling and missile attacks, a large amount of pollution consisting of carbon particles with heavy metals-iron, copper etc. and remains of organic molecules are formed. This is why modeling these particles and collecting them is important for understanding how they affect human health. Here the data on physical, chemical and neuroactive properties of the particles are presented. Earlier a method for obtaining nanohybrids based on carbon particles was developed in the Palladin Institute of Biochemistry NAS of Ukraine and applied for biochemical tasks [1].

The spectroscopic data showed that carbon particles with Cu and Fe of both valences are similar to property of carbon quantum dots with specific features. Size of particles are registered in wide regions from nm to tens of μm. Different molecular groups belonging to hazard aromatic molecules was observed. The data obtained allow us to conclude about the potential toxicity of these nanoparticles for human health not only in Ukraine and Europe but everywhere.

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9

Targeting TMPRSS2 with carbon nanostructures: an in silico study

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TMPRSS2 (transmembrane serine protease 2) is a key protein involved in SARS-CoV-2 entry into host cells by participating in membrane fusion. Therefore, TMPRSS2 represents a promising therapeutic target with a lower risk of resistance development as a host factor compared to viral proteins.

In this study, the in silico investigation was conducted to evaluate the possibility of interaction between C60 fullerene and TMPRSS2. First, four potential binding pockets were predicted by using the p2Rank tool. Based on structural features and residue decomposition, three pockets were selected for further analysis. The molecular docking simulations suggested strong interactions within pocket 1. However, long-scale (1000 ns) MD simulations indicate C60 fullerene migration from pocket 1 to pocket 2, showing thermodynamic stability insight that pocket.

RMSD and RMSF analyses confirmed the overall structural stability of the complexes, while PCA analysis indicated a significant reduction in conformational flexibility upon fullerene binding compared to the apo-TMPRSS2 structure. The MM/PBSA approach has shown that van der Waals interactions dominate in the binding between C60 fullerene and TMPRSS2. Pocket 2 exhibited the most favourable binding energy ($\Delta G \approx -30.7$ kcal/mol), whereas binding in the other pockets was weak.

To conclude, C60 fullerene can interact with TMPRSS2 via a non-classical, hydrophobic-driven mechanism and stabilize via van der Waals interactions. Obtained results suggest C60 fullerene as potential antiviral scaffolds targeting the TMPRSS2 protein. To find more details about this work, use this link: https://doi.org/10.3390/molecules30234586

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Change in orientation of the Ca2+ sensor protein hippocalcin in its membrane-bound state as a mechanism for the development of primary dystonia

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A detailed study of the collective behavior of the lipid bilayer in the presence of peripheral proteins is essential for understanding the molecular signaling processes that occur on membranes. The N75K mutation of the neuronal Ca2+ sensor protein hippocalcin, which is partially embedded in the inner layer of the plasmatic membrane, leads to the development of a severe disease, primary autosomal dystonia. However, how exactly the mutation changes the functioning of the protein remains unclear. In this work, we tested the hypothesis that the orientation of wild-type (WT) hippocalcin and its N75K mutant relative to the normal bilayer surface in a steady state of lipid parameters does differ, which may lead to steric hindrance of protein interaction with its membrane targets.
For simulations, a lipid bilayer model was created. It consists of POPC/DPPC/POPI25/DMPI25 lipids and cholesterol in ratios corresponding to a realistic mammalian plasma membrane. The wild-type hippocalcin model was obtained from the rcsb.org database under code 5G4P. Modeling of unstructured N-terminus and C-terminus and modification of N-terminus with myristoyl were performed using the CHARMM-GUI service. The following parameters were obtained to describe the lipid bilayer collective behaviour: order parameters and area per lipid. Analysis of the WT and N75K location data in the bound position shows a significant difference in their tilt angles, close to 45 degrees with a high spread of values for the N75K mutant. The high dispersion in the case of N75K is explained by low kinetic barriers to other equilibrium positions, which reduces the mutant's ability to self-stabilize through electrostatic interactions after introducing momentum into the system. Such differences in the dynamics of WT and N75K hippocalcin indicate the possibility of steric hindrance in protein-protein interactions with membrane targets and lower stability of the bound state.

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Quantum mechanical calculations in prediction of properties of π-conjugateded molecules

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The relevance of studies on π-conjugated molecular systems is determined by their wide application in modern organic electronics, photonics, sensing, and biomedical technologies. Quantum-mechanical calculations make it possible to predict the geometric, electronic, and spectral properties of π-conjugated molecules and their complexes with nanostructures at the stage of material design. This enables purposeful modification of molecular structures and control of the energy gap, charge transfer, and optical characteristics, which is important for the development of efficient organic semiconductors, photosensitive materials, nanocomposites, and bioactive systems.

Quantum-chemical calculations and spectral studies of π-conjugated molecules have revealed the features of the formation of their electronic structure and geometry. It has been shown that neutral 1,2-squaraines exhibit a polyene type of conjugation with pronounced bond-length alternation and a large energy gap, whereas isomeric 1,3-thiasquaraines demonstrate a polymethine type with nearly equalized bond lengths and a smaller energy gap. The introduction of heteroatoms and modification of donor–acceptor terminal groups significantly affect the geometry of the conjugated chain and the HOMO–LUMO gap. Charge injection into one-dimensional π-systems leads to the formation of soliton-like waves of charge and bond-length alternation and to the appearance of additional electronic states within the band gap. Studies of thin films of squaraine and merocyanine dyes have shown that intermolecular interactions between conjugated systems result in aggregates with different geometries, manifested as bathochromic or hypsochromic shifts of the absorption maxima.

It has been shown that the interaction of π-conjugated molecules with carbon nanostructures significantly modifies their electronic properties. In complexes of dyes with fullerene C60, graphene, and carbon nanotubes, charge transfer from the dye to the nanostructure occurs, accompanied by changes in bond lengths, shifts of electronic levels, and a reduction of the energy gap. Functionalization of fullerenes with covalent bridges or metal atoms breaks the symmetry of the C60 molecule, leading to the splitting of degenerate electronic levels and modification of vibrational spectra. Studies of metal doping and diffusion in C60 fullerite films revealed the possibility of forming dimeric and polymerized structures, accompanied by changes in X-ray diffraction patterns, vibrational spectra, and photoluminescence, and also demonstrated the possibility of complex formation between fullerenes and biologically active molecules.

The obtained results demonstrate that quantum-mechanical calculations are an effective tool for predicting the geometric, electronic, and spectral properties of π-conjugated molecules and their complexes with nanostructures. The revealed relationships between molecular structure, intermolecular interactions, and charge transfer can be used for the targeted design of new functional materials for organic electronics, photonics, and biomedical applications.

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How could a molybdenum metal atom get into biomolecules’ structure: mass spectrometry based version

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Modeling of formation of primary organic molecules in the course of prebiological biochemical evolution usually deals with assembling of H, C, O, N, S chemical elements. However, biomolecules of such importance as enzymes incorporate metal atoms. These could get into the structure of evolving organic molecules through direct contact with early Earth's minerals. This step of biochemical evolution was proposed in the framework of the “iron world hypothesis”. Enzymatic activity of minerals was considered, whereas direct reactions of metal inclusion into organic molecules, to the best of our knowledge, were not modeled.

In our studies of bionanohybrids of the transition metal dichalcogenide MoS2, we have considered combinations of this mineral with various organic compounds and biomolecules probed by means of laser desorption/ionization (LDI) mass spectrometry [1]. None of the studied compounds have shown cluster ions or associates with the Mo atom or ion, with the only exception: thio-derivatives of nucleic acid bases 6-thiopurine (TP), 2-thioadenine, and 6-thioguanine. Along with the expected signals corresponding to individual components, products of the bases oxidation and MoS2-related clusters, a new group of peaks appeared in the LDI mass spectra of these three systems. As an example, for the (TP + MoS2) nanohybrid, this group was recorded at m/z 410 418 in the positive ion mode and m/z 408 416 in the negative ion mode. Isotopic distribution in the peak group evidenced the presence of one molybdenum atom, two nitrogen bases, and an oxygen atom in the structure, while the recording of these species in both positive and negative ion modes in the protonated and deprotonated forms, respectively, indicated their molecular nature. The presumed composition of this molecule as {(2TP − 2H) + Mo + O} was proposed. Modeling of possible structures using the DFT quantum chemical approach revealed a set of configurations in which the centered Mo atom binds to two sulfur and two nitrogen atoms of two TP bases, and to one oxygen atom.

Formation of such a molecule implies a step of extraction of the Mo atom from the MoS2 crystalline lattice and its covalent attachment to definite sulfur-containing heterocyclic organic molecules during the direct contact of these compounds in an aqueous medium. We believe this is the first case of observation of such a process, which may occur during the creation of precursors to molybdenum-containing enzymes. Our further studies are directed toward modeling MoS2 systems with the organic components of the present-day enzyme's molybdenum-containing cofactors.

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Modeling aggregation of proteins on computers

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Protein aggregation refers to the process by which fully or partially unfolded proteins self-associate to make large and insoluble aggregates. Amyloid fibrils - a prominent example of the aggregates, is implicated in various neurodegenertive diseases and also has found multiple uses in technology. In this talk we will focus on what can be learned about amyloid formation using theoretical models and methods. First, we will give a broad overview of the problems and challenges facing theoretical approaches in the studies of protein aggregation, ranging from the description of small oligomers

[1], which are often considered kinetic intermediates to fibrils, continuing on to particlar details of amyloid structure [2]. Then, we will present a model - RAPID - specifically designed for simulations of protein aggregates [3] in water. Finally, we will discuss microscopic details of the aggregation pathway presented by the shortest amyloidogenic peptide reported so far - KFFE [1].

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Complex Formation in the ATP - Curcumin System in the Presence of Mg^{2+} and Ca^{2+} Ions

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Interactions between nucleotides, biologically active polyphenols, and metal ions play an important role in biochemical processes and molecular recognition in living systems. Adenosine triphosphate (ATP) is a key molecule involved in cellular energy metabolism, while curcumin, a natural polyphenolic compound derived from Curcuma longa, exhibits pronounced antioxidant, anti-inflammatory, and anticancer activity. Divalent metal ions such as Mg^{2+} and Ca^{2+} are essential cofactors in many enzymatic reactions and may significantly affect intermolecular interactions in aqueous solutions.

In this work, the mechanisms of heteroassociation between ATP, curcumin, and metal ions were investigated using fluorescence spectroscopy. Fluorescence emission and excitation spectra of aqueous ATP solutions were recorded at different temperatures (293–313 K) in the absence and presence of curcumin as well as Mg^{2+} and Ca^{2+} ions. The addition of curcumin to ATP solutions resulted in pronounced quenching of ATP fluorescence, indicating the formation of ATP–curcumin complexes.

Analysis of Stern–Volmer plots showed large quenching constants ($K_q \approx 10^{12}$ M^{-1} s^{-1}), which exceed the diffusion-controlled limit and therefore indicate a static quenching mechanism associated with complex formation. Binding parameters obtained from Hill analysis suggest the presence of approximately one binding site in the ATP–curcumin system.

The presence of Mg^{2+} and Ca^{2+} ions noticeably modifies the interaction between ATP and curcumin. Both ions promote the formation of heteroassociates, which is reflected in changes of Stern–Volmer constants, binding parameters, and thermodynamic characteristics. Thermodynamic analysis revealed negative Gibbs free energy values, confirming the spontaneous nature of the complexation process.

Overall, the results demonstrate that ATP, curcumin, and divalent metal ions form stable heteroassociates in aqueous solution. The formation of these complexes is governed by a combination of electrostatic interactions, coordination effects of metal ions, and molecular association processes. These findings provide new insight into nucleotide–polyphenol interactions in the presence of biologically relevant metal ions and may be important for understanding their behavior in biochemical systems.

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Mechanisms of Complex Formation Between Diphtheria Anatoxin CRM197 and Curcumin

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The development of efficient drug delivery systems is an important direction in modern biomedical research. Protein carriers are widely investigated as platforms capable of improving the stability, solubility, and targeted delivery of biologically active compounds. One such protein is CRM197, a non-toxic mutant of diphtheria toxin that retains receptor-binding ability while lacking enzymatic toxicity. Due to its structural stability and biocompatibility, CRM197 is widely used as a carrier protein in conjugate vaccines and is considered a promising candidate for drug delivery applications.

Curcumin is a natural polyphenolic compound extracted from Curcuma longa, known for its antioxidant, anti-inflammatory, and anticancer properties. However, its therapeutic application is limited by poor water solubility, low stability, and limited bioavailability. Complex formation with protein carriers may significantly enhance its physicochemical stability and pharmacological efficiency.

In this work, the mechanisms of interaction between diphtheria anatoxin CRM197 and curcumin were investigated using fluorescence spectroscopy and computational modeling. Fluorescence quenching analysis revealed a static quenching mechanism, indicating the formation of a stable CRM197–curcumin complex. Binding parameters obtained using the Hill model suggest the presence of approximately one binding site for curcumin on the CRM197 molecule. Thermodynamic analysis based on the Van't Hoff approach showed that the binding process is spontaneous and predominantly driven by hydrophobic interactions.

The Förster resonance energy transfer (FRET) method estimated the donor–acceptor distance between tryptophan residues of CRM197 and curcumin to be approximately 1.52 nm, confirming close spatial proximity between the interacting molecules.

Computational studies included molecular docking using AutoDock 4.2 and molecular dynamics simulations in Desmond software packages to analyze possible binding configurations and structural stability of the complex. The results revealed several energetically favorable binding modes of curcumin near exposed tryptophan residues (Trp50, Trp153, Trp398), with binding energies in the range of −7.7 to −5.5 kcal/mol. The interaction is mainly stabilized by hydrophobic and van der Waals forces.

Overall, the results demonstrate that CRM197 can form stable complexes with curcumin, supporting its potential use as a protein carrier for hydrophobic therapeutic compounds.

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Molecular Modeling of the Interaction Between Cytokine EMAPII and Titanium Dioxide Nanoparticles

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Protein-based therapeutics represent an important class of modern biopharmaceutical agents due to their high specificity and ability to regulate biological processes. One such molecule is the cytokine Endothelial Monocyte-Activating Polypeptide II (EMAPII), which exhibits antiangiogenic, proapoptotic, and immunomodulatory activity. However, its biomedical application is limited by aggregation in aqueous solutions, which reduces stability and efficiency. One possible strategy to overcome this limitation is the use of nanoparticles as stabilizing platforms and delivery carriers for protein molecules.

Titanium dioxide (TiO_2) nanoparticles are widely studied in nanomedicine due to their biocompatibility, chemical stability, and tunable surface properties. Their ability to interact with biomolecules makes them promising candidates for targeted delivery systems and nanocomposite therapeutic platforms.

In this study, the molecular interaction between EMAPII and a spherical TiO_2 nanoparticle (2 nm in diameter) was investigated using computational modeling. A two-step approach was applied: blind molecular docking was first performed to identify energetically favorable binding sites, followed by molecular dynamics simulations in an explicit aqueous environment.

Docking calculations revealed several possible binding modes on the EMAPII surface, with the most favorable conformations located within the hydrophobic pocket of the protein. The calculated binding energies ranged from −12.15 to −11.24 kcal/mol, indicating strong affinity between the nanoparticle and the protein. The interaction is primarily driven by electrostatic attraction between negatively charged oxygen atoms of the TiO_2 surface and positively charged residues such as Arg73, Lys123, and Lys166, while hydrogen bonds and hydrophobic contacts further stabilize the complex.

Molecular dynamics simulations (100 ns, GROMACS, CHARMM27 force field) demonstrated that the EMAPII–TiO_2 complex remains stable in aqueous solution. Structural deviations of the protein were minimal (RMSD < 0.2 nm), indicating that the nanoparticle does not significantly perturb the native structure of the cytokine. Stable contacts were observed with several residues, including Asp26, Arg73, Lys123, Lys166, Trp125, and Glu126. Analysis of interaction energies showed that electrostatic forces dominate the binding process, whereas van der Waals interactions provide a smaller contribution.

Overall, the results demonstrate that TiO_2 nanoparticles can form stable complexes with EMAPII without disrupting its structural integrity. These findings highlight the potential of TiO_2 nanostructures as carriers and stabilizing platforms for cytokine-based therapeutics.

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Simulation study of affinity-based cell sorting on switchable microstructured surfaces

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Affinity-based cell sorting on microstructured substrates offers a label-free route for separating heterogeneous cell populations based on differences in cell-surface interactions. In such systems, the efficiency of separation is controlled by the spatial distribution of adhesive regions together with the possibility of externally induced switching between adsorbing and desorbing surface states. This makes it possible to design multistage sorting protocols in which cell attachment and detachment are regulated in time. In this talk, I will present a computer simulation study of cell sorting on dynamic microstructured adhesive surfaces represented by a disordered array of circular adhesive domains. The interdomain regions are associated with a thermoresponsive polymer layer that induces a repulsive interaction facilitating cell detachment. Special attention is paid to the role of adhesive domain size at fixed surface coverage and to its influence on separation during successive

adsorption-desorption steps. Different regimes of surface switching are considered in order to examine how dynamic control of surface properties can improve sorting performance. The results help to clarify how the combination of surface microstructure and switching protocol affects the efficiency of label-free cell separation.

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Towards machine learning-based segmentation of zigzag patterns in BSA film micrographs

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Dried films of biofluids and biopolymer solutions are a promising object for querying the state of biomolecules and their interactions with biologically active substances, without requiring complex and expensive equipment. Particularly for express diagnostics, it is important that the resulting textures and patterns can be analyzed with relatively little time and effort. Changes in “zigzag” structures are one such indicative marker. These structures have been observed under certain drying conditions for saline solutions of DNA or BSA. Earlier studies quantified zigzag density using manual tracing. This study attempted to use machine learning to segment these patterns. A U-Net model was trained to predict segmentation masks for medium-sized patches of input images. The results agree well with manual markings on photographs with clearly visible zigzags, but in 63% of cases, the difference in segmentation exceeds 75%. This points to the need for more advanced architectures or training approaches.

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Conformational mobility of Trp125 in the EMAP II protein: molecular dynamics study

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Tryptophan fluorescence is one of the most widely used intrinsic probes of protein conformational dynamics, as the emission wavelength of a tryptophan residue is sensitive to its local environment. Although a red shift of the emission maximum is conventionally interpreted as an increase in solvent exposure of the indole ring, such interpretation may not always hold, particularly for tryptophans buried in the protein interior, where changes in the surrounding protein matrix can also modulate the emission.

Endothelial Monocyte-Activating Polypeptide II (EMAP II) contains a single tryptophan residue, Trp125, located within the functionally important tRNA-binding motif. Fluorescence measurements available in the literature indicate that its emission maximum shifts by 14 nm (from 335 to 349 nm) upon heating from 25 to 45 ℃, suggesting a major change in the residue's environment. However, the molecular mechanism behind this shift has remained unclear.

In this work, we carried out microsecond-long all-atom molecular dynamics simulations (CHARMM36m force field, at six temperatures, from 25 to 50 ℃) based on PDB 8ONG structure to investigate the conformational mobility of Trp125. The simulations reveal a temperature-driven coupled chi1/chi2 rotameric transition, confirmed by NMR data, with a midpoint matching the experimental fluorescence crossover at ˜42 ℃. Unexpectedly, the high-temperature flip-out state is more buried than the room-temperature flip-in state. Unbiased clustering of the residue's geometric environment shows that the rotameric switch repositions the indole between two distinct internal pockets. Based on the obtained data, an electrostatic emission model reproduces the experimental red shift trends, while the solvent-exposure model, based on solvent-accessible surface area (SASA), fails. The results establish a "buried flip-out" mechanism in which fluorescence is modulated by the protein matrix rather than by solvation, highlighting insightfulness of the molecular dynamics for the interpreting spectral signatures of tryptophan.

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Role of Internal conformation in the coupled deformation of DNA

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The mechanical response of DNA to external forces reveals several anomalous features, including the coupling between twisting and stretching and the unusually large deformation of specific sequence motifs. In this work, I present a theoretical model that incorporates both classical deformation modes of the DNA double helix (stretching, bending and twisting) and an internal conformational degree of freedom associated with sugar ring mobility. It is shown that this internal conformational component plays a key role in the coupled deformation of DNA and can explain the experimentally observed change in the sign of the twist–stretch coupling under applied force. The model also provides a natural interpretation of the unusually large deformation observed in the TATA-box fragment. These results highlight the importance of internal conformational dynamics for understanding anomalous mechanical behavior of DNA.

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Adsorption of the low density lipoptoteins on photo-sensitive polymer brushes: computer simulations

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Excessive concentration of the low density lipoproteins (LDLs) in blood increases the risk of cardiovascular diseases. One of the strategies to reduce its contents is the hemoperfusion therapy, when LDLs are selectively retracted by an external adsorber located outside the patient body. Recently, a photo-controllable smart surface was developed characterized by high selectivity and repeated cyclic usage. We examine the efficiency of such setup via computer simulation of a mesoscopic models for

both LDL and the azobenzene-containing polymer brush. It is found that the adsorption efficiency is seriously affected by the brush microstructure, with the bunch-like (bush-like) arrangement of its constituent chains being the most efficient.

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Counterions in DNA-Nanomaterials

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The DNA molecule consists of chains of nucleotides that, under physiological conditions, are bound by hydrogen bonds and form a double helix. The nitrogenous bases are located inside the helix, whereas the phosphate groups are exposed to the surrounding aqueous environment. This structural organization arises from the hydrophobic nature of the bases and the hydrophilic character of the phosphate groups. DNA phosphates carry a negative charge and are neutralized in solution by positively charged ions, known as counterions, which may be metal ions or molecular ions. Beyond its fundamental biological role, DNA possesses unique physical properties that make it attractive as a material for nanotechnological applications. Consequently, the fundamental properties of DNA-counterion systems are of considerable interest.

In this presentation, the results obtained using theoretical models, classical molecular dynamics simulations, and quantum chemical calculations for DNA in the presence of counterions will be discussed. In particular, DNA condensation induced by counterions of different valencies will be examined. DNA is known to condense in the presence of multivalent ions such as spermidine3+ and spermine4+, primarily due to effective charge neutralization, whereas condensation is usually not observed with monovalent ions like sodium or potassium. The analysis emphasizes that differences in DNA-counterion interactions are strongly influenced by the structure of the ion hydration shells and the ability of ions to form stable complexes with atoms of the DNA macromolecule. Understanding these hydration effects is essential for controlling the physical properties of DNA-ion systems and for the design of DNA-based nanomaterials.

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Molecular Dynamics Insights into the Stabilization of Nucleic Acid Quadruplexes

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Guanine-rich nucleic acid sequences can fold into G-quadruplexes (GQs), noncanonical DNA structures stabilized by stacked G-tetrads and monovalent cations, which play important roles in genome regulation and are widely investigated as drug targets. Despite extensive experimental and computational work, predicting G-quadruplex stability and ligand-induced stabilization remains difficult. Molecular dynamics simulations have shown that even for well-characterized telomeric GQs, apparent structural stability depends sensitively on the choice of ion parameters and water models, with

different parameterizations leading to distinct ion residence times, channel occupancies, and loop dynamics. This sensitivity underlies a key limitation of docking approaches: while docking can identify plausible ligand binding poses, it cannot predict whether ligand binding will stabilize or destabilize the GQ, as it neglects the dynamic coupling between ligands, ions, hydration, and flexible loop regions, and docking energies do not reflect GQ stability. Atomistic molecular dynamics simulations provide a way to address this limitation by explicitly capturing ligand-induced reorganization of the ionic environment and local structure. To overcome the gap between accessible simulation times and experimental denaturation times, simulations performed at variable temperature can be used to accelerate destabilization events. I will present studies combining docking and variable-temperature molecular dynamics simulations to clarify ligand effects on G-quadruplex stability.

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DNA Electromotors

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The human civilization runs on rotary motors, from cars to planes, from conveyer belts to power generators, from pumps to ice cream mixers. Surprisingly, very few examples of rotary motors exist at the nanoscale. This lecture will highlight our recent efforts to develop such nanoscale electromotors using DNA as a building material. First, I will show that a single DNA duplex can itself acts as a tiny electromotor, spinning billions of revolutions per minute when subject to external electric field. I will next describe our efforts to build more complex DNA electromotors and to realize them in practice. The lecture will highlight the applications of the all-atom molecular dynamics method to design molecular motors and to unravel microscopic phenomena that give rise to puzzling experimental observations.

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Drug repurposing: molecular modelling

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Measures to combat SARS-CoV-2 infection include the development of antiviral agents as well as the repurposing of existing drugs targeting key stages of the viral life cycle. Viral entry occurs through the interaction of the spike protein with host cell receptors and its subsequent proteolytic activation by host proteases. Identification of host cellular factors exploited during viral entry, replication, and activation enables the discovery of novel therapeutic targets. Molecular docking was employed to evaluate the binding affinity of pharmaceutical compounds to SARS-CoV-2 proteins, with particular emphasis on potential inhibitors of the furin protease and the impact of spike protein mutations on drug–protein interactions. Docking assesses the energetic favorability of ligand–target binding and supports early-stage drug repurposing. To further refine complex stability and structural features, molecular dynamics simulations were performed under physiologically relevant conditions, including explicit solvent, ions, and temperature control. Overall, our results confirm that computational modeling is an effective tool for virtual screening in antiviral drug repurposing.

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Computer simulation of cell sorting on dynamic microstructured surfaces

Cell sorting is a fundamental process in biology and biotechnology that enables the separation of heterogeneous cell populations based on their intrinsic properties. Among the various sorting strategies, affinity-based approaches exploit differences in cell-surface interactions to achieve selective cell attachment and detachment. Micropatterned adhesive surfaces provide a means to tune these interactions by controlling the surface coverage of adhesive domains, their geometry and adhesion strength. By combining these features with dynamic surface switching, the separation efficiency can be significantly enhanced through a multistage process in which the surface alternately promotes cell adsorption or desorption.

We report a computer simulation study of label-free cell sorting on dynamic microstructured adhesive surfaces, modelled as an array of randomly distributed circular adhesive domains. Cell detachment is induced by a repulsive force originating from a thermoresponsive polymer occupying the inter-domain regions. We investigate the effect of domain size on cell separation arising from sequential attachment-detachment events at fixed surface coverages of adhesive domains. For the multistage process, different scenarios of periodic surface switching are explored to optimize the efficiency of cell sorting.

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Soliton mediated long-range electron transport in Donor–Biopolymer–Acceptor systems

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Biopolymers demonstrate unique physical properties and are widely used in modern nanotechnologies long molecular bridges in Donor – Acceptor systems. There are numerous experimental evidences of the long-range electron transport in such systems.

Here we show that the mechanism of the long-range transport can be based on the soliton formation in biopolymers. It is shown that there exists a broad interval of the parameters for which an electron initially located on the donor, tunnels onto the chain where it forms a soliton-like state, which then travels to the opposite end, where it is captured by the acceptor. It is shown that the efficiency of the electron transport from the donor to the acceptor can reach 90%. Obtained results explain difference of charge transport efficiency in systems “Small Donor – Long Polymer” and “Long Polymer – Acceptor”.

These results explain also highly efficient long-range donor-acceptor electron transport in redox reactions in photosynthesis and cellular respiration in biological systems.

These results explain also highly efficient long-range donor-acceptor electron transport in redox reactions in photosynthesis and cellular respiration in biological systems.

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Spectroscopic markers of biological molecules and cells

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arious spectral methods-optical and vibrational spectroscopy, mass spectroscopy, luminescence, NMR, X-ray etc.- play a key role in analytical and prognostic research in various fields of science, industry, and medicine.In this report, we will focus on vibrational spectroscopy, its linear (IR, Raman) and nonlinear (CARS, SFG) methods, and a new method - surface-enhanced spectroscopy (SES).

In vibrational spectroscopy, spectroscopic markers are the intensity, half-width, frequency, polarization of bands, and their combinations, which are sensitive to changes in the structure of molecules or crystals under the influence of external factors. The establishment of spectral markers is an important direction in modern biophysics, because, thanks to the high specificity of vibrational spectra and their conformational sensitivity, it is possible to detect differences in the structure of DNA, proteins, lipids el without the additional labels, to determine the conformational states of biomolecules, structural rearrangements in the cell membrane, changes in the molecular composition of tissues, o to distinguish the normal state from the pathological, with an accuracy not available to other methods. Experimental and computational data obtained at the Institute of Physics of the NASU on markers of metastatic cells, lipids from resistant cells, cells interacting with the antiviral drug will be discussed. New data on CARS spectroscopy es will be presented here. Now and in the future, the main emphasis will be on mathematical processing of spectral information, correlations in spectra, machine learning and prediction.

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Photoluminescent MoS2 quantum dots surrounded by nucleotides

In this work, we have successfully dispersed MoS2 in aqueous solutions of canonical nucleotides (dAMP, or dGMP, or dCMP, or UMP) by ultrasound-assisted exfoliation. We report the first observation of visible-range photoluminescence (PL) registered from all suspensions, which we attribute to the presence of MoS2 quantum dots (QDs) in the suspensions. The comparison of PL band intensity, peak position, and spectral width suggests the essential role of MoS2-nucleic base interaction for MoS2 QDs exfoliation, colloidal stabilization, and the production of emissive quantum dots. Different structures of MoS2 QDs with dAMP are analyzed employing the DFT calculations. It is shown that dAMP can form coordination bonds with the Mo atoms located at the QD edges or at the defect sites, where direct contacts with these atoms can occur. The covalent bonds facilitate strong adsorption of dAMP on a MoS2 QD. The structural flexibility of the nucleotide adsorbed on the MoS2 QD enables a combination of noncovalent stacking interaction of the nucleobase and a coordination bond of the phosphate group with the Mo atoms located at the edges to occur. This leads to the formation of a very energetically stable complex.

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On measuring localization and delocalization patterns in molecules

After a brief introduction about the quantum 20 th century, and about the year of 2025 as the international year of quantum theory and quantum technology, according to the United Nations resolution, we begin to discuss the impact of the former and its two key narratives – the observer and the measurement - on quantum chemistry and its core concepts: the bond, localization and delocalization. We demonstrate that the latter two took the origin in the old quantum theory that started in 1900, in M. Planck’s hands. The above narratives were marked by J. Bell in his work “Against ‘measurement”, where he mentioned P.A.M. Dirac as the most distinguished of ‘why bother?’ers since P. Dirac in his paper “The Evolution of the Physicist’s Picture of Nature” considered the difficulties of quantum mechanics and divided them into two classes. Into the first one, he particularly attributed the problems of ‘observer’ and ‘measurement’ and suggested that these problems should be left for later. It is precisely the latter that is the goal of this work that splits into two goals. The first is to construct a logically consistent chain of reasoning to link to the above narratives. The second is to propose a new model of quantum measurement based on the concept that the state of a quantum system necessarily changes under measurement, that put forward in the works of Fock, von Neumann and De Broglie, and many others and that aims to measure quantum chemical localization and delocalization patterns. The latter particularly describes the formation of the hydrogen bond. The measuring protocol is performed via the measurement machine that particularly employs the architecture of neural networks.

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Quantum programming for the study of complex systems, and possible applications in biophysics

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Quantum programming fundamentally differs from classical programming, as it is based on using the properties of quantum systems in computing. Nowadays, quantum algorithms have been developed to solve a variety of fundamental and applied problems. It is expected that, with the advancement of quantum computing, quantum algorithms will outperform classical ones for a wide range of tasks.
Quantum algorithms for studying the properties of networks using quantum computers will be presented. We investigate multi-qubit quantum states that can be represented as graphs, including bipartite graphs [1], weighted graphs [2], and one-layer variational quantum graph states [3]. The entanglement of these states and their quantum correlators are calculated. We identify relationships between quantum properties and the characteristics of the corresponding classical graphs, providing a framework to study network properties using quantum programming [1–3].
Potential applications of quantum computing in biophysics will also be discussed. In particular, applications of quantum optimization algorithms, quantum algorithms for studying the properties of complex systems, and quantum machine learning for solving problems in biophysics will be considered.

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The effect of branching in modeling adsorption of impurities by polymeric adsorbents

We consider a generalized lattice model describing adsorption of dispersed obstacles on a set of branched polymer structures. There is a strong experimental evidence that branched adsorbents could be essentially more efficient than their linear counterparts. We focus on two the simplest representatives of the core-shell branched architectures: the star-like (with zero-dimensional point-like core) and comb-like polymers (with one-dimensional rigid core) with various number of branches, f, branch lengths, N, and branch separations, S (for the case of comb-like structure).
The quantitative estimates for adsorption capacity ⟨na⟩ in terms of adsorbed obstacles per monomer and the average number of bonds ⟨nbond⟩ per adsorbed obstacle (average adsorption strength) have been evaluated in a wide range of parameters f, N, and S. Both the case of implicit
diffusion of obstacles (with averaging over different arrangements of immobilized obstacles), and explicit diffusion of obstacles (allowing to study dynamics of adsorption process) have been analyzed. We found that comb-like polymers display the higher adsorption capacity but lower adsorption strength, comparing to the star-like polymers, and these effects are more pronounced with increasing branches separations S. Our analysis indicates essential role of bridging between adjacent branches by shared adsorbed particles.

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Molecular dynamics insights into the stabilization of nucleic acid quadruplexes

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Guanine-rich nucleic acid sequences can fold into G-quadruplexes (GQs), noncanonical DNA structures stabilized by stacked G-tetrads and monovalent cations, which play important roles in genome regulation and are widely investigated as drug targets. Despite extensive experimental and computational work, predicting G-quadruplex stability and ligand-induced stabilization remains difficult. Molecular dynamics simulations have shown that even for well-characterized telomeric GQs, apparent structural stability depends sensitively on the choice of ion parameters and water models, with different parameterizations leading to distinct ion residence times, channel occupancies, and loop dynamics. This sensitivity underlies a key limitation of docking approaches: while docking can identify plausible ligand binding poses, it cannot predict whether ligand binding will stabilize or destabilize the GQ, as it neglects the dynamic coupling between ligands, ions, hydration, and flexible loop regions, and docking energies do not reflect GQ stability. Atomistic molecular dynamics simulations provide a way to address this limitation by explicitly capturing ligand-induced reorganization of the ionic environment and local structure. To overcome the gap between accessible simulation times and experimental denaturation times, simulations performed at variable temperature can be used to accelerate destabilization events. I will present studies combining docking and variable-temperature molecular dynamics simulations to clarify ligand effects on G-quadruplex stability.

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Modeling aggregation of proteins on computers

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Protein aggregation refers to the process by which fully or partially unfolded proteins self-associate to make large and insoluble aggregates. Amyloid fibrils - a prominent example of the aggregates, is implicated in various neurodegenertive diseases and also has found multiple uses in technology. In this talk we will focus on what can be learned about amyloid formation using theoretical models and methods. First, we will give a broad overview of the problems and challenges facing theoretical approaches in the studies of protein aggregation, ranging from the description of small oligomers [1], which are often considered kinetic intermediates to fibrils, continuing on to particlar details of amyloid structure [2]. Then, we will present a model - RAPID - specifically designed for simulations of protein aggregates [3] in water. Finally, we will discuss microscopic details of the aggregation pathway presented by the shortest amyloidogenic peptide reported so far - KFFE [1].

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DNA Electromotors

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The human civilization runs on rotary motors, from cars to planes, from conveyer belts to power generators, from pumps to ice cream mixers. Surprisingly, very few examples of rotary motors exist at the nanoscale. This lecture will highlight our recent efforts to develop such nanoscale electromotors using DNA as a building material. First, I will show that a single DNA duplex can itself acts as a tiny electromotor, spinning billions of revolutions per minute when subject to external electric field. I will next describe our efforts to build more complex DNA electromotors and to realize them in practice. The lecture will highlight the applications of the all-atom molecular dynamics method to design molecular motors and to unravel microscopic phenomena that give rise to puzzling experimental observations.

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Counterions in DNA-nanomaterials

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The DNA molecule consists of chains of nucleotides that, under physiological conditions, are bound by hydrogen bonds and form a double helix. The nitrogenous bases are located inside the helix, whereas the phosphate groups are exposed to the surrounding aqueous environment. This structural organization arises from the hydrophobic nature of the bases and the hydrophilic character of the phosphate groups. DNA phosphates carry a negative charge and are neutralized in solution by positively charged ions, known as counterions, which may be metal ions or molecular ions. Beyond its fundamental biological role, DNA possesses unique physical properties that make it attractive as a material for nanotechnological applications. Consequently, the fundamental properties of DNA-counterion systems are of considerable interest.

In this presentation, the results obtained using theoretical models, classical molecular dynamics simulations, and quantum chemical calculations for DNA in the presence of counterions will be discussed. In particular, DNA condensation induced by counterions of different valencies will be examined. DNA is known to condense in the presence of multivalent ions such as spermidine3+ and spermine4+, primarily due to effective charge neutralization, whereas condensation is usually not observed with monovalent ions like sodium or potassium. The analysis emphasizes that differences in DNA-counterion interactions are strongly influenced by the structure of the ion hydration shells and the ability of ions to form stable complexes with atoms of the DNA macromolecule. Understanding these hydration effects is essential for controlling the physical properties of DNA-ion systems and for the design of DNA-based nanomaterials.

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Drug repurposing: molecular modelling

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Measures to combat SARS-CoV-2 infection include the development of antiviral agents as well as the repurposing of existing drugs targeting key stages of the viral life cycle. Viral entry occurs through the interaction of the spike protein with host cell receptors and its subsequent proteolytic activation by host proteases. Identification of host cellular factors exploited during viral entry, replication, and activation enables the discovery of novel therapeutic targets. Molecular docking was employed to evaluate the binding affinity of pharmaceutical compounds to SARS-CoV-2 proteins, with particular emphasis on potential inhibitors of the furin protease and the impact of spike protein mutations on drug–protein interactions. Docking assesses the energetic favorability of ligand–target binding and supports early-stage drug repurposing. To further refine complex stability and structural features, molecular dynamics simulations were performed under physiologically relevant conditions, including explicit solvent, ions, and temperature control. Overall, our results confirm that computational modeling is an effective tool for virtual screening in antiviral drug repurposing.

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Collective behavior of the lipid bilayer and the role of PIP_2 in binding the neuronal Ca^{2+} sensor protein hypocalcin

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Protein Interactions with bioactive molecules and oxide nanoparticles: spectroscopic and computational studies

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Quantum Programming for the Study of Complex Systems, and possible applications in Biophysics

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Quantum programming fundamentally differs from classical programming, as it is based on using the properties of quantum systems in computing. Nowadays, quantum algorithms have been developed to solve a variety of fundamental and applied problems. It is expected that, with the advancement of quantum computing, quantum algorithms will outperform classical ones for a wide range of tasks.
Quantum algorithms for studying the properties of networks using quantum computers will be presented. We investigate multi-qubit quantum states that can be represented as graphs, including bipartite graphs [1], weighted graphs [2], and one-layer variational quantum graph states [3]. The entanglement of these states and their quantum correlators are calculated. We identify relationships between quantum properties and the characteristics of the corresponding classical graphs, providing a framework to study network properties using quantum programming [1–3].
Potential applications of quantum computing in biophysics will also be discussed. In particular, applications of quantum optimization algorithms, quantum algorithms for studying the properties of complex systems, and quantum machine learning for solving problems in biophysics will be considered.

[1] Kh. Gnatenko, Phys. Lett. A 566, 131191 [7 p.] (2026)
[2] Kh. Gnatenko 2025 IEEE International Conference on Quantum Computing and Engineering (QCE), Albuquerque, NM, USA, 2025, 470–471 (2025)
[3] Kh. Gnatenko Eur. Phys. J. Plus 140(3), 241 [7 p.] (2025)

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Quantum programming for the study of complex systems, and possible applications in biophysics

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