9th International Conference

NANOBIOPHYSICS: Fundamental and Applied Aspects

NBP-2025

BOOK OF ABSTRACTS

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9th International Conference
NANOBIOPHYSICS: Fundamental and Applied Aspects

Organized by: B. Verkin Institute for Low Temperature Physics and Engineering
of the National Academy of Science of Ukraine

6-9 October 2025, Kharkiv. Ukraine

9th International Conference NANOBIOPHYSICS: Fundamental and Applied Aspects
(6-9 October 2025, Kharkiv): Conference Program and Book of Abstracts./
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This book contains 86 peer-reviewed abstracts of reports presented at the 9th International Conference NANOBIOPHYSICS: Fundamental and Applied Aspects 2025. The materials represent current results of multidisciplinary studies in the field of nanobiophysics, including data on nanobiohybrids formed by 1-D or 2-D nanomaterials with biomolecules, properties of biomolecules on nanoparticles and nanostructured surfaces, physical properties of biomolecular nanosystems, theoretical calculations and computer modeling of nanobiosystems, and various applied aspects of nanobiophysics. Also abstracts of the talks given within the framework of the NanoBioPhysics-2025 round table "History of Biophysics in Kharkiv" are presented.

A collection of the accepted conference manuscripts will be published in the special issues of “Biophysical Bulletin” and “Low Temperature Physics” journals as the conference proceeding.

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PREAMBLE

Dear Participants of the NBP-2025 Conference,

It is our great pleasure to welcome you to the 9th International Conference **"NANOBIOPHYSICS: Fundamental and Applied Aspects"** (NBP-2025) which will be held from October 6 to 9, 2025 in Kharkiv, Ukraine at the B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine.

"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. Previous eight conferences were organized biennially in Kyiv and Kharkiv alternately.

The aim of our conferences is to enlighten urgent problems in a modern scientific field combining biophysics and nanotechnology, to evaluate its progress and advances, and to discuss prospects of its further development. These topical issues will be debated at the NBP-2025 during the following sessions:

1. Nanobiohybrids of 1-D or 2-D nanomaterials with biomolecules
2. Biomolecules on nanoparticles and nanostructured surfaces
3. Physical properties of biomolecular nanosystems
4. Theoretical calculations and computer modeling of nanobiosystems
5. Applied aspects of nanobiophysics
6. Round table "History of Biophysics in Kharkiv"

It is expected that the NBP-2025 conference will provide opportunities to share up-to-date information obtained in the fields of biophysics and nanosciences, to exchange new ideas, and to tighten existing or to gain new collaboration. A special attention will be devoted to problems of professional promotion of young researchers. The conference will bring together colleagues from the international scientific community.

We wish the conference participants fruitful work, high-quality scientific presentations, and long-awaited meeting with the colleagues.

Organizing Committee
of the 9th International Conference
**"NANOBIOPHYSICS:
Fundamental and Applied Aspects"**

9th International Conference
NANOBIOPHYSICS: Fundamental and Applied Aspects
NBP - 2025

CONFERENCE PROGRAM

6 OCTOBER, MONDAY

10.00-10.15	**OPENING OF THE CONFERENCE**	

Physical properties of biomolecular nanosystems

Chair	***Victor Karachevtsev***	
10.15-10.45	**BIOPHYSICS OF GFP PROTEIN – A MARKER COMMONLY USED AS A FLUORESCENT LABEL** Krasowska J., Bzowska A., Breer K., **Wielgus-Kutrowska B.**	**PL6**
10.45-11.05	**MECHANICAL PROPERTIES OF THE MEMBRANE OF CIRCULATING METASTATIC TUMOR CELLS AS A DIAGNOSTIC MARKER** **Gnatyuk O.P.**, Olenchuk M.V., Romanenko S.V., Monastyrskyi G.P., Solyanik G.I., Kolesnik D.L., Dovbeshko G.I.	**O10**
11.05-11.25	**CORE-SHELL Au@PEtOx-PBuOx COLLOIDS WITH TUNABLE LCST TRANSITION FOR THERMALLY SWITCHABLE OPTICAL APPLICATIONS** Yeshchenko O., Daoud L., **Fedotov O.**, Khort P., Krupka O.	**O8**
11.25-11.30	***General Conference Photo (online)***	
11.30-11.40	***Technical break***	

Physical properties of biomolecular nanosystems

Chair	***Victor Karachevtsev***	
11.40-12.10	**FROM UV TO IR: STRATEGIES FOR COMPLETE SOLAR ENERGY CAPTURE IN PHOTOSYNTHESIS** **Freiberg A.**	**PL1**
12.10-12.30	**INTRINSIC DISORDER OF THE bHLH-PAS FAMILY OF TRANSCRIPTION FACTORS** Kolonko-Adamska M., **Greb-Markiewicz B.**	**O11**
12.30-12.50	**FEATURES OF EXCITATION OF NUCLEIC ACIDS COMPONENT ON THE MATRIX SURFACE BY ELECTRON BEAM** **Sukhoviya M.I.**, Shafranyosh M.I., Kovach V.V., Shafranyosh I.I.	**O27**
12.50-14.00	***Time for Lunch***	

Applied aspects of nanobiophysics

Chair	***Marina Kosevich***	
14.00-14.30	**COUNTERIONS IN DNA-NANOMATERIALS** **Perepelytsya S.M.**	**PL4**
14.30-14.50	**SYNERGISTIC THREAT TO THE NERVOUS SYSTEM FROM COMBINED EXPOSURE TO COPPER AND WOOD SMOKE PARTICULATE MATTER** Dovbeshko G.I., Krisanova N.V., Pozdnyakova N.G., Pastukhov A.O., Dudarenko M.V., Tarasenko A.S., Borysov A.A., Bezkrovnyi O., Gnatyuk O., Tolochko A., Boiko V., **Borisova T.O**	**O4**
14.50-15.10	**ARTEMISININ: AN ANTIMALARIAL AGENT DISRUPTING NANOCRYSTAL HEMOZOIN FORMATION, WITH ANTITUMOR AND IMMUNE-MODULATING PROPERTIES** **Skorokhod O.**, Valente E., Mandili G., Ulliers D., Schwarzer	**O29**
15.10-15.20	***Technical break***	
15.20-15.40	**NANOBIOHYBRIDS OF 2D MoS_2 WITH ANTICANCER DRUGS: EXPERIMENTAL & THEORETHICHAL CHARACTERIZATION, APPLICATION PROSPECTS** **Pashynska V.A.**, Kosevich M.V., Stepanian S.G., Kuzema P.O., Boryak O.A., Voloshin I.M., Karachevtsev V.A.	**O24**

15.40-16.00	**APPLICATION OF NIR-REDUCED GRAPHENE QUANTUM DOTS FOR BIOSENSING OF NEUROTRANSMITTERS/ HORMONES** **Sharma P.**	**O28**
16.00-16.20	**BIOLOGICAL AND MECHANICAL PROPERTIES OF THE COMPOSITES CONTAINING GRAPHENE FLAKES OBTAINED FROM MINERAL GRAPHITE** **Głuchowski P.**, Grabowska A., Bartczak N., Junka A., Kowalczyk J., Stręk W.	**O9**
16.20-16.40	**SURFACE AND INTERFACE EFFECTS IN THE ANTIBACTERIAL ACTIVITY OF NANO- AND MICROSCALE OXIDES OF ZINC AND GALLIUM** **Strzhemechny Y.M.**, Brannon J.H., Johnson D.A., McGillivray S.M., Wiglusz R.J., Watras A., Boiko V.V., Danchuk V.V.	**O30**
16.40-18.00	**Poster Session 1** *Moderator Marina Kosevich*	**P1-P15**

7 OCTOBER, TUESDAY

Theoretical calculations and computer modeling of nanobiosystems

Chair	***Vlada Pashynska***	
10.00-10.30	**SARS-COV-2 EVOLUTION FROM 2021 TO 2025: GENERAL FACTS AND RESEARCH FINDINGS** Khmil N.V., **Shestopalova A.V.**	**PL4**
10.30-10.50	**ACCURATE MACHINE LEARNING APPROACH TO PROTEIN-LIGAND DOCKING** **Voitsitskyi T.**, Koleiev I., Starosyla S., Yesylevskyy S.	**O34**
10.50-11.10	**STABILITY OF COMPLEXES OF Ag^+ IONS WITH NITROGENOUS BASES OF THE DNA MOLECULE** **Osokin Y.S.**, Perepelytsya S.M.	**O23**
11.10-11.30	**FTIR SPECTROSCOPY BASED IDENTIFICATION OF SPECTRAL BIOMARKERS ASSOCIATES WITH BIOLOGICAL AGE USING MACHINE LEARNING** **Kot O.**, Kyrylenko R., Melnychenko M., Midlovets K., Makhnii T., Krasnenkov D.	**O17**

11.30-11.40	***Technical break***	
11.40-12.00	**PARTIAL LEAST SQUARES ANALYSIS OF ATR-FTIR SPECTRA FOR INTRAOPERATIVE CHARACTERIZATION AND RAPID BIOCHEMICAL PROFILING OF BRAIN TUMORS** **Gubareni Ie.V.**, Gnatiuk O.P., Shmeleva A.A., Malysheva T.A., Vaslovich V.V., Dovbeshko G.I.	**O12**
12.00-12.20	**A PHYSICALLY INTERPRETABLE NEURAL NETWORK MODEL FOR DETERMINING THE ENERGY OF BIOMOLECULES BASED ON THEIR STRUCTURE** **Terets A.D.**, Nikolaienko T.Yu.	**O31**
12.20-12.40	**DFT STUDY OF TERNARY COMPLEXES OF MoS_2 WITH URACIL AND NOBLE METAL CLUSTERS: STRUCTURE, STABILITY AND SPECTRA** **Stepanian S.G.**	**O26**
12.40-14.00	***Time for Lunch***	

Biomolecules on nanoparticles and nanostructured surfaces

Chair ***Stepan Stepanian***

14.00-14.30	**ON POSSIBILITIES OF MINERAL MOS_2 PARTICIPATION IN PREBIOLOGICAL CHEMICAL EVOLUTION** **Kosevich M.V.** , Shelkovsky V.S., Boryak O.A., Pashynska V.A., Kuzema P.O., Stepanian S.G., Karachevtsev V.A.	**PL2**
14.30-14.50	**FROM CHAOS TO THE FIRST STORED INFORMATION AND ORIGIN OF LIFE** **Krasnokutski S.A.**	**O18**
14.50-15.10	**PMMA:PVP BLENDED NANOFIBERS LOADED WITH ANTIBIOTIC LEVOFLOXACIN FOR ANTIBACTERIAL APPLICATION** **Karachevtsev V.A.**, Plokhotnichenko A.M., Trufanov O.V., Stepanian S.G.	**O14**
15.10-15.20	***Technical break***	
15.20-15.40	**BSA-PERSISTENT NANOPARTICLES INTERACTION: LINKING OPTICAL PROPERTIES TO STRUCTURAL PROTEIN CHANGES** **Boiko V.V.**, Fandzloch M., Bezkrovnyi O., Foley S.	**O3**

15.40-16.00 **BEYOND LIGAND BINDING: DECODING GPCR ACTIVATION ON BUDDED BACULOVIRUS NANOPARTICLES VIA FLUORESCENCE ANISOTROPY AND CONFORMATIONAL BIOSENSORS.** **O16**
Kopanchuk S., Veiksina S., Joandi E., Leht R.R, Rinken A.

16.00-17.30 **Poster Session 2** **P16-P30**

Moderator Olena Gnatyuk

8 OCTOBER, WEDNESDAY

Physical properties of biomolecular nanosystems

Chair ***Galina Dovbeshko***

10.00-10.30 **ON THE TELOMERE MODEL OF AGING: UNRAVELLING THE HYDROGEN BONDING PATTERNS IN G-QUADRUPLEXES. FROM STRUCTURE TO FUNCTION.** **PL3**
Kryachko E.S., MacDougall P.J., Neal S.

Nanobiohybrids of 1-D or 2-D nanomaterials with biomolecules

Chair ***Galina Dovbeshko***

10.30-10.50 **MOLYBDENUM DISULFIDE QUANTUM DOTS EXFOLIATED WITH NUCLEOTIDES: SPECTROSCOPY AND AFM CHARACTERIZATION, ANALYSIS OF TEMPORAL STABILITY** **O20**
Kurnosov N.V., Voloshin I.M., Lytvyn O.S., Valeev V.A., Plokhotnichenko A.M., Karachevtsev V.A.

10.50-11.10 **MANGANESE OXIDE NANOCRYSTALS INDUCE ERYPTOSIS, A REGULATED CELL DEATH OF MATURE RED BLOOD CELLS** **O32**
Tkachenko A.S., Yefimova S.L., Kot Yu.G., Klochkov V.K., Onishchenko A.I., Prokopiuk V.Yu.

11.10-11.30 **Mn_3O_4 NANOCRYSTALS ACTIVATE CASPASE-3 IN ERYTHROCYTES** **O25**
Prokopiuk V.Yu., Yefimova S.L., Klochkov V.K., Kot Yu.G., Onishchenko A.I., Tkachenko A.S.

11.30-11.40 *Technical break*

Applied aspects of nanobiophysics

Chair ***Nikita Kurnosov***

11.40-12.00 **STRUCTURE-ACTIVITY RELATIONSHIPS IN $Cu_xCo_{1-x}WO_4$ SYSTEMS FOR DEGRADATION OF ACETAMINOPHEN UNDER SOLAR LIGHT** **O15**
Czekanowska D., Grzegórska A., Zielińska-Jurek A., Salazar H., Murauskas T., Głuchowski P.

12.00-12.20 **MODEL-BASED QUANTIFICATION OF SURFACE PASSIVATION EFFECTS INDUCED BY BIOGEL IMMOBILIZATION IN FIELD-EFFECT BIOSENSORS** **O7**
Karpenko Y.V., Dzyadevych S.V.

12.20-12.40 **COMPARATIVE MECHANISMS OF MICROVESICULATION IN RED BLOOD CELLS AND BACTERIA** **O1**
Volobuiev D.O., **Berest V.P.**

12.40-14.00 *Time for Lunch*

Applied aspects of nanobiophysics

Chair ***Nikita Kurnosov***

14.00-14.20 **DEVELOPMENT AND CRYOPRESERVATION OF PROBIOTIC-ENRICHED ALGINATE HYDROGEL FILMS FOR WOUND CARE APPLICATIONS** **O33**
Trufanov O.V., Ananina H.E., Martsenyuk V.P., Abrafikova L.G., Nardid E.O.

14.20-14.40 **A RAPID, GREEN AND COST-EFFECTIVE SYNTHESIS OF PH- AND HYDROXYL GROUP SENSITIVE CARBON DOTS FOR SENSING APPLICATIONS** **O20**
Kujawa D., Ptak M., Głuchowski P.

14.40-15.00 **ON LIGANDS FOR «GREEN» SYNTHESIS OF LUMINESCENT Ag-In-Se NANOPARTICLES** **O22**
Nikolaienko A., Kapshuchenko O., Karlash A., Dmytruk A.

15.00-15.20 **TUNING OF ANTIBACTERIAL ACTION OF ZnO MICROCRYSTALS BY MODIFYING SURFACE DEFECTS WITH Fe-DOPING** **O5**

Brannon J.H., Rubio E.H., Cohens N.S., Hattarki M.N., Strzhemechny Y.M., McGillivray S.M., Sobierajska P., Pinchuk N., Wiglusz R.J., Watras A., Boiko V.V., Danchuk V.V.

15.20-15.30 ***Technical break***

Round table "History of Biophysics in Kharkiv"

15.30-17.30 ***Moderator Marina Kosevich***

PL7
RT1

Nanobiophysics at the B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine: a historical review
Karachevtsev V.A.

RT2

How the Biophysics in IRE started and progressed: according to the memoirs by V. Ya. Maleev
Shestopalova A.V.

RT3

Biophysicists of Kharkiv National University and the Advance of Biophysics
Berest V.P.

RT4

Tribute to academician B.I. Verkin – the founder of the biophysical and biomedical research at the Institute for Low Temperature Physics and Engineering
Kosevich M.V.

RT5

Contribution of Professor Blagoi Yu.P. to molecular biophysics of nucleic acids
Kosevich M.V.

RT6

In memoriam: Yu.V. Malyukin, the founder of nanobiophysics in the Institute for Scintillation Materials of STC "Institute for Single Crystals"
Yefimova S.L., **Lisetski L.N.**

RT7

Tribute to Professor O.M. Ogurtsov
Bliznyuk O.M.

General discussion

9 OCTOBER, THURSDAY

Applied aspects of nanobiophysics

Chair *Valentina Zobnina*

10.00-10.20	**POTENTIAL OF Eu^{3+} AS A LUMINESCENT MARKER FOR RAPID MONITORING OF THE Ce^{4+}/Ce^{3+} TRANSITIONS IN CeO_2 CATALYST** **Bezkrovnyi O.**, Szymczak M., Marciniak L., Vorochta M.	**O2**
10.20-10.40	**HIGH-RESOLUTION SEM MICROSCOPY FOR STUDYING LIPOSOMES AND MODEL CIRCULATING TUMOR CELLS INCUBATED WITH M_OS_2 AND WS_2 NANOPARTICLES** **Monastyrskyi G.**, Olenchuk M., Gnatyuk O., Solyanik G., Kolesnyk D., Karakhim S., Dovbeshko G.	**O21**
10.40-11.00	**THE EFFECTS OF SYNGAP KNOCKDOWN ON THE AMPA RECEPTOR SURFACE MOBILITY** **Hnatiuk S.I.**, Ignácz A., Daburon S., Breillat C., Sainlos M., Choquet D.	**O13**
11.00-11.10	***Technical break***	
11.10-11.30	**EXPERIMENTAL AND THEORETICAL INVESTIGATION OF THE LEVIFLOXACIN-PVP COMPLEX** **Bulova A.G.,** Glamazda A.Yu., Stepanian S.G., Plokhotnichenko A.M., Karachevtsev V.A.	**O6**
11.30-11.50	**SELF-FORMATION OF COHERENT CORRELATED STATES OF INTERACTING PARTICLES IN BIOMOLECULES FOR THE REALIZATION OF NUCLEAR FUSION IN BIOSYSTEMS** **Vysotskii V.I.**	**O35**
11.50-13.00	**Poster Session 3**	**P31-P45**
13.00	***Closing Ceremony***	

POSTER SESSION 1
6 October, Monday

POSTER SESSION 2
7 October, Tuesday

POSTER SESSION 3
9 October, Thursday

Plenary lectures

PL1

FROM UV TO IR: STRATEGIES FOR COMPLETE SOLAR ENERGY CAPTURE IN PHOTOSYNTHESIS

Freiberg A. [1,2]*
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Photosynthesis powers nearly all life on Earth, yet optimizing light energy utilization across the entire solar spectrum remains a key scientific challenge with far-reaching implications for sustainability [1]. While canonical systems capture primarily visible light, a large fraction of solar energy lies in the infrared region, and ultraviolet photons—though scarce—can profoundly affect pigment–protein architectures. Here, we investigate how photosynthetic bacteria extend light harvesting across an extraordinary range (200–1100 nm) through a combination of native adaptations and engineered modifications. By resolving the dynamic interplay between pigments and their protein scaffolds, we reveal strategies that push the theoretical limits of photosynthetic efficiency. These insights chart a path toward bioinspired energy technologies capable of leveraging the full breadth of solar radiation.

1. K. Timpmann, M. Rätsep, A. Freiberg, Scientific Reports, **13**, 22299 (2023).

PL2

ON POSSIBILITIES OF MINERAL MoS_2 PARTICIPATION IN PREBIOLOGICAL CHEMICAL EVOLUTION

Kosevich M.V. [1]*, Shelkovsky V.S.[1], Boryak O.A. [1], Pashynska V.A.[1], Kuzema P.O. [2],
Stepanian S.G. [1], Karachevtsev V.A. [1]
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Some events of prebiotic biochemical evolution can be approached in terms of nanoscience, as they occur at the level of single molecules, clusters, and nanoparticles. The method of choice for studying these objects and related processes is mass spectrometry.

Within a long chain of chemical evolution events, spanning from the primary synthesis of simple organic molecules to the assembly of biopolymers [1], in the present work, we addressed a stage of simple biomolecules interactions with the Earth's natural minerals containing transition metal dichalcogenides, molybdenum disulfide in particular. The presumable evolutionary scenario in such systems is known as the “iron-sulfide world” hypothesis [2]. It states that initially metal sulfides acted as “external” catalysts for simple organic molecules transformations; then the metals were captured into biomolecules mainly as enzymes’ cofactors.

We have applied laser desorption/ionization (LDI) mass spectrometry to characterize a set of systems composed of MoS_2 nanopowder and simple biomolecules: amino acids, nucleic acid nitrogen bases, and thiols. The LDI results were interpreted from the standpoint of searching for transformations of biomolecules in these systems. Noticeable effects were observed for thiol-containing compounds.

Three main findings were achieved. Firstly, the expected results of MoS_2-biomolecule interactions were redox transformations of redox-active organic compounds due to the known catalytic and redox activity of MoS_2. Some of these reactions led to the formation of covalent dimers, i.e., to the complication of the biomolecules. E.g., cystine amino acid was formed due to covalent dimerization of cysteine and, similarly, hexapeptide was formed from two glutathione tripeptides. MoS_2 served as a nanozyme here. The next step in molecular evolution was the incorporation of such inorganic cofactors (nanozymes) into biological enzymes. Our second finding was related to this step. Namely, two of the studied compounds – 6-thiopurine and 6-thioguanine nitrogen bases – have formed complexes with the Mo atom (associated with O and S ligands) on their contacts with MoS_2 material. Thus, the selectivity of Mo extraction from MoS_2 mineral by certain heterocyclic compounds was observed, since no complexes with Mo with other types of studied biomolecules were registered. Thirdly, the release of ligand-free Mo^+ ions from the MoS_2 nanosheets under the effect of simple thiols was detected. Such naked Mo^+ ions may cause their own biological effect.

DFT quantum chemical calculations were performed to determine the structures of noncovalent and covalent associates of the biomolecules with the MoS_2 nanosheet fragment.

The results obtained demonstrate several options of MoS_2 participation in the transformation of organic matter, which may be related to ancient biochemical evolution.

Acknowledgements: This work was supported by the National Academy of Sciences of Ukraine Grant N0123U100628. LDI mass spectrometric studies were performed at the Center for the collective use of scientific instruments/equipment "Mass spectrometry and liquid chromatography" of the National Academy of Sciences of Ukraine.

1. A. Longo, B. Damer, Life*,* **10(**5), 52 (2020).
2. G. Wächtershäuser, Prog Biophys Mol Biol, **58**(2), 85(1992).

PL3

ON THE TELOMERE MODEL OF AGING: UNRAVELLING THE HYDROGEN BONDING PATTERNS IN G-QUADRUPLEXES. FROM STRUCTURE TO FUNCTION

Kryachko E.S.[1*], MacDougall P.J.[2], and Neal S.[2]
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The paradigm of aging (*vs.* longevity) is now on everyone's lips and thoughts. People wish to live longer, and this is natural: life matters! Scientists all over the world are trying to slow down aging. It is real: suffice to remember that in the epic of any nation there have always been people's dreams to prolong youth and even acquire immortality. If we turn to the Bible, Adam gave his wife the name Eve that means "life." The Bible says that Adam himself lived 930 years, his son Seth 912 (he was born when Adam was already 330 years old), Adam's grandson Enosh - 905. What happened in human evolution that cut the limit of aging to about one hundred years? And when João Pedro de Magalhães proposed a theory [1] dubbed him as 'the longevity bottleneck hypothesis', stating that a long time ago (over 100 million years ago, in the Mesozoic era), evolutionary pressure on mammals by dinosaurs, as the dominant predators, led to the loss or inactivation of so called 'longevity genes' and pathways associated with long life. The cure for aging/longevity has long been the Holy Grail of medicine that these days were joined by physics and quantum chemistry. In 2009, the Nobel Prize in Physiology or Medicine was awarded to E.H. Blackburn, C.W. Greider, and J.W. Szostak "for the discovery of how chromosomes are protected by telomeres...". Actually, they solved a major problem in biology of how the chromosomes can be copied in a complete way during cell divisions and how they are protected against degradation. It was demonstrated that the solution is to be found in the caps of the chromosomes – the telomeres – and in an enzyme that forms them – telomerase: the long, thread-like DNA molecules that carry our genes are packed into chromosomes, capped by telomeres. The latter contain G (for guanine)-rich repeat sequences that are capable to fold into four-stranded so-called G-quadruplexes or G4 structures unveiled in X-ray diffraction experiments conducted in 1962 and "initially considered a structural curiosity".

In this work [2], we investigate the molecular basis of the telomere model of ageing. Its key trait is the hydrogen (H-) bonding patterns of G-tetrads that serve a top of G-quadruplexes composing telomeres. The surprising result is the differing chemical nature of the hydrogen-bonding interactions of the over-coordinated oxygen (OCO) atoms in the ‘naked’ G-quadruplex. These insights are gained via performing topological analysis of the Laplacian of the charge density, $\nabla^2\rho(\mathbf{r})$, identifying regions of local charge concentration and depletion, in the vicinity of the over-coordinated oxygen atoms, and overlay this topology over the bond paths found via topological analysis of $\rho(\mathbf{r})$. Of the two hydrogen bonds to each over-coordinated oxygen atom, one is conventional and presumably stronger, while the other is longer and presumably weaker. But topological analysis reveals that the longer H-bond is unconventional in that the hydrogen bond is *not* coordinated to either of the lone pairs on oxygen, but rather is aligned with the *minimum* in charge concentration between them! That is, the subatomic features of the over-coordinated oxygen atoms in the ‘naked’ G-quadruplex reveal that the unconventional hydrogen bonds are actually examples of chalcogen bonding where the donor atom is hydrogen. We thus show that these patterns demonstrate a variety of bonding characters – from classic hydrogen bonds to so called ‘over-coordinated oxygen’ bifurcated H-bonds that thus result in non-rigidity (floppiness) of G-tetrad structures. This work has implications for the functionality of G-quadruplexes and, in turn, for the *complexity* of the quadruplex-based telomere model of aging.

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PL4

COUNTERIONS IN DNA-NANOMATERIALS

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The structure of the DNA molecule is strongly influenced by environmental conditions due to the presence of both hydrophobic (nitrogenous bases) and hydrophilic (phosphate groups) components in its structure. The phosphates of DNA carry a negative charge (-e) and in an aqueous environment are neutralized by positively charged counterions, usually metal K^+, Mg^{2+} or molecular ions such as polyamines (spermidine^{3+} and spermine^{4+}). The counterions condense onto DNA, forming a layer of ionic atmosphere around the macromolecule. Together with surrounding water molecules, they create an ion-hydration shell that stabilizes the structure of the double helix. The properties of the DNA ion-hydration shell are crucial for understanding the physical mechanisms underlying DNA's biological functions. At the same time, the unique physicochemical characteristics of DNA make it an attractive material for various nanotechnological applications. Moreover, the total amount of DNA on Earth is comparable to the amount of oil, which highlights its potential as a practically abundant and sustainable material for future technologies [1]. The talk will outline various types of DNA-based materials with potential applications in nanotechnology, including metallized DNA, DNA origami, and DNA nanomotors. Particular attention will be given to the use of DNA in lithium-ion supercapacitors [2,3]. The role of counterions in determining material properties will be discussed, with a focus on molecular dynamics results for the structure of DNA in the presence of metallic and molecular counterions, including modeling of DNA gels with LiCl salt [4-8]. In this context, the effects of counterion-induced DNA condensation will be highlighted, and a newly observed phenomenon of DNA aggregation induced by Li^+ counterions will be presented, along with the physical mechanism proposed to underlie the formation of DNA-Li^+-DNA crosslinks. These findings provide important insights into the potential of DNA as a novel material for a wide range of technological applications.

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PL5

SARS-COV-2 EVOLUTION FROM 2021 TO 2025: GENERAL FACTS AND RESEARCH FINDINGS

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COVID-19, caused by the SARS-CoV-2 coronavirus, may have faded from the headlines but has not disappeared, as SARS-CoV-2 continues to evolve. The Omicron variant (lineage B.1.1.529), first designated as a SARS-CoV-2 Variant of Concern on 26 November 2021, rapidly became the dominant strain due to a high number of spike protein mutations that enhanced transmissibility and immune evasion compared with earlier lineages. The exact number of new subvariants of Omicron is difficult to determine, as their classification is continuously updated, and their total number has increased significantly since 2022–2023. As of August 2025, at least 10–12 active or newly detected subvariants can be highlighted, including subvariants BA.2.86 and its descendant JN.1, XBB lineages, NB.1.8.1 (Nimbus), and XFG (Stratus).

Efforts to fight the coronavirus SARS-CoV-2 include the development and investigation of vaccines, monoclonal antibodies, and specific antiviral drugs targeting key stages in the viral life cycle. Most studies focus on the numerous structural and nonstructural viral proteins encoded by SARS-CoV-2, including the SARS-CoV-2 spike glycoprotein (S protein), papain-like, and the main proteases. Additionally, studying human cell proteases such as furin and type II transmembrane serine protease (TMPRSS2) is crucial for understanding the mechanisms involved in the activation of the SARS-CoV-2 S protein. The attachment of SARS-CoV-2 to the host cell is a critical step in the infection process, mediated by interactions between the S protein and the host cell's angiotensin-converting enzyme 2 receptor (ACE2). The proteolytic activation of the S protein by host proteases is necessary to convert its precursor form into a biologically active form, enabling the subsequent fusion of viral and cellular membranes. The S protein has a cleavage site that is processed by host furin to prime it for TMPRSS2 protease processing. The furin cleavage site is unique to the SARS-CoV-2 S protein, making it particularly efficient at utilizing host proteases for entry. Thus, furin inhibition can block this important activation step, preventing the virus from effectively infecting host cells.

Our study aims to evaluate the binding affinity of glucocorticoids to the S protein–ACE2 complex in two SARS-CoV-2 variants: the wild-type Wuhan strain and the JN.1 subvariant of Omicron, in order to identify potential glucocorticoid binding sites and the amino acid residues involved in interactions through molecular docking. In moderate and severe cases of COVID-19, the therapeutic benefits of glucocorticoids are attributed to their ability to mitigate immune-mediated lung injury and suppress the cytokine storm. Docking results show that the glucocorticoids under investigation bind to specific sites on the S protein–ACE2 complex, involving both A and B chains in the wild type but only the A chain in the mutated JN.1 Omicron subvariant. These glucocorticoids may block viral entry in addition to their anti-inflammatory effects. Identifying these binding sites is key to developing antiviral strategies and designing drugs to disrupt S protein–ACE2 interactions or adapt to viral mutations.

Another aim is to investigate the potential sites of furin protease binding to the S protein in different conformations and to evaluate the binding affinity of non-specific antiviral drugs to the S protein–furin protease complex using a molecular docking approach. The results demonstrate that furin can interact with the S protein in both "open" and "closed" conformations, even outside the canonical furin cleavage site. This study also shows that, regardless of furin's binding location on the S protein, inhibitors preferentially bind to furin, particularly at its catalytic site, rather than to the S protein within the investigated SARS-CoV-2 S protein–furin complexes, thereby preventing S protein processing. A detailed atomic-level understanding of S protein–furin interactions with antiviral agents, enabled by molecular docking technologies, could support the development of new therapeutic agents or drug combinations to combat COVID-19. Therefore, both studies provide valuable insights for assessing these compounds as potential antiviral drugs against SARS-CoV-2.

PL6

BIOPHYSICS OF GFP PROTEIN – A MARKER COMMONLY USED AS A FLUORESCENT LABEL

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Green Fluorescent Protein (GFP) and its enhanced variants, such as EGFP, are indispensable tools in molecular and cellular biology, widely employed as fluorescent labels in live-cell imaging, protein localization, and folding studies. While GFP is routinely used for its visible green fluorescence arising from a buried chromophore within its β-barrel structure, the full complexity of its folding, aggregation and interactions with the environment remains underexplored.

In our study, we addressed several biophysical aspects of GFP, focusing on folding mechanisms, chromophore maturation, and the influence of environmental factors such as pH and the surrounding medium. Using a combination of spectroscopic techniques (UV-VIS, fluorescence, circular dichroism, analytical ultracentrifugation, and kinetic studies via stopped-flow pH-jump methods), we investigated the differences between the de novo folding of EGFP (from a never-folded state) and its refolding after denaturation. Our results show that these processes differ not only in folding kinetics but also in their tendency to aggregate - the presence of the chromophore significantly influences folding pathways, with aggregation being more pronounced during refolding [1].

Using electron spin resonance and spin-trapping techniques, we also demonstrated that correctly folded EGFP effectively quenches reactive oxygen species. This suggests a photoprotective role for this protein. However, excessive ROS can damage the chromophore, impairing fluorescence [2].

Our findings shed new light on the biophysical properties of GFP and its role in nature. Researchers need to be aware of the slow maturation process of the chromophore and the propensity of GFP to aggregate. Understanding these factors is crucial for the properly interpreting of GFP-based assays and designing optimized fluorescent tools for use in biotechnology and bioimaging.

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Oral presentations

O1

COMPARATIVE MECHANISMS OF MICROVESICULATION IN RED BLOOD CELLS AND BACTERIA

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Microvesicle release represents a conserved membrane remodeling strategy across biological systems. In red blood cells (RBCs), microvesiculation is a hallmark of physiological aging and storage lesions, while in bacteria, outer membrane vesicle (OMV) formation supports stress adaptation and intercellular communication. Although these processes occur in evolutionarily distant systems, they share biophysical determinants such as membrane curvature, surface charge heterogeneity, and compositional asymmetry. In this study, we present a comparative analysis of vesiculation mechanisms in RBCs and bacteria, integrating lipidomics, peptidomics, and surface chemistry approaches.

In erythrocytes, vesicle release is driven by cytoskeletal destabilization, oxidative modifications of hemoglobin and membrane proteins, and lipid asymmetry collapse (notably externalization of phosphatidylserine). Zeta potential reduction lowers electrostatic repulsion, promoting membrane budding. Lipidomic analyses confirm selective enrichment of lysophospholipids and sphingomyelin in RBC-derived vesicles, while proteomic profiling highlights accumulation of oxidatively modified band 3 protein and cytoskeletal fragments.

In bacterial OMVs, vesiculation is linked to local defects in peptidoglycan–outer membrane interactions and curvature stress induced by phosphatidylglycerol, cardiolipin, and lipopolysaccharides. Using lipidomics and peptidomics, we show that bacterial vesicles are enriched in anionic phospholipids, outer membrane proteins, and stress-related peptides, reflecting their role in host-pathogen interactions. High-resolution X-ray photoelectron spectroscopy (XPS) allowed precise quantification of surface chemical composition, confirming that OMVs exhibit an increased ratio of negatively charged lipids and proteinaceous components compared to intact bacterial envelopes.

Despite contextual differences, both systems demonstrate that vesiculation is strongly governed by membrane charge distribution and biophysical instabilities. While RBC vesiculation primarily eliminates damaged components to preserve circulation competence, bacterial OMVs act as vehicles for communication, antimicrobial resistance, and immune evasion. Importantly, compositional analyses reveal convergent features: enrichment in oxidized or stress-modified molecules, asymmetric lipid distribution, and surface charge reduction as common drivers of vesiculation.

By combining lipidomics, peptidomics, and surface-sensitive methods such as XPS, our work provides a comprehensive molecular-level characterization of vesicles across domains of life. This comparative biophysical framework not only advances understanding of universal principles of membrane remodeling but also suggests translational applications: monitoring RBC vesicles as quality markers in transfusion medicine, and targeting OMV pathways in antimicrobial strategies.

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O2

POTENTIAL OF Eu^{3+} AS A LUMINESCENT MARKER FOR RAPID MONITORING OF THE Ce^{4+}/Ce^{3+} TRANSITIONS IN CeO_2 CATALYST

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The chemical state of a Ceria-based catalyst is one of the most important factors determining its activity. Thus, developing a new remote and relatively simple technique to monitor the Ce^{4+}/Ce^{3+} transitions in ceria under operating conditions is an important task in applied science. Traditional techniques for direct determination of the chemical state of materials (X-ray photoelectron spectroscopy (XPS), X-ray absorption near edge structure (XANES), and electron energy loss spectroscopy (EELS)) are very accurate but very expensive and complex. Thus, our work is focused on investigating the possibility of using luminescence techniques to monitor the dynamics of Ce^{4+}/Ce^{3+} transitions in ceria catalysts under in-situ conditions. Our idea is based on the strong sensitivity of the luminescence spectra of Eu^{3+} ions to the local environment of cationic centers. The intensity of the $^5D_0 \rightarrow {}^7F_2$ electronic transition strongly depends on the local ions' environment whereas the intensity of the emission bands associated with the $^5D_0 \rightarrow {}^7F_1$ magnetic dipole transition is independent of the ions' symmetry.

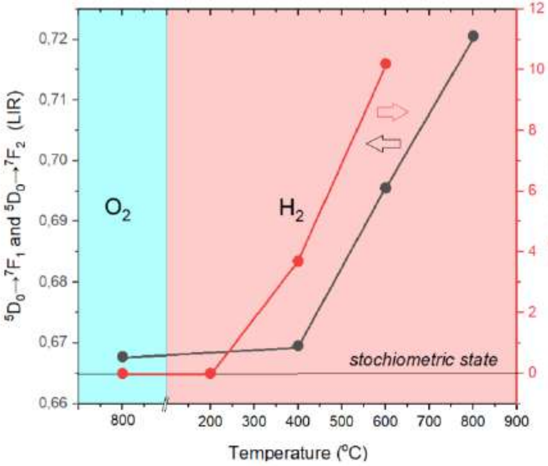

Fig. 1. Luminescent intensity ratio (LIR) between $^5D_0 \rightarrow {}^7F_1$ and $^5D_0 \rightarrow {}^7F_2$ bands and Ce^{3+} percentage from NAP-XPS as function of annealing temperature for $Ce_{0.95}Eu_{0.05}O_2$ catalyst

Thus, the $^5D_0 \rightarrow {}^7F_2/{}^5D_0 \rightarrow {}^7F_1$ ratio can be used as a structural, luminescence-based optical probe of the changes in the local ions environment, which in turn is associated with the number of oxygen vacancies. In our work, we demonstrated the applicability, advances and limitations of this approach for monitoring the dynamic Ce^{4+}/Ce^{3+} transitions in ceria exposed to reductive atmosphere[1,2] - a common type of atmosphere for variations in structurally important reactions like methane steam reforming, hydrogenation reactions, etc.

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O3

BSA-PERSISTENT NANOPARTICLES INTERACTION: LINKING OPTICAL PROPERTIES TO STRUCTURAL PROTEIN CHANGES

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Persistent luminescence nanoparticles (PersL NP), particularly $ZnGa_2O_4$ (ZGO) doped with Cr and Fe, are promising materials for use as fluorescent labels due to their emission in the deep red and near-infrared regions. These features enable the omission of autofluorescence and minimize absorption by biological molecules [1].

In the present work, we investigate the optical properties arising from the interaction between ZGO and bovine serum albumin (BSA). PersL NPs were synthesized using hydrothermal methods with additional surface modification [2, 3]. Comprehensive optical characterization, including absorption, photoluminescence emission (PL), excitation (PLE), and lifetime measurements, was performed for both BSA and ZGO separately as well as for the ZGO-BSA complex. Additionally, Raman spectroscopy was used to determine changes in BSA's secondary structure and to identify possible interaction/binding sites in the ZGO–BSA complexes.

The results indicate that BSA conformation is sensitive to both the presence and surface charge of NPs. The physical properties of BSA and ZGO dispersions in water are also discussed in detail.

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O4

SYNERGISTIC THREAT TO THE NERVOUS SYSTEM FROM COMBINED EXPOSURE TO COPPER AND WOOD SMOKE PARTICULATE MATTER

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Trace metal cooper and carbonaceous airborne particulate matter are hazardous neuro pollutants.

In this study, water-suspended wood smoke particulate matter preparations (SPM) were obtained under laboratory conditions. Cu^{2+} influenced particle size and surface properties of SPM that was shown using microscopy, DLS, and IR spectroscopy. A capability of Cu^{2+} to modulate acute neurotoxicity signs induced by SPM and vice versa was assessed during their combined application in presynaptic rat cortex nerve terminals (synaptosomes). It was demonstrated that Cu^{2+} alone and SPM alone increased the extracellular levels of L-[^{14}C] glutamate and [^{3}H] GABA, which are key excitatory and inhibitory neurotransmitters in the central nervous system, respectively. Combined application of Cu^{2+} and SPM significantly enhanced SPM- or Cu^{2+}-induced increase, respectively, in the extracellular levels of neurotransmitters, thereby demonstrating cumulative synergistic effect and substantial interference of Cu^{2+}- and SPM-related neurotoxicity. Also, Cu^{2+} and SPM demonstrated harmful cumulative synergistic effects on the plasma membrane and mitochondrial membrane potential, synaptic vesicle acidification and spontaneous generation of reactive oxygen species [1]. Therefore, it was concluded that Cu^{2+} and SPM demonstrated acute synergistic harmful effect on key presynaptic processes in nerve terminals. This multipollutant neurological threat was realized through disturbance of the excitation and inhibition balance, synaptic vesicle acidification, generation of reactive oxygen species in nerve terminals, and depolarization of the plasma membrane and mitochondrial membrane. An association of increased neuropathology expansion around the world with underestimated synergistic interference of the neurotoxic effects of Cu^{2+} and carbonaceous smoke particulate matter on the nervous system was suggested.

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O5

TUNING OF ANTIBACTERIAL ACTION OF ZNO MICROCRYSTALS BY MODIFYING SURFACE DEFECTS WITH FE-DOPING

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ZnO is an inexpensive II-VI wide-bandgap semiconductor that is used in many fields, from LED technology, gas sensors, and piezoelectric devices to pharmaceuticals and biomedicine. In particular, ZnO demonstrates a strong antibacterial action to both Gram-positive (e.g., *Staphylococcus Aureus*) and Gram-negative (e.g., *Escherichia Coli*) bacteria. At this time, there remains a significant controversy regarding the predominant mechanisms of antibacterial action of ZnO. To investigate the impact of ZnO on *Staphylococcus Aureus*, we implement an incremental Fe doping of microscale ZnO in order to change the surface defect concentration. We compare morphologies and surface defect concentrations in our samples before and after interaction with bacteria. The tools employed to characterize the pre- and post-assay ZnO doped specimens include scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray photoelectron spectroscopy, X-ray diffraction spectroscopy, and photoluminescence spectroscopy. Our experimental results provide detailed information about the changes in ZnO surface properties, specifically defect-related.

O6

EXPERIMENTAL AND THEORETICAL INVESTIGATION OF THE LEVIFLOXACIN-PVP COMPLEX

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Levofloxacin (LEV), a broad-spectrum fluoroquinolone antibiotic, effectively treats various bacterial infections by targeting bacterial DNA gyrase and topoisomerase IV, but its low aqueous solubility and chemical instability limit its bioavailability and use in drug delivery systems like medicated bandages. To overcome these challenges, pharmaceutical science has turned to developing drug-polymer complexes using polyvinylpyrrolidone (PVP), a biocompatible and water-soluble polymer. PVP forms inclusion complexes with LEV, significantly enhancing the antibiotic's solubility, stability, and controlled release. This approach is particularly beneficial for creating advanced wound dressings and bandages, where the molecular interactions—driven by hydrogen bonding, hydrophobic interactions, and van der Waals forces—create stable LEV dispersions within the PVP matrix. This not only ensures gradual, prolonged antibacterial activity at the wound site but also allows for the creation of flexible, durable, and breathable bandages.

The present work is dedicated to the complex experimental and theoretical approach, using Raman spectroscopy to provide a molecular fingerprint of the LEV-PVP complex and Density Functional Theory (DFT) calculations to model its structure and intermolecular forces. This synergistic use of techniques provides a comprehensive understanding of the LEV-PVP interaction, which is crucial for the rational design of effective new LEV formulations for wound management. The performed analysis of Raman spectra of LEV-PVP complex showed that the interaction between the components is non-covalent in nature. That is explained by the minor shifts, intensity modulations, and broadening of bands due to the perturbation of bond strengths and electron density polarization in the complex. We have revealed that levofloxacin molecules prevent polymer collapsing. The binding of LEV to PVP results in conformational changes of the polymer structure. The performed calculation predicted the most probable molecular structures of the complexes. The theoretical Raman spectra of the predicted molecular complexes LEV-PVP are in good agreement with the experimental data. In conclusion, the performed detailed analysis of non-covalent interactions and conformational changes within the LEV-PVP complex provides a critical molecular-level insight, essential for optimizing its therapeutic potential.

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O7

STRUCTURE-ACTIVITY RELATIONSHIPS IN $Cu_xCo_{1-x}WO_4$ SYSTEMS FOR DEGRADATION OF ACETAMINOPHEN UNDER SOLAR LIGHT

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Photocatalysis is an advanced oxidation process that harnesses light energy to activate semiconductor materials, generating reactive oxygen species capable of degrading organic pollutants. This approach offers a sustainable and efficient alternative to conventional water treatment methods, particularly for contaminants of emerging concern such as pharmaceuticals. To further enhance performance, photocatalysis can be coupled with peroxymonosulfate (PMS), which acts as a co-oxidant and is readily activated to produce highly reactive sulfate radicals, thereby improving degradation efficiency under visible light.

This study systematically investigates the structure-activity relationships within the $Cu_xCo_{1-x}WO_4$ (where x: 0, 0.2, 0.4, 0.6, 0.8 1.0) solid-solution system for visible-light-driven photocatalytic degradation of acetaminophen (ACT), with and without PMS assistance. A series of powders were synthesized via hydrothermal method and characterized using XRD, TEM, Raman, XPS, diffuse reflectance spectroscopy (DRS), photocurrent, and electrochemical impedance spectroscopy. The results reveal a strong dependence of photocatalytic activity on composition, crystal structure, and surface chemistry.

Among the tested compositions, $CuWO_4$, $Cu_{0.8}Co_{0.2}WO_4$, and $CoWO_4$ exhibited highest photocatalytic activity and were selected for more detailed photocatalytic studies. $CuWO_4$ exhibited the highest activity due to its narrow bandgap (2.3 eV), strong visible-light absorption, efficient charge transport, and Cu^{2+}/Cu^{+} redox cycling that effectively activated PMS, producing sulfate and hydroxyl radicals. The as-prepared $CuWO_4$ sample degraded ~34% of ACT under simulated solar irradiation in 60 min, which increased to nearly complete removal in PMS-assisted conditions. Partial Co^{2+} substitution (e.g., $Cu_{0.8}Co_{0.2}WO_4$) introduced structural tunability but reduced photocatalytic efficiency due to less favorable band alignment and increased charge recombination, although PMS addition partially compensated for this loss. $CoWO_4$ displayed the weakest photocatalytic activity despite generating the highest amount of $^{\bullet}OH$ reactive oxygen radicals, indicating that radical concentration alone is not a sufficient predictor of performance. Thermal treatment at 500 °C enhanced crystallinity and charge separation, improving PMS-free photocatalysis but slightly reducing PMS-assisted efficiency, likely due to loss of surface hydroxyl groups critical for PMS activation. Band structure analysis confirmed that all compositions had valence band positions favorable for $^{\bullet}OH$ generation, while conduction band potentials generally allowed PMS reduction to $^{\bullet}SO_4^{-}$, except for Cu-rich annealed samples where surface redox cycling dominated.

This work highlights the importance of balancing electronic structure, crystallinity, and surface chemistry to optimize mixed-metal tungstate photocatalysts. The findings provide key insights for the rational design of visible-light-responsive PMS-assisted systems for environmental remediation of pharmaceutical pollutants.

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O8

CORE-SHELL Au@PEtOx-PBuOx COLLOIDS WITH TUNABLE LCST TRANSITION FOR THERMALLY SWITCHABLE OPTICAL APPLICATIONS

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Au@PEtOx$_{1-x}$-PBuOx nanoparticles with gold core coated with a thermoresponsive polymer shell composed of statistical copolymers α-methyl-ω-hydroxy poly(2-ethyl-2-oxazoline)-*stat*-poly (2-*n*-butyl-2-oxazoline) were synthesized in aqueous colloidal form. These hybrid nanostructures were designed as potential materials for thermo-optical systems, particularly as thermally tunable optical absorbers. The polymer shell is thermosensitive due to the lower critical solution temperature (LCST) behavior, which can be precisely modulated by adjusting the ratio of hydrophobic (PBuOx) to hydrophilic (PEtOx) components in the copolymer. It was observed that increasing the hydrophobic content in the copolymer from 0 to 0.3 causes a decrease in the LCST point from 81 °C down to 17 °C. Remarkably, at a composition with $x = 0.19$, the transition temperature coincides with human body temperature (37 °C), making the system particularly relevant for biomedical applications. During temperature variation, the nanoparticles exhibit a noticeable change in hydrodynamic diameter. This change includes an initial size reduction which is a result of the polymer shell contracting at the LCST transition followed by size increase occurring due to aggregation of NPs. The temperature cycling induces significant alterations in the optical properties of the nanoparticles. The localized surface plasmon resonance (LSPR) absorption peak undergoes a red shift, broadening, and intensity enhancement as a response to heating. These spectral changes highlight the system's sensitivity to thermal stimuli. Additionally, the LCST transition was confirmed by SERS from polymer shell, which showed an enhanced signal after a heating-cooling cycle due to strengthening of plasmonic enhancement during structural transformations in the polymer shell.

O9

BIOLOGICAL AND MECHANICAL PROPERTIES OF THE COMPOSITES CONTAINING GRAPHENE FLAKES OBTAINED FROM MINERAL GRAPHITE

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Graphene, a two-dimensional (2D) material consisting of sp^2-hybridized carbon atoms arranged in a hexagonal honeycomb lattice, possesses unique structural, mechanical, and electronic properties that make it an attractive additive for multifunctional composites. In this study, graphene flakes were synthesized from mineral graphite by electrochemical and mechanical exfoliation methods, assisted by ultrasound treatment [1]. The morphology, crystallinity, and chemical structure of the obtained graphene were comprehensively characterized using X-ray diffraction (XRD), Raman and Fourier-transform infrared (FTIR) spectroscopy, and scanning and transmission electron microscopy (SEM/TEM). Additional surface functionalization strategies were employed to enhance dispersibility and stability of the flakes within polymer and coating matrices.

Graphene-based composites were subsequently fabricated by incorporating the flakes into polyamide 6 (PA6) via melt intercalation [2], as well as into acrylic paint, enamel, and varnish systems at varying concentrations (0.5, 1, and 3 wt.%) [3]. Mechanical testing revealed a pronounced increase in elastic modulus and micro-hardness with graphene addition, although a trade-off was observed in terms of reduced impact resistance for some formulations. SEM analysis confirmed that the degree of dispersion and interfacial adhesion between the graphene flakes and the host matrix strongly influenced fracture morphology and load-transfer efficiency. Beyond mechanical reinforcement, functional properties of the composites were systematically investigated. Wettability studies indicated modified surface characteristics upon graphene incorporation, while antimicrobial assays against *Staphylococcus aureus* (ATCC 33591), *Pseudomonas aeruginosa* (ATCC 15442), and *Candida albicans* (ATCC 10231) demonstrated pronounced bactericidal and fungicidal activity. These effects are attributed to a synergistic mechanism involving oxidative stress induction and physical membrane disruption by the sharp edges of graphene flakes.

Overall, the results establish a direct correlation between the synthesis route, structural characteristics of the graphene flakes, and the resulting composite performance. The findings confirm that graphene incorporation not only enhances mechanical strength but also imparts antimicrobial functionality, highlighting its strong potential for next-generation multifunctional coatings, biomedical devices, and high-performance polymer composites.

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O10

MECHANICAL PROPERTIES OF THE MEMBRANE OF CIRCULATING METASTATIC TUMOR CELLS AS A DIAGNOSTIC MARKER

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It is known that metastasis is one of the most complex consequences of cancer. The important and early stage of the metastatic cascade is the detachment of metastatic cells from the extracellular matrix and migration both within and outside the primary tumor. Unlike normal cells, the separation of which from the extracellular matrix leads to their death metastatic cells survive and retain the ability to proliferate. During this process, the cell undergoes profound structural and biochemical changes. That is why the determination of the biophysical and biochemical characteristics of circulating metastatic cells may give us the new conception of antimetastatic therapy.

In this work we investigate the problem of metastasis using the unique cell model of the Lewis lung carcinoma (LLC). We used two types of tumor cells that differ significantly in their proliferative, angiogenic and metastatic potential. LLC is the original strain, LLC/R9 is a modified variant of Lewis lung carcinoma obtained in the R.E. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology, as a result of tumor progression in vivo. LLC/R9 is a resistant variant obtained after nine courses of cis-platinum chemotherapy. LLC/R9 cells are characterized by three times lower metastatic potential compared to LLC cells. In addition, LLC/R9, in comparison with LLC, is characterized by a high rate of primary tumor growth and high angiogenic potential.

To model the process of metastasis, two methods of cell cultivation were used adhesive and deadhesive cells growth. In our previous work [1, 2] it was shown that the transition from adhesive to deadhesive growth is accompanied by differences in glucose consumption, lactate production, intracellular level of ROS and proliferative heterogeneity of LLC cells.

An important characteristic of the cell membrane is its mechanical properties. To determine the mechanical characteristics of cells, in particular the general ability to deform and effective elastic constants, the micropipette aspiration method was used. 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. I would like to pay special attention to the aspiration setup. It was assembled at the O.O. Bogomoletz Institute of Physiology. The setup includes an optical system, micromanipulators, capillaries, and back pressure supply systems. Visualization and control of the process is carried out using Fiji-based software.

The study shows that cells grown by the deadhesive method have more rigid cell membranes, including due to the presence of numerous microvilli on the membrane surface - lamellopodia, filopodia, etc. The effect of glycolysis inhibitors on changes in the mechanical properties of the cell membrane is discussed.

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O11

INTRINSIC DISORDER OF THE bHLH-PAS FAMILY OF TRANSCRIPTION FACTORS

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The basic helix–loop–helix/Per-ARNT-SIM (bHLH–PAS) proteins constitute a family of transcription factors (TFs) ubiquitously expressed in vertebrates and invertebrates. They play essential roles in regulating a wide range of developmental and physiological processes [1]. Despite their functional diversity, bHLH–PAS proteins share a relatively well-conserved N-terminal domain structure: the bHLH domain located at the N-terminus, followed by the PAS domain, which is divided into two conserved regions, PAS-A and PAS-B, located in the central part of the protein. The PAS-A and PAS-B regions are separated by a poorly conserved linker [2]. The PAS-A region is critical for dimerization partner selection and ensures target gene specificity, whereas the PAS-B region senses diverse exogenous and endogenous signals, accompanied by energetic and conformational changes that regulate protein activity [3].

In contrast to the conserved domains, the C-termini of bHLH–PAS proteins exhibit significant variability and contain diverse transcriptional activation/repression domains (TAD/RPD). Importantly, these C-terminal regions specifically modulate protein function through interactions with a wide range of partners, enabled by their intrinsically disordered character (IDRs) [2]. IDRs and IDPs (intrinsically disordered proteins) have been identified as key components of cellular signaling, governing regulatory mechanisms and protein interaction networks [4].

Recently, the propensity of IDRs to undergo liquid–liquid phase separation (LLPS) has been recognized as a crucial feature that allows regulation of fundamental cellular processes, including transcription, DNA repair, and others [5]. Despite their importance, the structural characterization of these regions remains challenging and is still incomplete. In the presentation, the current state of knowledge regarding IDRs and their significance for the flexibility and function of bHLH–PAS proteins will be discussed.

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O12

PARTIAL LEAST SQUARES ANALYSIS OF ATR-FTIR SPECTRA FOR INTRAOPERATIVE CHARACTERIZATION AND RAPID BIOCHEMICAL PROFILING OF BRAIN TUMORS

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Rapid intraoperative tissue diagnostics, performed directly next to the surgical table, is critically important for determining tumor type, stage, and guiding the therapeutic strategy. Fourier-Transform Infrared (FTIR) spectroscopy with Attenuated Total Reflection (ATR) represents a promising adjunctive method to conventional cytology, providing fast biochemical information on tissue samples without complex preparation.

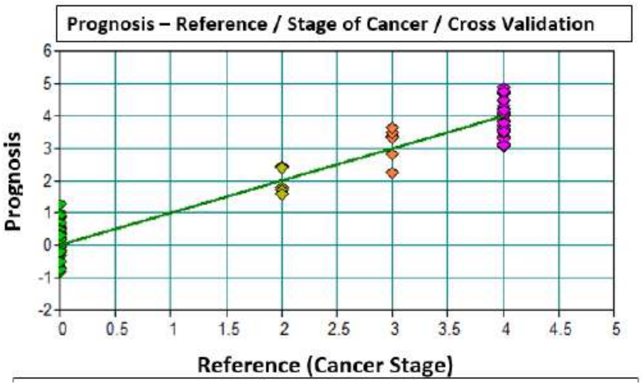

Fig. 1. Results of the PLS model for predicting glioblastoma stage based on FTIR spectra of brain tissue

Surgical samples of brain tumor tissue (glioblastoma) and non-tumor samples were collected from patients aged 6 to 70 years, representing both genders and different tumor stages. Samples were dried and analyzed using ATR-FTIR spectroscopy on a Tensor 27 spectrometer (Bruker Optics) in the 4000–600 cm^{-1} range. For each specimen, 2–6 spectra were recorded. Data analysis was carried out using Partial Least Squares (PLS) regression in OPUS Quant 2 (Bruker).

PLS analysis is a multivariate statistical method widely used in spectroscopy to model relationships between spectral features and reference variables. It projects high-dimensional spectral data into a reduced latent space, simultaneously maximizing the covariance between predictors (spectra) and responses (biological or clinical variables). This approach not only improves prediction accuracy but also provides information about the chemical regions of the spectra that contribute most strongly to the modeled property.

- The age prediction model achieved a correlation coefficient of 77% with an RMSECV of 8.4 years.
- Predictive spectral regions for patient age and tumor stage included protein bands (amide I, II – 1650–1550 cm^{-1}), lipid-associated CH_2/CH_3 vibrations (2800–3000 cm^{-1}), and phosphate-related bands (1000–1150 cm^{-1}). Variations in the 3300–3000 cm^{-1} range (O–H, N–H stretching) reflected age-related changes in hydration.
- The PLS model for tumor stage prediction demonstrated strong performance ($R^2 = 92.3\%$, RMSECV = 0.52, RPD = 3.6). The 1740–1700 cm^{-1} region (C=O carbonyls) was linked to lipid peroxidation in progressive tumors.
- Models predicting patient gender performed poorly (correlation coefficient \~25%), consistent with the absence of stable biochemical gender markers in the brain tumor tissues.

ATR-FTIR spectroscopy combined with PLS regression enables the identification of biochemical changes associated with patient age and glioblastoma stage. The most informative spectral features correspond to protein structures, lipid content, and nucleic acids. Importantly, PLS analysis not only facilitates prediction but also reveals chemical patterns in the spectra and their relative ranking (importance), making it a powerful tool for exploring complex biomedical data.

O13

THE EFFECTS OF SYNGAP KNOCKDOWN ON THE AMPA RECEPTOR SURFACE MOBILITY

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Learning, memory, and cognition are governed by highly dynamic processes in the brain, involving a spectrum of molecular players. The cellular mechanism underlying these functions is called synaptic plasticity, e.g. the ability of synapses to change the efficacy of their transmission in an activity dependent manner — primarily strengthening and weakening of the synaptic connection [1]. The effects of synaptic plasticity largely converge on AMPA-type glutamate receptors (AMPARs) present in excitatory synapses [2, 3].

SynGAP is a Ras/Rap GTPase-activating protein highly enriched in the postsynaptic density (PSD) – a part of the neuron that is a primary hub for the receptors and other molecules involved in synaptic transmission. SynGAP specifically plays an important role in regulating synaptic strength and dendritic spine maturation [4]. Among its multiple isoforms, SynGAP-α1 directly interacts with the scaffold protein PSD-95 in the PSD [1]. This interaction competitively regulates access of AMPARs to postsynaptic binding "slots" on PSD-95, thereby decreasing synaptic strength. While SynGAP has long been considered a bidirectional regulator of strengthening and weakening of the synapse through its GAP activity, recent studies suggest that its binding to PSD-95 may be more directly responsible for modulating AMPAR recruitment.

In this study, we used CRISPR-Cas9 mediated knockdown of endogenous SynGAP in rat hippocampal neuronal cultures to investigate SynGAP's role in AMPAR surface dynamics. For this we used a cutting edge high-resolution single-molecule tracking called uPAINT microscopy. The acquisition was done with a Leica DMi8 dSTORM setup. For the recordings I used two lasers: 488 nm to identify transfected cells expressing GFP and 642 nm laser to image the AMPARs. We were able to track individual AMPA receptors, tagged with directly labelled fluorescent probes. Using FIJI application to analyse the data we determined the fractions of AMPARs which were immobile and the mobile (receptors which were freely moving and were not bound to PSD-95).

We found that SynGAP knockdown significantly reduced AMPAR mobility, indicating increased receptor trapping which might promote synaptic strengthening. Our results support the growing theory that SynGAP's competitive binding to PSD-95 plays a crucial role in regulating AMPAR entrapment in the synapse. This offers a mechanistic explanation for the hyperexcitable synaptic states frequently seen in neurodevelopmental diseases linked to SYNGAP1 dysregulations and offers a new insight into the structural mechanisms by which SynGAP regulates synaptic plasticity.

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O14

PMMA:PVP BLENDED NANOFIBERS LOADED WITH ANTIBIOTIC LEVOFLOXACIN FOR ANTIBACTERIAL APPLICATION

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Nanofibers prepared by electrospinning have a high surface area-to-volume ratio, tunable porosity, are flexible, strong, biocompatible, and have unique physicochemical properties. These properties of nanofibers play an important role in the production of antibacterial materials. Nanofiber mats are also used extensively in healing wounds, as this mat is a scaffold with similar morphological structures to natural extracellular matrices. In addition, drug delivery systems can be developed from these nanofibers as they can be functionalized by embedding drugs, bioactive agents, and nanoparticles (as antimicrobial agents).

In this study, a novel electrospun nanofiber mat incorporating the antibiotic levofloxacin (LV) was prepared from a blend of hydrophilic polyvinylpyrrolidone (PVP) and hydrophobic polymethyl methacrylate (PMMA) [1]. A microphotograph of a thin PMMA:PVP:LV nanofiber mat showed that the nanofiber diameter is in the range of 1–4 μm. SEM images taken before and after soaking in water reveal uniform, bead-free fibers with smooth surfaces. LV release in water was monitored by UV–vis absorption spectroscopy, showing that PVP enhances both drug loading and release. About half of the LV was released within the first 5 min, followed by an additional quarter over the next 2–3 h. The complete release of LV from PMMA nanofibers is impossible, as a certain part of the nanopores remains closed, rendering drug release impossible. After the release of the drug and PVP, the nanofiber mat remains in the form of a PMMA framework, which is insoluble in water, indicating the potential use of this mat for wound dressing. In the composite mat, PMMA contributes mechanical strength, ensures sustained release, and resists degradation in water and against microorganisms. The PMMA:PVP blended nanofiber mat can serve as an effective delivery system for the antibiotic LV, maintaining its bactericidal effects, as evidenced by the growth inhibition of both Gram-positive and Gram-negative bacteria. It was found that the LV released from the nanofiber mat more strongly inhibited the growth of *E. coli B* compared to *S. aureus* and *P. aeruginosa.*

Figure 1 shows the growth inhibition zones around LV-loaded nanofiber mat disks. The average diameters of the growth inhibition zones around disks were 21 mm for *S. aureus* 209, 26 mm for *P. aeruginosa* 9027, and 30 mm for *E. coli* B, while the negative control disks (without LV) exhibited no inhibitory effect on any of the tested microorganisms.

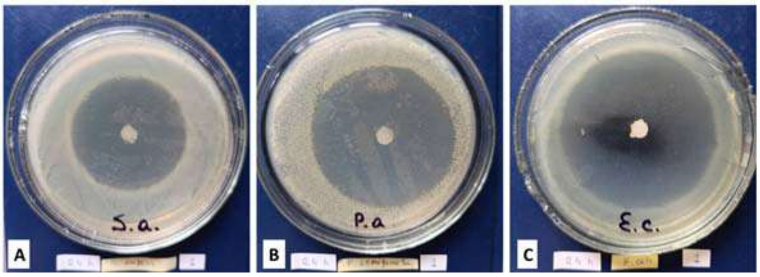

Fig. 1. Sensitivity of three bacterial strains to LV released from nanofiber mat disks. (A) *S. aureus* 209, LV; (B) *P. aeruginosa* 9027, LV; (C) *E. coli* B, LV.

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O15

MODEL-BASED QUANTIFICATION OF SURFACE PASSIVATION EFFECTS INDUCED BY BIOGEL IMMOBILIZATION IN FIELD-EFFECT BIOSENSORS

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Immobilization of biogels on gate surfaces of field-effect biosensors introduces not only selective biochemical functionality but also alters the electrochemical interface that governs signal transduction. We develop and apply an advanced modeling framework to quantify the passivation of surface ionizable groups caused by biogel deposition – both enzymatic and inert – on SiO_2/Si_3N_4-based gate dielectrics in pH-sensitive ISFETs.

The model is based on site-binding equilibrium and Gouy-Chapman-Stern electrostatics and captures how surface charge density (σ_0), potential (φ_{eo}), and capacitance (C_H) are affected by enzymatic reaction products while enzyme is immobilized in biogel [1]. A critical factor revealed by our analysis is the ionic strength of the buffer, which modulates the Debye length and alters the electrical double layer, thereby attenuating surface potential changes and pH sensitivity.

We propose that biogel immobilization leads to partial passivation of ionizable surface silanol N_{Si} and amine groups N_{Nit}, changing the effective surface charge modulation in response to analyte-induced pH shifts. This effect is accounted for using a passivation factor α_p, which scales the accessible surface group density N_{Si}, N_{Nit} in the model without altering intrinsic *pKa`s* or dielectric constants. Importantly, this effect is shown to be independent of enzymatic activity, indicating that non-specific matrix properties – such as swelling, hydration layer formation, and steric hindrance – play a substantial role in transducer behavior. Simulated drain current responses were compared to experimental measurements, revealing good agreement under varying buffer ionic strengths and gel compositions. These findings highlight the importance of modeling electrostatic surface phenomena independently from biochemical kinetics to accurately predict biosensor performance and interpret experimental variation due to immobilization protocols and ionic environments.

Additionally, we analyze how the presence of the biogel influences the effective double-layer capacitance C_{DL}, potentially reducing the sensor's electrostatic sensitivity by introducing a dielectric decoupling layer. These findings provide critical insights into biosensor signal generation mechanisms and establish a generalized methodology for deconvoluting biochemical signal from interfacial electrostatic modulation.

Our results offer a pathway to improved design and calibration of biosensors by explicitly accounting for immobilization-induced surface passivation effects in modeling and interpretation.

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O16

BEYOND LIGAND BINDING: DECODING GPCR ACTIVATION ON BUDDED BACULOVIRUS NANOPARTICLES VIA FLUORESCENCE ANISOTROPY AND CONFORMATIONAL BIOSENSORS

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G protein-coupled receptors (GPCRs) represent 34% of FDA-approved drug targets, yet characterizing their ligand-binding kinetics and activation mechanisms remains challenging. Budded baculoviruses (BBVs) have emerged as a powerful nanoscale platform for studying GPCRs in near-native lipid environments. Here, we present an integrated strategy that combines BBV-based fluorescence anisotropy (FA) ligand binding assays [1] with receptor-activation-sensitive conformational biosensors (GRABs) [2], opening new avenues for GPCR drug discovery and mechanistic biophysics.

BBVs are rod-shaped membranous nanoparticles produced during insect cell infection, displaying GPCRs embedded in native-like lipid bilayers. Compared to conventional membrane preparations or whole-cell systems, BBVs provide isotropic receptor orientation, high receptor density, and minimal autofluorescence—enabling homogeneous FA assays without separation steps and meeting High-Throughput Screening (HTS) robustness criteria. We pioneered the BBV-FA approach for melanocortin MC_4 receptors using Cy3B-NDP-α-MSH, enabling real-time monitoring of ligand binding [3]. Global kinetic analysis—accounting for nonspecific interactions and ligand depletion—allows simultaneous determination of affinity, association/dissociation rates, and allosteric modulations.

This platform has since been extended to diverse GPCRs, including different peptide receptors (e.g., neuropeptide Y, neurotensin) and monoamine receptors (e.g., dopamine, serotonin). BBVs immobilized on functionalized coverslips, enable also single-particle sensitive ligand binding quantification and validation of affinity measurements using total internal reflection fluorescence (TIRF) microscopy [4].

While BBV-FA excels in resolving ligand binding kinetics, conformational biosensors add complementary insight into state-specific transitions underlying receptor activation. Incorporating GRAB biosensors into BBVs unifies ligand binding and conformational changes in a single platform, enabling HTS for conformation-selective compounds that stabilize therapeutically relevant states (e.g., G-protein-biased agonists). We demonstrate potential of this approach using dopamine, serotonin, and norepinephrine receptor GRABs, revealing distinct biosensor signatures that reflect dynamic activation landscapes often inaccessible to traditional assays.

Integration of these conformational signatures with structural data, offers a framework for classifying pharmacological efficacy (e.g., superagonism, inverse agonism, antagonism) and identifying mechanistic classes of receptor modulations. Together, BBV-based FA and GRAB assays provide a versatile and scalable platform that bridges traditional gap between binding and functional assays.

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O17

FTIR SPECTROSCOPY BASED IDENTIFICATION OF SPECTRAL BIOMARKERS ASSOCIATES WITH BIOLOGICAL AGE USING MACHINE LEARNING

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Biological aging is a complex process involving progressive molecular and physiological deterioration, which often does not associated directly with chronological age. Accurate assessment of biological age is crucial for early detection of age-related pathologies and for evaluating the effectiveness of anti-aging interventions. While genetic and epigenetic clocks are informative, they remain expensive and labor-intensive. Fourier-transform infrared (FTIR) spectroscopy, a rapid and non-invasive technique, offers the potential to capture comprehensive biochemical signatures of aging from biofluids such as blood. We aim to identify informative FTIR spectral biomarkers that correlate with biological age, leveraging advanced machine learning (ML) methodologies to create predictive and interpretable models of aging.

A dataset comprising 955 dried blood smear FTIR spectra (range 1000–1720 cm^{-1}) was collected using ATR-FTIR spectroscopy (mean age 56±16 years). Spectral data underwent a rigorous preprocessing pipeline, including baseline correction, Savitzky-Golay smoothing, and peak deconvolution using pseudo-Voigt curve fitting across 53 characteristic spectral regions. To predict biological age, multiple machine learning models were trained via H2O AutoML, enabling automatic model selection and hyperparameter optimization. SHAP (SHapley Additive exPlanations) analysis was performed to determine the contribution of each spectral feature to model output, ensuring biological interpretability.

A range of distinct FTIR spectral regions demonstrated correlation with age, including:

- **1491 cm^{-1}** – Resonating with aromatic amino acid residues (phenylalanine, tyrosine, tryptophan), decreased peak sharpness suggests oxidative modifications of aromatic side chains. It also suggests decline in choline phospholipid, reflecting membrane aging.
- **1618 cm^{-1}** – Assigned to intermolecular β-sheet structures (Amide I band), showing increasing intensity with age, reflecting protein misfolding, aggregation, and amyloidogenic processes.
- **1682 cm^{-1}** – Linked to antiparallel β-sheet formations and β-turn structures, increasing with age, indicative of altered protein secondary structures and loss of ordered β-structures.
- **1042 cm^{-1}** – May suggest simplification of the blood glycome, likely reflecting reduced glycosylation diversity and accumulation of AGEs (Advanced Glycation End-products).
- **1697 cm^{-1}** – Decreasing amplitude with age hint at declining oligomeric protein intermediates, marking a transition from soluble aggregates to mature fibrillar forms

Identified peaks are aligned with known molecular hallmarks of aging, particularly protein aggregation, membrane lipid alterations, and carbohydrate structure remodeling, supporting the translational potential of FTIR spectroscopy in aging research, diagnostics, and geroprotective intervention monitoring.

O18

FROM CHAOS TO THE FIRST STORED INFORMATION AND ORIGIN OF LIFE

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The most common attribute of life is the capability of self-replication, meaning the capability to store and reproduce information. The first stored information in nature appeared when atomic gas in the interstellar medium (ISM) condenses at low temperatures forming first molecules and solids. The prevailing perspective has been that this rudimentary, chemically-encoded information required a substantial evolutionary progression to initiate the encoding of the property of self-replication. In contrast, recent studies suggest that these earliest solids, originating from the direct condensation of interstellar gas, may exhibit properties that position them remarkably near this critical threshold for life [1-5].

Our studies reveal that the condensation of atomic carbon onto cold solid particles (cosmic dust) in translucent molecular clouds initiates the barrierless surface reaction $CO + C + NH_3 \rightarrow NH_2CH{=}C{=}O$. These reactive fragments subsequently undergo low-temperature oligomerization, yielding glycine-based oligopeptides [1,6]. Remarkably, this peptide synthesis follows a previously unrecognized pathway that bypasses the intermediate stage of free amino acid formation. It proceeds efficiently under cryogenic interstellar conditions on the surfaces of nanoparticles present in space, without requiring energetic processing or liquid water. Further investigations demonstrate that the presence of other abundant interstellar molecules during condensation does not largely affect the peptide formation [2].

The presentation reviews the low-temperature condensation of atomic gases in the ISM and explores how the resulting peptides may have contributed to prebiotic chemistry that ultimately enabled the emergence of life on rocky planets.

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O19

A RAPID, GREEN AND COST-EFFECTIVE SYNTHESIS OF PH- AND HYDROXYL GROUP SENSITIVE CARBON DOTS FOR SENSING APPLICATIONS

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Carbon dots (CDs) represent promising luminescent nanomaterials owing to their tunable photophysical properties and straightforward surface modification, which make them highly attractive for sensing applications [1]. However, most CD-based pH sensors are characterized by narrow operational ranges and rely predominantly on fluorescence intensity variations rather than emission wavelength shifts. Furthermore, conventional synthetic routes frequently require complex procedures or toxic reagents [2]. In this work, we introduce a rapid, sustainable, and cost-efficient strategy for synthesizing CDs with dual environmental sensitivity, effectively overcoming these limitations.

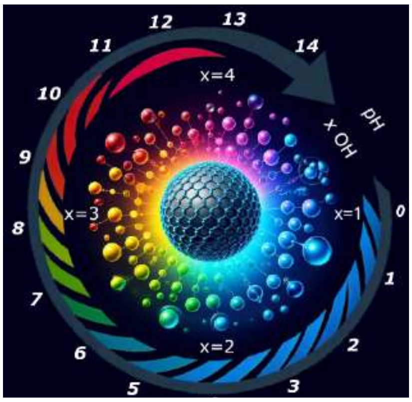

Fig. 1. Spectroscopic properties of the CDs depend on pH and the number of OH groups in the environment.

CDs were synthesized through a simple combustion method using low-cost and non-toxic precursors: citric aids, urea, and sodium hydroxide. The synthesis was carried out by heating at 260°C. Structural and optical features were examined using X-ray diffraction (XRD), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy with ATR attachment (IR-ATR), and UV-Vis and photoluminescence (PL) spectroscopy. PL studies included time-dependent emission measurements in aqueous and alcoholic media, as well as in solutions of different pH.

The synthesized CDs showed strong and tunable photoluminescence, high photostability, and excellent dispersibility in water. XRD analysis indicated a partly amorphous structure with a graphene- like core and polymeric surface groups. Their emission responded continuously across a wide pH range (1-14): increasing pH in water induced a blue shift, whereas red shifts were observed in alcoholic media. IR measurements revealed dynamic surface interactions during solvent evaporation, occurring more rapidly in methanol than in ethanol. Quantum yields were 15% in water, 11% in methanol, 22% in ethanol, and 13.5% at pH 13.

Overall, this sustainable and scalable synthesis produced multifunctional CDs with dual sensitivity to pH and hydroxyl-rich environments, enabling selective discrimination between methanol and ethanol. Their time-dependent emission behavior further points to dynamic surface equilibria, underscoring their promise as cost-effective environmental and biomedical sensors.

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O20

MOLYBDENUM DISULFIDE QUANTUM DOTS EXFOLIATED WITH NUCLEOTIDES: SPECTROSCOPY AND AFM CHARACTERIZATION, ANALYSIS OF TEMPORAL STABILITY

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Currently, transition metal dichalcogenides (TMDCs) such as MoS_2, WS_2, $MoSe_2$ are being widely studied by researchers from various scientific areas. Due to the layered structure of TMDCs, the ultrasound-assisted liquid-phase exfoliation [1] is one of the most facile and cost-effective methods of downscaling of in particular bulk MoS_2 into low-dimensional nanostructures with unique physical properties. These include so-called zero-dimensional quantum dots which electronic structure is governed by quantum confinement effects. The study of interaction of MoS_2 nanostructures, including MoS_2 quantum dots (MoS_2 QDs), with biomolecules is of high research interest due to potential use in biomedicine as drug delivery agents, therapeutic, or bioimaging agents, as well as biosensors [2].

In this work, we have successfully dispersed MoS_2 in aqueous solutions of deoxyadenosine monophosphate (dAMP), deoxyguanosine monophosphate (dGMP), deoxycytidine monophosphate (dCMP), and uridine monophosphate (UMP) by ultrasound-assisted exfoliation. UV-Vis absorption spectroscopy study of these samples has shown characteristic MoS_2 bands which confirm presence of exfoliated MoS_2 nanostructures, the spectral parameters of bands match rather closely. We report the first observation of visible-range photoluminescence (PL) registered from all suspensions, which we attribute to the presence of MoS_2 QDs in the suspensions. The comparison of PL band intensity, peak position, and spectral width suggests the essential role of MoS_2-nucleic base interaction for MoS_2 exfoliation, colloidal stabilization, and producing of emissive quantum dots. Notably, the MoS_2-dAMP suspension displayed the highest PL intensity and relative PL quantum yield. Therefore, additional experiments were carried out for this sample. By means of UV-Vis absorption and Raman spectroscopy, as well as AFM characterization, we show that consecutive use of two sonication methods followed by several stages of centrifugation provides separation of larger two-dimensional MoS_2 nanostructures with lateral size of ~1 µm (MoS_2 nanoflakes) from MoS_2 QDs. As a result, the MoS_2-dAMP suspension with improved emission properties of MoS_2 QDs was obtained. Finally, we have studied the temporal stability of this MoS_2-dAMP suspension. The long-term storage (~1.5 years) revealed exceptional PL stability (intensity drop not more than 15%). Analysis of PL spectrum also suggests the essential role of defect-mediated emission, the relative contribution of which further increased over time.

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O21

HIGH-RESOLUTION SEM MICROSCOPY FOR STUDYING LIPOSOMES AND MODEL CIRCULATING TUMOR CELLS INCUBATED WITH MoS_2 AND WS_2 NANOPARTICLES

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Understanding membrane–nanoparticle interactions is essential for evaluating their role in cancer progression and potential therapeutic applications. Liposomes serve as versatile biomimetic systems that replicate lipid bilayer organization and allow controlled investigation of exogenous particle incorporation. Circulating tumor cells (CTCs), modeled by Lewis lung carcinoma (LLC) cells grown under de-adhesive conditions, represent a relevant system, as their survival strongly depends on membrane integrity and remodeling. SEM data were supplemented with confocal microscopy data.

High-resolution scanning electron microscopy (SEM) provides a direct means to visualize cells surface morphology and nanoparticle distribution with nanometer precision. In this study, SEM was applied to investigate liposomes and LLC cells incubated with two-dimensional transition metal dichalcogenides, molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2). These nanomaterials were selected for their distinctive physicochemical properties and prospective biomedical applications, including biosensing and targeted drug delivery.

The objective of this work is to establish a structural framework for understanding how 2D nanoparticles interact with lipid membranes in both simplified and cellular systems. Such an approach bridges the gap between model and biological membranes, emphasizing SEM as a valuable tool for cancer diagnostics, CTC monitoring, and the design of functional nanocarriers.

SEM imaging of liposomes in secondary (SE) and backscattered electron (BSE) modes enabled detailed visualization of surface morphology, vesicle integrity, and nanoparticle localization. Liposomes exhibited membrane deformations and heterogeneous contrast patterns associated with nanoparticle adsorption or partial embedding within the bilayer.

For LLC cells, SEM revealed morphological features typical of de-adhesive growth, including near-spherical shapes, membrane roughness, and abundant surface projections. Nanoparticles were detected at the plasma membrane and within infoldings, often co-localizing with vesicular protrusions. Complementary energy-dispersive X-ray spectroscopy (EDS) confirmed the elemental composition of Mo and W clusters, validating their presence.

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O22

ON LIGANDS FOR «GREEN» SYNTHESIS OF LUMINESCENT Ag-In-Se NANOPARTICLES

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Ternary chalcogenide Ag–III–VI nanoparticles (for example, AgInS and AgInSe) have drawn significant attention in recent years due to their distinctive optical characteristics, low toxicity, and broad potential for use in biological and optoelectronic applications. Among these, AgInSe (AISe) is particularly promising thanks to its direct band gap energy of 1.24 eV for bulk crystals, which enables tunable photoluminescence (PL) across a wide spectral range from visible to near-infrared one by adjusting its chemical composition, particle size, and synthesis conditions. This makes AISe nanoparticles (NPs) highly attractive for applications requiring controlled emission properties, including biomedical imaging where their high luminescence and tunable emission make them strong candidates for *in vitro* optical imaging as versatile fluorescent probes. They can be considered as a safer alternative to Cd-/Pb-containing NPs and organic dyes. The clinical application of in vivo fluorescence imaging is still hampered by the lack of effective contrast agents. In this context, AISe have been investigated and show significant potential as contrast agents for fluorescence imaging. Experiments confirm their effectiveness for in vivo imaging, especially of the cardiovascular system, due to their long circulation time in blood vessels [1]. However, synthesizing such NPs remains challenging, as conventional methods require high temperatures or pressures, organic solvents, and long growth times to achieve proper quality. To address this, we recently proposed a simplified approach for more accessible and efficient AISe NPs production using L-cysteine (Cys) as a ligand [2].

In this work we expand the choice of ligands and study the role of their functional groups in the synthesis of the NPs. Namely, N-acetyl-L-cysteine (NAC) and L-cysteine hydrochloride (Cys-HCl) are of particular interest. We find that the thiol functional group facilitates controlled synthesis by coordinating metal ions and stabilizing the surface of the NPs, thereby improving particle homogeneity, while the acetate group provides colloidal stability of the NPs in water.

PL properties of the synthesized particles were investigated using the 2nd harmonic of Ti:Sa laser (400 nm, 150 fs) for excitation. PL spectra of Ag-In-Se NPs with In/Ag molar ratios of 9 and 6, synthesized using different stabilizers (Cys, NAC, and Cys-HCl), revealed a redshift toward the near-infrared region with increasing silver content. For the In/Ag = 9 samples, the emission peaks were observed at 670 nm for NAC, 685 nm for Cys, and 695 nm for Cys-HCl. For other samples, the peaks shifted further to 675 nm, 695 nm, and 720 nm, respectively. The magnitude of the spectral shift upon changing the In/Ag ratio also depended on the stabilizer: 5 nm for NAC, 10 nm for Cys, and 25 nm for Cys-HCl.

These results indicate that both the In/Ag ratio and the choice of stabilizing ligand significantly influence the emission properties of Ag-In-Se NPs. In particular, stronger redshifts were observed with stabilizers containing protonated amino groups (e.g., Cys-HCl), suggesting their more pronounced effect on the surface environment and band structure of the nanoparticles.

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O23

STABILITY OF COMPLEXES OF Ag$^+$ IONS WITH NITROGENOUS BASES OF DNA MOLECULE

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Despite the key role of DNA in biological processes, this molecule is increasingly being considered as a material that can have practical applications in various technologies. Among such materials, it is worth noting the so-called metallized DNA with cations of heavy d-metals (Au, Hg, Cu, Pt and Ag) located between nitrogenous bases. In particular, the data of X-ray structural analysis for Ag-DNA showed that Ag$^+$ ions form long one-dimensional chains in the center of DNA helix [1]. In this case, Ag$^+$ ions form bonds only with guanine, thymine and cytosine, while adenine nucleotide bases are pushed out of the double helix. At the same time, such a system is periodic and twisted into a double-stranded helix, inside which the ions are next to each other within the van der Waals radii. This chain of silver ions inside DNA is stabilized by the formation of argentophilic interaction, which is currently not sufficiently studied. In the presented work, quantum-chemical modeling of Ag$^+$ ion complexes with nitrogenous base residues was carried out in order to establish their geometric and electronic structure. DFT method with the Def2-TZVP ECP basis set for Ag atoms and 6-311++G(d,p) for nitrogenous base atoms was used. The calculations of energy characteristics of the system, and QTAIM-analysis of the electron distribution between Ag$^+$ ions and nitrogenous bases were performed. As a result, a regularity of change in interatomic distances between the Ag$^+$ ion and the nitrogenous base ligand is observed within the framework of both B3LYP/PCM and B3LYP/SMD methods. The smallest interatomic distance is observed for Ag$^+$–T pair (2.167 Å and 2.181 Å, respectively). It is also shown that for all the considered complexes, the presence of critical points (3;–1) is observed, which confirm the presence of a bond between Ag$^+$ and the nitrogenous base (Fig. 1). It is also shown that the largest value of the interatomic distance is observed in Ag$^+$ complexes with adenine (2.252 Å and 2.238 Å, respectively), i.e. they are less stable than complexes with thymine, cytosine and guanine, which is additionally confirmed by the results of QTAIM analysis. The obtained results are important for the understanding of the physical properties of metalized Ag-DNA.

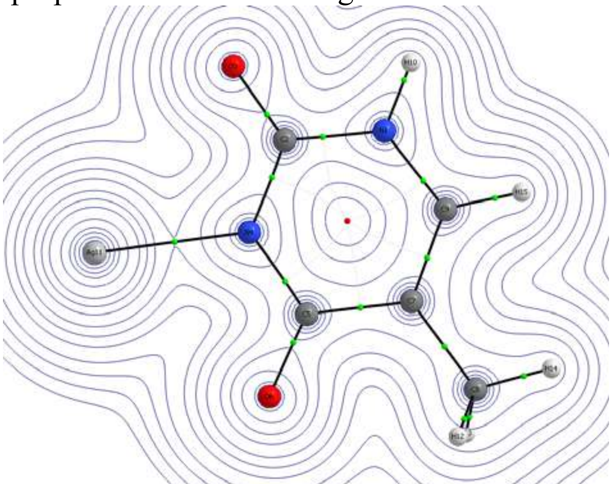

Fig.1. Molecular graph with electron density surface in the space of Ag-thymine complex

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O24

NANOBIOHYBRIDS OF 2D MoS_2 WITH ANTICANCER DRUGS: EXPERIMENTAL & THEORETHICHAL CHARACTERIZATION, APPLICATION PROSPECTS

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2D nanomaterials, including MoS_2 nanosheets, are in the focus of current nanobiophysical research due to the great prospects of these materials' applications in biosensing, drug delivery, biocatalysis, and other biomedically related nanotechnologies. The unique physicochemical properties and biocompatibility of 2D MoS_2 offer the possibility of utilizing this nanomaterial as an anticancer drug delivery platform and in photothermal therapy (PTT) of tumors. Thus, the characterization of the physicochemical properties of nanobiohybrids of MoS_2 nanosheets with anticancer drugs and the evaluation of the nanocomposites' applicability in cancer treatment can be considered as a task of current importance in modern nanobiophysics.

In the present work we report on combined experimental and theoretical study of the nanocomposites of MoS_2 nanosheets with a set of widely used anticancer drugs including doxorubicin (DOX), 6-thiopurine (TP), 2-thioadenine (TA), 5-fluorouracil (FU), as well as with biologically active derivatives of nucleobases – 6-thioguanine (TG), 2-thiopyrimidine (TPm), adenine (A). The nanocomposites obtained by ultrasound treatment were examined experimentally using laser desorption/ionization (LDI) mass spectrometry (MS). 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 composites with MoS_2, which is crucial for maintaining biological activity and the therapeutic effectiveness of these drugs. At the same time, the observed changes in the spectra, particularly in the intensity distribution of the MoS_2 characteristic peaks (described in detail in [1]), pointed to the active exfoliating role of these drugs in the ultrasound technology for producing the MoS_2 nanosheets. Interestingly, that we revealed spectral confirmations of some chemical transformations (covalent dimerization or oxidation) of sulfur-containing anticancer drugs and active agents (TP, TA, TG, TPm) induced by catalytically active MoS_2. We believe that such chemical transformations of drug molecules can reduce their therapeutic activity, which is mostly related to the thio-groups in the molecules.

Ab initio DFT/M06-2X theoretical modelling of nanobiohybrids of MoS_2 nanosheets with anticancer drugs were performed to examine the possible structures of such nanocomplexes. In particular, the structures of the complexes of MoS_2 with anticancer thioderivatives of purine nucleobases – TP and TA – were determined, and the energies of such complexes were calculated. Based on the modelling results, the biologically significant peculiarities of sulfur-containing agents with MoS_2 nanosheets are discussed. We suppose that the data obtained should be considered at the development and application of MoS_2-based nanobiohybrids in biomedical practice.

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O25

Mn_3O_4 NANOCRYSTALS ACTIVATE CASPASE-3 IN ERYTHROCYTES

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Unlike nucleus-containing cells, erythrocytes have been found to have only two caspases, namely caspase-3 and caspase-8. Their contribution to cell death of erythrocytes is less critical compared to nucleated cells. Nevertheless, activation of caspases in mature erythrocytes definitely results in cell death (eryptosis) via promotion of phosphatidylserine externalization.

In this research, we investigated the effects of Mn_3O_4 nanocrystals on caspase-3 activity in mature erythrocytes.

Erythrocytes were treated with the newly synthesized Mn_3O_4 nanoparticles (40 and 80 mg/L) during 24 h. The fluorogenic indicator DEVD-ProRed was used to detect caspase-3 activity using laser scanning confocal microscopy.

Mn_3O_4 nanocrystals were found to activate caspase-3 in both studied concentrations. Of note, the effects were comparable for 40 and 80 mg/L. Our study has revealed that Mn_3O_4 nanocrystals are erythrotoxic at high concentrations and their erythrotoxicity is mediated by caspase-dependent eryptosis.

O26

DFT STUDY OF TERNARY COMPLEXES OF MoS_2 WITH URACIL AND NOBLE METAL CLUSTERS: STRUCTURE, STABILITY AND SPECTRA

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We used the quantum-mechanical DFT method with the meta-hybrid M06-2X density functional to characterize structure, interaction energies and vibrational spectra of ternary complexes MoS_2-Au_{10}-uracil and MoS_2-Ag_{10}-uracil nanobiohybrides. In the calculations, we used the Stuttgart RSC 1997 ECP basis set for gold and silver atoms, the 6-31+G* basis set for uracil, the LanL2DZ basis set for molybdenum atoms and LanL2DZdp basis set for sulphur atoms. First we located all possible structures of silver and gold particles consist of 10 metal atoms eacch. For clusters of this size, both flat and 3D stable structures are possible. We found 15 stable structures for Au_{10} and 21 for Ag_{10}. Next, for the most stable metal particles, calculations of their binary complexes with uracil and MoS_2 were performed. We demonstrated that interaction with uracil and especially with MoS_2 significantly changes both geometry and electron structure of the noble metal clusters. Thus, it was discovered that the most of Au_{10} clusters, when interacting with the MoS_2 surface, are transformed into pyramidal structures, as shown in Fig. 1. It is important to note that for individual (isolated) Au_{10} clusters, such a pyramidal structure is not stable. The calculated ZPVE and BSSE corrected interaction energies between MoS_2 and the metal clusters reach -100 kcal/mol for the MoS_2-Au_{10} and -150 kcal/mol for the MoS_2-Ag_{10} binary complexes. This is significantly higher than the similar interaction energies of these clusters with graphene (-20 — -40 kcal/mol for the graphene-Au_{10} and and -35 — -45 kcal/mol for the graphene-Ag_{10}). We performed the natural bond orbital (NBO) population analysis to elucidate the nature of the interactions in the binary complexes. The results of this analysis showed that the in the MoS_2-Au_{10} and MoS_2-Ag_{10} complexes the covalent coordination bonds between gold or silver atoms and the surface sulfur atoms of the MoS_2 fragment are formed. These covalent bonds provide strong interactions within the complexes. It should be noted that the noble metal cluster complexes with graphene are stabilized by the cation-π interactions, which are weaker than covalent bonding.

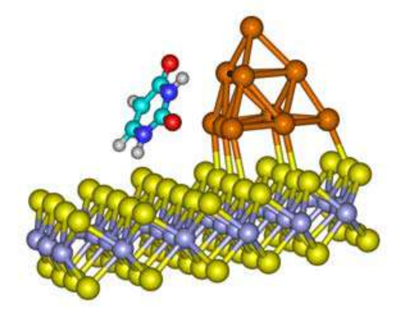

Fig. 1. Structure of the MoS_2-Au_{10}-uracil complex.

It was also found that the interaction between MoS_2 and noble metal clusters is accompanied by significant charge transfer between them (up to 0.7e). It results in enhanced interaction between the uracil molecule and metal clusters placed on the MoS_2 surface (ternary complexes) as compared to the interaction in binary uracil-Au_{10} and uracil-Ag_{10} complexes. An important consequence of this is the enhanced spectral effects of uracil interactions with metal clusters placed on the MoS_2 surface compared to the binary complexes. Thus, in IR and especially in Raman spectra, a stronger increase in band intensities/activities is observed in ternary complexes. This shows that the placement of metal clusters on the surface of MoS_2 can improve the performance of the corresponding nanohybrids used for biosensors.

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O27

FEATURES OF EXCITATION OF NUCLEIC ACIDS COMPONENT ON THE MATRIX SURFACE BY ELECTRON BEAM

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The aim of this report is to study the luminescence of the nucleic base thymine under the action of electrons in conditions when these molecules are on the surface of a graphite matrix. Similar studies were previously performed by us for the base cytosine [1].

The experiments were carried out using the electron-photon spectroscopy method, which is sensitive to the properties of the surface layer, which allows creating a high concentration of excited states of biomolecules. Immobilization of thymine molecules was carried out by their precipitation from an aqueous solution onto the surface of a graphite matrix with subsequent heating to 110 °C at $P \leq 10^{-1}$ Pa. Measurement of electron luminescence spectra was carried out under ultrahigh vacuum conditions - $P \leq 5\ 10^{-7}$ Pa. An electron beam with energies of 500-800 eV and a current density on the graphite surface of ~ 0.05-0.30 mA/mm was generated by an electron gun.

Intense luminescence of thymine molecules immobilized on the graphite surface was detected experimentally in the wavelength range of 200-800 nm. The luminescence spectra were represented by three broad molecular bands. The absolute photon yield at the maxima of these spectral bands was estimated. The molecular bands are due to the excitation of π-electrons of thymine molecules from the ground singlet state to the excited singlet and triplet states with their subsequent deactivation.

It should be especially noted that the fragmentation of the thymine molecules in the solid phase under the action of the primary electron beam and secondary electrons is very small, in contrast to that in the gas phase. Therefore, the adsorption of nucleobase molecules to the porous surfaces of a solid can protect them from degradation in the environment.

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O28

APPLICATION OF NIR-REDUCED GRAPHENE QUANTUM DOTS FOR BIOSENSING OF NEUROTRANSMITTERS/HORMONES

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Early detection and monitoring of neurotransmitters and hormones are essential for accurate diagnosis, individualized treatment, and real-time physiological assessment. Physiological problems such as neurological, psychiatric, cardiovascular, and metabolic problems are linked to dopamine, cortisol, oxytocin, and serotonin dysregulation. Traditional technologies like high-performance liquid chromatography (HPLC) and mass spectrometry (MS) are sensitive but expensive, intrusive, and unsuited for continuous or point-of-care applications. In this study, we present a biosensing platform for the detection of biological analytes (dopamine, serotonin, cortisol, and oxytocin), using near-infrared (NIR) fluorescent reduced graphene quantum dots (RGQDs). The study also uses artificial intelligence (AI) to analyze unique spectral fingerprints produced through fluorescence quenching in NIR emission spectra (800–1050 nm) for each analyte. Precise identification without surface functionalization is possible with artificial intelligence algorithms that distinguish small spectral differences for each biological analyte. Our lab synthesizes RGQDs with intense NIR fluorescence, high water solubility, and great biocompatibility for wearable or implanted diagnostic systems. Nanomaterial engineering and machine learning provide a cost-effective, scalable, and non-invasive biosensing system that could increase diagnostic access in clinical and underprivileged settings.

O29

ARTEMISININ: AN ANTIMALARIAL AGENT DISRUPTING NANOCRYSTAL HEMOZOIN FORMATION, WITH ANTITUMOR AND IMMUNE-MODULATING PROPERTIES

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Malaria remains an important life-threatening disease caused by *Plasmodium* parasites, with *P. falciparum* (*P.f.)* being the most dangerous. The parasite induces anemia, disrupts the immune system balance, and deposits malarial pigment hemozoin (HZ), a bioactive nanocrystal [1].

Among numerous substances exhibiting antimalarial activity, artemisinin has emerged as one of the most widely used compounds. Artemisinin-based combination therapy (ACT) is the globally recommended treatment for *P.f.* malaria. Beyond its antimalarial effects, artemisinin is under investigation for its antitumor, immunomodulatory, and other therapeutic applications. Various mechanisms of action have been suggested for dihydroartemisinin (DHA), the active metabolite of artemisinin, including the induction of oxidative stress in target cells. We track the production of reactive oxygen species (ROS) and the lipid peroxidation product 4-hydroxynonenal (4-HNE), along with protein alkylation by 4-HNE, in *P.f.*-infected human erythrocytes after DHA treatment. At nanomolar DHA concentrations, the disruption of HZ crystal formation began, and progressively, at low micromolar concentrations, DHA induced 4-HNE-adduct formation, which proved detrimental to parasite proteins. Mass spectrometry of proteins from young ring-stage parasites revealed extensive modifications of the *P.f.* cysteine proteinase falcipain-1 by 4-HNE conjugation. This suggests that the post-translational modification of crucial *P.f.* proteins by 4-HNE may contribute to DHA-induced parasite death. While significant 4-HNE accumulation was detected following DHA treatment, its concentrations were well above pharmacologically effective levels for malaria treatment but within the ranges observed for antitumor activity. Notably, human cathepsins B, K, and S enzymes sharing active site similarities with falcipain-1, are potential targets of DHA in tumor treatment [2].

Thus, lipid peroxidation with subsequent conjugation of functionally relevant proteins by 4-HNE may represent a unifying mechanism by which DHA enhances the efficacy of antimalarial drugs within ACT, modulates tumor progression and immune response.

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O30

SURFACE AND INTERFACE EFFECTS IN THE ANTIBACTERIAL ACTIVITY OF NANO- AND MICROSCALE OXIDES OF ZINC AND GALLIUM

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The growing global issue of antibiotic resistance has sparked interest in alternative antibacterial agents, such as metal oxide particles. While the antibacterial properties of many metal oxides are well-documented, the mechanisms behind their effectiveness remain largely unclear. These mechanisms may involve the production of reactive oxygen species, the release of toxic cations, or interactions that disrupt cell walls, leading to osmotic stress. It is believed that bacteria cannot develop resistance to oxide-based treatments because the antimicrobial action occurs through multiple pathways. The targeted use of these oxide antibacterials is also limited by a lack of understanding regarding the local bacterial environment's role in mediating or impeding antibacterial interactions.

To explore this, our expansive research focuses on the interactions between oxide surfaces, bacterial cell membranes, and growth media. We use hydrothermally synthesized nano- and microparticles of undoped and Fe-doped ZnO, β-Ga_2O_3, and GaOOH. Our method enables precise control over particle morphology and the distribution of polar surface areas.

To assess the antibacterial activity, we conduct biological assays using *Escherichia coli* and *Staphylococcus aureus*. In addition, we perform pre- and post-assay comparative studies of the oxide particles using advanced characterization techniques, including X-ray diffraction spectroscopy, scanning electron microscopy, energy dispersive X-ray spectroscopy, X-ray photoelectron spectroscopy, Raman spectroscopy, photoluminescence spectroscopy, surface photovoltage, Fourier-transform infrared spectroscopy, thermoluminescence spectroscopy, and impedance spectroscopy.

Our findings demonstrate that there exist significant interactions at the free crystalline oxide surfaces, which are highly dynamic and complex. We present evidence of competitive interactions between bacteria and environmental species, mediated by defect states. We suggest that multiple competing mechanisms of antibacterial action in oxides may be at play. Additionally, the dominant inhibitory mechanism may be influenced by factors such as particle size and morphology.

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O31

A PHYSICALLY INTERPRETABLE NEURAL NETWORK MODEL FOR DETERMINING THE ENERGY OF BIOMOLECULES BASED ON THEIR STRUCTURE

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Designing novel molecules and enhancing synthesis routes critically relies on our ability to infer molecular properties and energies from structural data. In this context, machine learning (ML) has increasingly become an essential tool that automatically generalizes large datasets of molecular data in order to relate molecular structures to their properties much faster than traditional quantum chemical calculations, while achieving comparable accuracy. Despite growing interest in ML-based models for molecular energy prediction [1], many existing approaches provide accurate outputs without offering insight into the underlying physics, thus becoming the „black boxes". Lack of interpretability limits their scientific use, where understanding of underlying physics matters as much as accuracy. This is in contrast to the physics-based models that build confidence, reveal failure modes, transfer to unseen chemical spaces, and deepen understanding of molecular interactions. To overcome these limitations of ML models, we integrate concepts from quantum-chemical description of molecular structure with graph-based neural network architectures. Our approach decomposes the energy prediction task into two sequential steps. Initially, it learns descriptors of atoms and bonds by being trained to predict physically meaningful localized quantities related to the electron density distribution and kinetic energy of electrons. These intermediate features are then fed into a secondary network, which task is predicting parameters of an explicit interatomic potential. This two-stage approach balances the contributions from different pairs of atoms in physically sound manner. Evaluated on publicly available datasets, the proposed model exhibits strong predictive performance, achieving mean absolute errors of 2.2 kcal/mol for total molecular energy and 6.1 kcal/mol for electronic kinetic energy. The model also attains a mean squared error of 1.7 kcal/mol in the prediction of intermolecular interaction energies, despite these not being included as explicit training targets. This suggests a high degree of physical consistency in the learned representations and indicates the model's capacity to generalize effectively to related tasks and previously unseen molecular configurations.

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O32

MANGANESE OXIDE NANOCRYSTALS INDUCE ERYPTOSIS, A REGULATED CELL DEATH OF MATURE RED BLOOD CELLS

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A compelling body of evidence indicates that red blood cells are a suitable model for assessing the toxicity of nanomaterials associated with alterations of the redox metabolism. This is linked to the differences between the sources of reactive oxygen species (ROS) in erythrocytes and enucleated cells. Thus, the assessment of the ability of nanomaterials to trigger ROS production in erythrocytes might provide novel insights into the redox pathways involved in their toxicity.

Herein, we tested how newly synthesized Mn_3O_4 nanocrystals affected ROS production in mature erythrocytes.

The investigated Mn_3O_4 nanocrystals were incubated at 40 and 80 mg/L with red blood cells for 24 h. Thereafter, Cellular ROS/RNS Detection Assay Kit was applied to quantify ROS production. Fluorescence was detected by laser scanning confocal microscopy.

It has been found that Mn_3O_4 nanocrystals trigger ROS production in a dose-dependent fashion. Thus, Mn_3O_4 nanocrystal-triggered toxicity against red blood cells is mediated by oxidative stress, suggesting that Mn_3O_4 nanocrystals exert erythrotoxicity at high concentrations.

O33

DEVELOPMENT AND CRYOPRESERVATION OF PROBIOTIC-ENRICHED ALGINATE HYDROGEL FILMS FOR WOUND CARE APPLICATIONS

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Alginate hydrogels are well-established biomaterials for wound dressings due to their biocompatibility. The therapeutic efficacy of these dressings can be significantly enhanced by incorporating probiotic lactic acid bacteria, such as *Lactobacillus* and *Bifidobacterium*, known for their antagonistic activity against common wound pathogens. However, preserving bacterial viability alongside the hydrogel's functional properties throughout production and long-term storage remains a significant challenge.

This study aimed to develop a comprehensive protocol for the immobilization, cultivation, and low-temperature storage of probiotic bacteria within an alginate-based hydrogel film, ensuring the preservation of cell viability, mechanical stability, and antimicrobial effectiveness.

Lactobacillus bulgaricus 1Z 03501 and *Bifidobacterium bifidum* LVA-3 were immobilized in an alginate hydrogel matrix fortified with either pectin or starch. The films were produced using an aerosol application of calcium chloride. Following immobilization, the films underwent a cultivation period of up to six days in Blaurock medium. Subsequently, they were saturated with cryoprotectants (glycerol or DMSO) and stored for seven days across a range of temperatures from +25°C to -80°C. Key performance indicators, including the mechanical and organoleptic properties of the films, viable probiotic cell counts, and antagonistic activity against *Staphylococcus aureus* 209, *Pseudomonas aeruginosa* 9027, and *Escherichia coli* B, were systematically evaluated.

The addition of pectin or starch significantly enhanced the mechanical integrity of the alginate films. Although the initial immobilization captured a high density of bacterial cells, their antagonistic properties were temporarily reduced. A subsequent two-day cultivation period was critical, leading to a substantial increase in viable cell counts (up to 100-fold) and restoring potent antagonistic activity against the tested wound pathogens. The study established that freezing the films at -80°C after saturation with 20% glycerol was the optimal condition for preserving both high cell viability and the films' essential functional characteristics post-thaw.

In conclusion, we have developed a robust method for fabricating alginate-pectin/starch hydrogel films loaded with viable and functionally active lactic acid bacteria. The developed protocol for cultivation and cryopreservation ensures the final product retains its therapeutic potential, making it a promising candidate for application as an advanced wound dressing for the management of infected wounds.

O34

ACCURATE MACHINE LEARNING APPROACH TO PROTEIN-LIGAND DOCKING

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Classical protein-ligand docking has been a cornerstone technique in computational drug discovery for decades, but has reached an accuracy and performance plateau. Recently introduced Machine Learning (ML)-based docking methods offer a promising paradigm shift; however, accuracy-to-speed trade-offs, inadequate benchmarking standards, and questionable chemical validity of predicted poses hinder their practical adoption.

In this work, we introduce an ML-based docking technique optimized for high-throughput virtual screening applications (Figure 1).

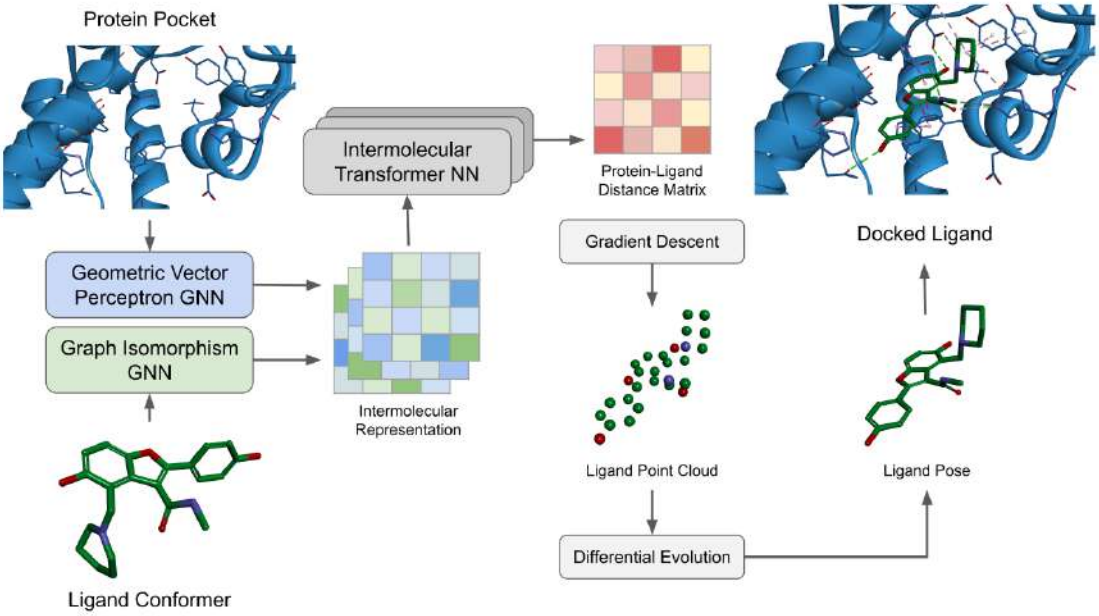

Fig. 1. General scheme of the docking ML model architecture and inference pipeline.

To ensure an unbiased evaluation, we retrained the model on the PLINDER dataset [1]. This dataset contains a large and diverse predefined training subset from the Protein Data Bank. The train-test splitting process is cluster-based, which minimizes both the data leakage between the sets and the test set redundancy. We assessed the final performance on the PLINDER test set and compared results to leading open-source and commercial classical docking techniques such as AutoDock [2], [3], Vina [4], and Glide [5]. The evaluation covers docking accuracy, chemical and geometric validity of the predicted poses, and computational efficiency.

We demonstrate that our method is 29-38% more accurate in terms of deviation between experimentally determined and predicted ligand poses compared to classical docking techniques, while providing a low computational cost.

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O35

SELF-FORMATION OF COHERENT CORRELATED STATES OF INTERACTING PARTICLES IN BIOMOLECULES FOR THE REALIZATION OF NUCLEAR FUSION IN BIOSYSTEMS

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The traditional point of view is that the nanostructure of biological molecules is important only for the implementation of specific biophysical functions associated with biochemical and bioinformational processes. The formation and functioning of such biomolecules in any living system has a purely "consumer" and passive character and in the absence of the necessary micro or macroelements these processes become impossible. Detailed analysis and successful experiments [1-6] show that under such critical conditions, biosystems are capable of switching to partial self-sufficiency by stimulating local nuclear processes that ensure the nuclear synthesis of essential microelements. Obviously, such processes cannot be realized using thermonuclear fusion, which require giant temperatures or accelerated particles to overcome the Coulomb barrier of nuclei.

On the other hand, multiple studies (e.g. [1,2,6]) have shown that such processes are effectively realized at room temperature n living biosystems using very large energy fluctuations of $\delta E \approx 30\text{-}100$ keV, which correspond to the Schrödinger-Robertson uncertainty relations $\delta E \delta t \geq \hbar / 2(1-r^2)^{1/2}$ and $\delta p \delta q \geq \hbar / 2(1-r^2)^{1/2}$ for coherent correlated states (CCS) with large ($|r| \to 1$) coefficient of correlation for interacting particles. Such states are formed, for example, during the natural modulation of nanoscale potential wells in the volume or near the surface of dynamic biomolecules (e.g., during DNA replication in the region of the replication fork or in the region of cell division). In such systems, the state of a proton (or other particle) located in the volume of these nanowells corresponds to a coherent quantum superposition with a large correlation coefficient, which leads to large energy fluctuations δE that exist for an anomalously long time δt. These parameters are many orders of magnitude larger than the similar characteristics corresponding to the Heisenberg uncertainty relation $\delta E \delta t \geq \hbar / 2$ for uncorrelated states, for which $r = 0$. Nuclear reactions stimulated by fluctuations of energy and momentum are fundamentally different from reactions involving real accelerated particles. In such reactions the channels that form radioactive isotopes are suppressed and gamma radiation is also very strongly suppressed [7].

Such biostimulated nuclear fusion can be effectively implemented in the cultivation of microbiological cultures with the present in water environment of light, medium and heavy stable isotopes (e.g. $Mn^{55}+d=Fe^{57}$, $Na^{23}+P^{31}= Fe^{54}$ and $Cs^{133}+p=B^{134}$). The most important results relate to the experimentally confirmed possibility of deactivation of long-lived radioactive isotopes and reactor waste in growing syntrophic microbiological associations (e.g., Cs^{137} in the reaction $\mathrm{Cs}^{137}+\mathrm{p}=\mathrm{Ba}^{138}$ which reduced the deactivation time from 30 years of natural decay to 10 days.

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Posters

P1

NEW APPROACHES IN THE METHODOLOGY FOR ASSESSING NANOPARTICLES OF METALS, ASBESTOS, AND PLASTICS STABILIZED BY BIOLOGICAL MOLECULES IN MODEL SOLUTIONS

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Modern advances in biomedical technologies, such as biotechnology, genetic engineering, and nanotechnology, offer unprecedented opportunities for enhancing human health and prolonging our lives. Nanoparticles of noble metals have a wide range of applications in various industries, making them important materials that have a significant impact on technology, healthcare, and environmental sustainability [1-3]. For example, one of the strategies for synthesizing homogeneous Au and Ag nanostars with tunable optical properties using adenosine monophosphate (AMP) as a capping ligand is discussed. AMP plays an important role as a ligand, providing colloidal and thermal stability, controlling precursor reduction, and mediating anisotropic growth of Au and Ag nanostars through selective adsorption on different faces of Au and Ag nanoparticles [3].

The unique qualities of nanomaterials, such as their tiny size, biocompatibility, and ability to cross cell membranes for drug delivery, make them useful for a variety of biological applications [4]. At the same time, there is another problem of studying the dangers of nanoparticles of other substances, such as asbestos and plastic. Increased emissions of such substances into the atmosphere, as well as metal nanoparticles during traditional industrial processing also require new methodological approaches [5-6].

Thus, the method used in this study was to create colloidal solutions capable of maintaining the stability of nanoparticles of various natures – metal oxides, asbestos, and plastic – in model solutions. The following research methods were used to identify and study the stability and structure of the nanoparticles.

The condensate structure elements and the surface of asbestos were studied in scanning electron microscope (SEM) CamScan-4 (Cambridge, Great Britain). Distribution of metal oxide nanoparticles (Ag, Fe, Cu), asbestos fibers and plastic particles dimensions in the colloidal solutions was studied by the method of dynamic light scattering (DLS) in laser correlation spectrometer (LCS) “Zeta Sizer - 3” (Malvern, Great Britain). Metals concentrations were determined by the method of inductively coupled plasma optic emission spectroscopy (ICP-OES methods) in Optima 2 100 DV (USA).

An important characteristic powders of Ag, Cu, and Fe oxide nanoparticles obtained by electron beam evaporation in a vacuumis the stability of metal concentrations in colloidal solutions, especially when it comes to powdered nanomaterials. The study of the distribution of NPs by the LCS method showed that the particle size distribution in colloidal solutions was as follows: for Ag_2O – 32 nm, CuO – 6-30 nm and Fe_2O_3 – 92 nm. The stability of the concentrations of Ag, Cu and Fe in dispersed systems in colloidal solutions of NP metal oxides determined by OES-ICP showed satisfactory results for dispersed systems using polyvinylpyrrolidone (PVP), dextran and serum albumin. The good stability of Ag concentration in fructose, citric acid, phosphate and citrate buffers was found during storage for 21 days.

Modern methods such as Fourier transform infrared spectroscopy with attenuated total reflection (FTIR-ATR), X-ray diffraction, and scanning electron microscopy [4,5] allow asbestos to be detected in samples and its type to be determined. Here, the main focus is on long fibers (>5-10 µm). However, the question of sampling often arises. Here, it is important to select an aqueous or colloidal solution. In our study, SEM revealed asbestos fibers measuring up to 100 μm. When sampling atmospheric air in a citrate solution using LCS method, fiber sizes ranging from 5 to 100 μm were detected. Another threat to the environment is plastic. Its various types (from PET to PFAS) actively pollute the environment and, according to various sources, enter the human body and have a destructive effect similar to organic substances and are also often described in scientific literature as endocrine disruptors. Methods for detecting them in the environment, particularly in drinking water and the tissues of living organisms, are currently under development and implementation. One such approach to detection in solutions is the LCS method. Bimodal distribution of PET plastic particles in succinic acid model solutions (0.1% solution) was detected. The distribution of particles ranged from 15.70 to 50-75 nm, although particles of 59-91 nm and 255-342 nm were also found, indicating polymer degradation processes.

Important parameters when determining the size of nanoparticles are the refractive index, brightness and absorption coefficient . For plastic, the refractive index was 1.569, for asbestos – 1.53-1.72, for low-frequency metals – 2.3-2.63 (for, silver, copper, ferrum). The buffer system used, based on citrates or tartrates, proved to be important.

Summarizing the results obtained, it should be noted that when studying nanoparticles using LCS method, it is important to choose the method of the sample preparation, and the physical properties of solutions, such as the absorption index, refractive index, and viscosity. The LCS method is well suited for studying metal, mineral, and polymer nanoparticles under certain model conditions. Thus, by selecting a colloidal system and gradually "dissolving" the condensate of metal/metal oxide nanoparticles, minerals (asbestos) or polymers (PET) in a liquid medium, it is possible to change the hydrodynamic size of nanoparticles. Currently, there are no internationally recognized standards regulating the content of microplastics in drinking water. The LCS method may be one such approach.

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P2

INHIBITION OF *PSEUDOMONAS AERUGINOSA* GROWTH BY “GREEN” SYNTHESIZED SILVER NANOPARTICLES

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The development of nanotechnology attracts now special attention due to the wide range of applications of nanomaterials in technology, medicine, and agriculture. So-called "green" synthesis, which involves the use of extracts from living organisms, in particular, plants, to obtain metal nanoparticles (NPs) is one of the practically used methods. The method is environmentally friendly because it does not require toxic chemicals. The shape and size of NPs depend on the type of plant extract, reaction temperature, pH of the medium, and precursor concentration. Phytochemical compounds contained in plant extracts can stabilize nanoparticles, preventing their aggregation. The NPs have high surface activity, which contributes to their biological effectiveness. They can interact with the cell membrane of microorganisms, causing its damage and dysfunction.

In this work, we investigated the antimicrobial activity of silver nanoparticles obtained by “green” synthesis using an extract from biotechnological roots of *Bidens pilosa* plants.

The presence of antibacterial properties in the nanoparticle samples was checked using the test strain *Pseudomonas aeruginosa* UCM B-907 (ATCC 27853 (F-51) from the Ukrainian Collection of Microorganisms (UCM, D.K. Zabolotny Institute of Microbiology and Virology of the National Academy of Sciences of Ukraine) which is recommended by the State Pharmacopoeia of Ukraine for controlling the accuracy of determining susceptibility to antibiotics. Cultivation of microorganisms was carried out on Mueller-Hinton agar - MXa (Conda) at the temperature of 37°C for 18-24 h, which is a requirement of EUCAST for the methodology of conducting microbiological studies of the sensitivity of microorganisms to antimicrobial drugs. Using serial tenfold dilutions, suspensions with a titer of $2\text{-}5\times10^5$ CFU/ml were obtained, which were used in further studies. Incubation was performed in 24-well culture plates. When determining the bactericidal activity, 50 µl of nanoparticle sample was added to individual wells of the plates and 450 µl of a suspension of bacteria with a titer of $2\text{-}5\times10^5$ CFU/ml was added. As a positive control, 450 µl of a similar suspension of the test strain of microorganisms with the addition of 50 µl of sterile saline solution was used. Cultivation was carried out at 37°C for 18-24 h, after which the titer of the bacteria was determined.

The results of the study showed that after 18-24 h of contact of nanoparticles in dilutions of 1:10, 1:100 and 1:1000 with *P. aeruginosa* UCM B-907 in the studied suspension with a volume of 100 µl, no viable bacteria were detected. When nanoparticles in a dilution of 1:10000 interacted with indicated microorganisms, the final titer of bacteria was 5.1×10^4 CFU/ml. The quantity of *P. aeruginosa* UCM B-907 in the control sample without the addition of nanoparticles after 18-24 h of incubation was 5.3×10^6 CFU/ml. Considering the given indicators of the titers of microorganisms in the experimental and control samples and the dilution factor, it can be stated that the nanoparticles reduced the number of *P. aeruginosa* UCM B-907 cells by 1039215 times.

Thus, it was found that nanoparticles derived from biotechnological roots do indeed have a high level of antimicrobial activity against test strain *P. aeruginosa* UCM B-907.

P3

MASS SPECTROMETRIC ASSESSMENT OF TRANSITION METAL DICHALCOGENIDES FUNCTIONING AS NANOZYMES

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Transition metal dichalcogenides (TMD) exhibit catalytic activity in biological systems, being constituents of enzymes' cofactors. A trend in modern nanobiotechnology is the substitution of biological enzymes with their simpler and cheaper inorganic analogues, called nanozymes [1]. TMD-based 2D nanomaterials are promising for this application [2, 3].

In this communication, we evaluate the catalytic redox activity of 2D TMD MoS_2 and WS_2 in relation to a set of biologically significant organic molecules – amino acids, nitrogen bases, dyes, and simple thiols – based on information obtained using the laser desorption/ionization (LDI) mass spectrometric experimental technique. LDI permits the desorption of components and products of redox reactions directly from the surface of 2D nanosheets; the high sensitivity of the method allows detection of small quantities of substances.

The catalytic activity of TMD was probed in the systems obtained by sonication of mixtures of TMD with organic compounds in aqueous medium. LDI (337 nm) analysis was performed for dried solid samples, applying low laser power required for non-damaging desorption mode. LDI mass spectra were recorded both in positive and negative ion modes. In the negative ion mode, a set of $Mo_xS_yO_z^-$ or $W_xS_yO_z^-$ clusters characteristic of the nanomaterials [4] dominated the spectra. Species related to organic compounds were registered mostly in the positive ion mode.

The strongest effect was observed in cases of MoS_2 interactions with organic compounds that contain thiol groups. For the cysteine amino acid, tripeptide glutathione, thioderivatives of nitrogen bases, and thioglycerol the oxidation reaction was catalyzed at the MoS_2 surface, resulting in the formation of covalent dimers bound by a disulfide bond. Interestingly, in the mixture of cysteine with thioglycerol, a heterodimer of two different thiols was formed.

However, for practical applications of TMD as nanozymes for definite types of reactions, the conditions for the elimination of some accompanying effects are to be established. Namely, the deepening of organics transformations may lead to fragmentation and destruction of organic molecules, which products are also observed in the mass spectra of glutathione and some polymers. In addition to interactions at the 2D planes, organic molecules can bind to the edges of 2D nanosheets; the outcomes of these interactions differ from those with the surface.

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P4

COMPLEX FORMATION IN AQUEOUS SOLUTIONS OF BSA WITH IBUPROFEN AND SILVER NANOPARTICLES

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Ibuprofen is a non-steroidal anti-inflammatory drug with high lipophilicity and significant protein-binding properties, especially to serum albumins. Bovine serum albumin (BSA) is commonly used as a model protein for evaluating drug–protein interactions due to its structural similarity to human serum albumin. In this work, we investigate the interaction between ibuprofen and BSA in aqueous solutions using both experimental and computational methods.

Fluorescence quenching experiments were performed for aqueous BSA solutions at fixed protein concentration (2 μM) and varying ibuprofen concentrations in the range of 0–1.5 μM at three different temperatures (293, 303, and 313 K). Similar experiments were performed for aqueous solutions of BSA and ibuprofen with addition of Ag nanoparticles at fixed concentrations of ibuprofen and BSA and varying concentrations of nanoparticles.

Quenching behavior followed the Stern–Volmer relationship and revealed static quenching with binding constants increasing with temperature, suggesting a hydrophobic interaction mechanism. The calculated binding constants ranged from 4.3 to 5.0 with a binding stoichiometry close to 1:1. Thermodynamic analysis using the van’t Hoff equation revealed positive values of ΔH and ΔS, confirming the spontaneous and entropy-driven binding.

Molecular docking simulations using AutoDock 4.2.6 identified three main binding clusters with 20 binding modes in total. The most energetically favorable modes are formed by all types of interactions (van der Waals, hydrogen-bonding, hydrophobic and electrostatic), but the most numerous are contacts with hydrophobic amino acid residues of BSA. The proximity of some binding modes to tryptophan residues supports the observed fluorescence quenching.

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P5

FEMTOSECOND LASER PROCESSING OF TITANIUM DIOXIDE FILMS FOR PHOTOCATALYTIC AND SELF-CLEANING APPLICATIONS

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The current report presents analysis of the properties of the developed functional titanium dioxide (TiO_2) films on glass substrates and their subsequent processing with femtosecond laser radiation. The self-cleaning and photocatalytic properties of TiO_2 films are crucial for removing organic compounds of biological origin from optical elements operating in harsh environmental conditions. TiO_2 is of particular interest due to its multiple polytypes (in particular, anatase and rutile) which can transform into one another. The anatase-rutile mixture exhibits better photocatalytic properties due to improved separation of charge carriers as the conduction band electrons are captured in the rutile phase. Laser treatment of sol-gel-derived TiO_2 films offers broad opportunities to tailor film characteristics such as thickness, crystalline or amorphous structure, grain size, residual stress, and defect density [1]. Compared to other surface treatment methods, laser processing uniquely combines time, temperature, and other conditions that are otherwise unattainable, and it offers high selectivity. Unlike thermal processing, laser irradiation is extremely fast and affects only the thin surface film.

The TiO_2 sols prepared with sol-gel method were applied on the substrates (glass) using spin-coating method followed by drying and calcination. Before annealing, the film of about 250 nm of thickness is porous with significant roughness. After annealing, the film becomes significantly thinner (around 90 nm) and denser. The films exhibit a band gap of 3.9 eV before annealing, which decreases slightly to 3.7 eV after annealing. Laser modification of TiO_2 films has been performed with a Ti:sapphire femtosecond laser using ultrashort laser pulses with fundamental wavelength of 800 nm. The pulse irradiation energy density was in the range of 0.025 - 0.225 $J\ cm^{-2}$ that resulted in different transparency of the TiO_2 film. Femtosecond laser treatment of TiO_2 films caused the formation of laser-induced periodic surface structures (LIPSS), nanoparticles, nano-cracks, and other features. We tried to select femtosecond laser treatment conditions to preserve sufficient transparency of the TiO_2 film while achieving the desired hydrophobic– hydrophilic balance. The laser treated surface demonstrates super hydrophilic properties. Photoluminescence (PL) spectra have been studied for each regime of ultrashort laser treatment of TiO_2 films deposited on glass. PL intensity presents the recombination efficiency of photogenerated charges that is an important factor for photocatalytic efficiency of TiO_2 films. PL spectra of TiO_2 films (both as grown and laser-treated) contain intense broad bands, namely green band at around 520 nm caused by the radiative recombination of free electrons with holes trapped around surface oxygen vacancies and red band at around 700 nm related to the defects of interstitial titanium ions. The relative intensities of these bands depend significantly on the parameters of laser processing of TiO_2 films. Weak PL band at about 340 nm corresponds to the exciton recombination in TiO_2.

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P6

THE STUDY OF THE SAFETY OF IRON OXIDE NANOPARTICLES

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Nanoparticles and nanomaterials are actively introduced into various areas of human activity. In particular, nanoparticles (NPs) of iron oxides Fe_2O_3 are widely used in medicine and pharmacy. As is known, NPs are more active and toxic than substances in their normal state, so studying their safety is a serious issue.

The aim of the study was assessment of Fe_2O_3 NPs effect of on the viability and functional activity of peritoneal macrophages in rats.

The studies were performed on peritoneal macrophages of rats in vitro and in vivo experiments. This object for the experiments was chosen due to the fact that macrophages are cells that are present in various tissues, take part in the formation of the immune response. Phagocytosis is the main process in protecting the organism from foreign agents.

The effect of Fe_2O_3 NPs (size 19 and 75 nm) on cell viability was studied using the MTT test, functional activity by phagocytosis and NBT test (spontaneous and stimulated). Fe_2O_3 NPs were obtained by chemical synthesis at the Chuiko Institute of Surface Chemistry of the NAS of Ukraine.

Studies have shown that incubation of macrophages with Fe_2O_3 NPs in vitro caused the death of 30% of cells, while its introduction into the body of rats did not significantly affect. At the same time, Fe_2O_3 NPs in vitro incubation with peritoneal macrophages during 24 hours caused activation of their phagocytic activity and bacterial ability compared with the control cells. Smaller Fe_2O_3 NPs 19 nm showed more stimulating effects than large NPs 75 nm. The phagocytic activity of peritoneal macrophages in the exposed rats after intraperitoneal administration of iron oxide NPs did not change significantly as compared to the control animals. However, NPs of both size in vivo equally stimulated bacterial ability with development of reactive oxygen forms in both versions of NBT-test (Fig. 1).

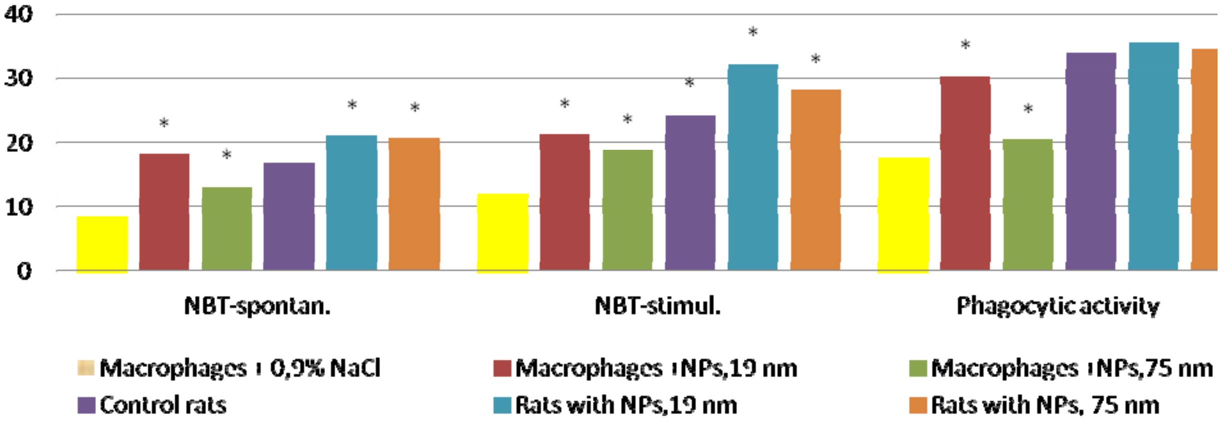

Fig. 1. The functional activity of macrophages (%) after 24 hour exposure with Fe_2O_3 NPs in vitro and in vivo.* Indicate significant differences compared with the control, $P < 0.05$.

The obtained data allow us to conclude that one of the ways of penetration of Fe_2O_3 NPs into the cell is phagocytosis. Nanoparticles, entering the body of rats, stimulated a nonspecific immune response (phagocytosis and the formation of reactive oxygen species in macrophages), which is aimed at their elimination and neutralization as foreign agents. Stimulation of macrophage activity after the introduction of Fe_2O_3 NPs indicates their positive effect on the viability and functional activity of cells and may be one of the signs of their safety for rats organism. The biological activity of Fe_2O_3 NPs depended on their size. Nanoparticles of 19 nm had a greater effect on the activity of macrophages, in particular on the synthesis of free radicals.

P7

STRUCTURE AND MECHANICAL PROPERTIES OF THE POLYMER BASE OF MEDICAL SPONGES WITH THE ADDITION OF METHYLURACIL

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The interaction between the gelatin-based polymer matrix, used as the base for medical sponges, and methyluracil – a filler with wound-healing and regenerative properties – was studied.

Gelatin surgical sponges are sterile porous products made from purified animal-derived gelatin, a biocompatible and biodegradable material [1]. They are primarily used during surgical procedures to stop bleeding [2]. Such sponges do not require removal, as they gradually dissolve in the body over the course of several days. Surgical sponges are often supplemented with medicinal agents (such as methyluracil) that exhibit antiseptic, antimicrobial, and wound-healing properties. When developing topical drugs based on polymer matrices incorporating pharmaceutical agents, a critical aspect is the interaction between the polymer base and the active pharmaceutical ingredients. It is essential that the polymer matrix does not interfere with the drug, alter its molecular structure, or reduce its functional activity [3].

Analysis of IR absorption spectra showed that methyluracil does not interact with gelatin, indicating that gelatin can be used as a neutral base for sponges. Examination of the structure and thermomechanical properties of medical sponge samples with varying methyluracil content, using optical microscopy and thermomechanical analysis, confirmed that the addition of methyluracil does not affect the structure or mechanical properties of the gelatin polymer matrix. Thus, the compatibility of methyluracil with the gelatin-based polymer matrix of surgical sponges was demonstrated.

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P8

STABILITY OF PROTONATED FORMS OF MONONUCLEOTIDES IN ALKALINE ENVIRONMENTS

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To date, the vast majority of spectral studies of mononucleotides have focused on their deprotonated (salt) forms. However, the properties of protonated nucleotide forms may differ from those of salt forms. It is believed that, in an alkaline intracellular environment, protonated nucleotides instantly transition to a salt state. Nevertheless, studies conducted in our laboratory have demonstrated the biological activity of protonated nucleotide forms. This suggests that protonated forms of nucleotides may be more stable in the intracellular environment than previously thought. In this study, we investigated the stability of protonated forms of mononucleotides using fluorescence spectroscopy.

We measured fluorescence spectra using Horiba FluoroMax 4P+ (HORIBA Scientific Jobin Yvon, USA). The integration time was 0.1 s, the slit width was 5 nm, the measurement step was 1 nm, the optical path length was 10 mm and the cuvette was made of quartz. The measurement temperature was 30 °C. Protonated and deprotonated mononucleotides were dissolved in 1x PBS and 0.05 M Tris buffers with a pH of 7.4–7.5 at concentrations of 2.9 and 14.5 mM/L. Spectra were measured for 80 minutes from the moment of dissolution.

The results showed that nucleotides in their protonated form, dissolved in alkaline buffers, exhibited different spectral properties as compared to nucleotides in their deprotonated form, primarily in terms of fluorescence intensity. Protonated nucleotides exhibited higher fluorescence intensity than deprotonated nucleotides. Additionally, the fluorescence intensity of protonated nucleotides depended strongly on concentration, whereas this was not observed for deprotonated nucleotides. Within 80 minutes of dissolution, protonated nucleotides with purine bases did not change their spectral properties. As for nucleotides of the protonated form with pyrimidine bases, the spectrum of uridine monophosphate gradually changed, and the spectrum of cytidine monophosphate was similar to that of its deprotonated form.

Therefore, most nucleotides in their protonated form are sufficiently stable in an alkaline environment, making them promising candidates for use in medical practice.

P9

A NANOCONJUGATE OF POLY-β-MALIC ACID WITH CYANINE-BASED DUAL INHIBITOR PF TELOMERASE AND TOPOISOMERASE I

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Modern anticancer strategy is based on the use of bioactive compounds interacting with molecular targets specific for tumor cell. A number of enzymes of nucleic acid biosynthesis, including the topoisomerase I (TopoI) and telomerase, are tumor-associated targets for anticancer drugs. Topoisomerase I is responsible for DNA relaxation during its replication, transcription and recombination. Due to high expression in tumor cells, TopoI is an established antitumor target [1]. Promising new target is telomerase, an enzyme performing the synthesis of telomeric DNA [2]. 85-90% of tumors exhibit high telomerase activity, in contrast to normal somatic cells.

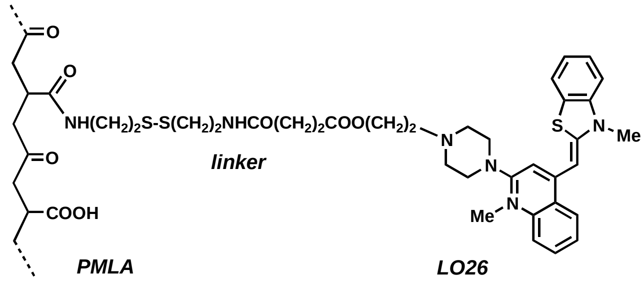
Multitarget approach is a new strategy in drug design. Since both TopoI and telomerase are biological targets for anticancer agents, the search for compounds simultaneously inhibiting these two enzymes may lead to the development of more potent anticancer drugs.

We have identified a series of 2-aminosubstituted cyanine derivatives with high inhibition activity against both TopoI and telomerase, with IC_{50} *in vitro* in the range 2-10 μM. Efficient dual inhibitors demonstrated high antiproliferative activity in tumor cell cultures (HeLa and U87MG lines), with nanomolar EC_{50} values (200-800 nM) for the most efficient compounds.

Low-molecular anticancer agents often suffer from low specificity, high toxicity and low water solubility. To overcome these drawbacks, the drugs can be attached to nanocarriers, including the biocompatible hydrophilic polymers, either natural (polysaccharides) or synthetic (polyethylene glycol, polylactic acid, dendrimers, etc.). Such conjugates allow the targeted delivery of drugs to release the attached bioactive compound inside the tumor cell.

Here, we synthesized a polymer conjugate of one of the active cyanines, **LO26**, to improve its cellular delivery. **LO26** was attached to poly-β-malic acid (PMLA), a natural polycarboxylated water-soluble polymer known as highly efficient carrier for drug delivery to the tumor cells [3].

COOH groups of PMLA (MW 50 kDa) were modified with cystamine by the active ester approach to get the amine-modified polymer. **LO26** derivative containing the OH group was functionalized by the treatment with succinic anhydride, and N-hydroxysuccinimide active ester of carboxyalkyl-cyanine was coupled with aminated polymer via the amide bond under mild reaction conditions (50 mM carbonate buffer, pH 7.5, room temperature). The final product was purified by gel filtration on Sephadex G-25. The cyanine content in various samples of nanoconjugate was in the range 100-150 μmol/g. Drug is attached to the carrier by the linker containing the biolabile S-S bond. This bond is easily cleaved in the cell by reducing agents like glutathione allowing the drug release after the conjugate uptake. The overnight treatment of PMLA-**LO26** with dithiothreitol (50 mM, pH 7.5) resulted in almost complete cleavage of cyanine inhibitor from the polymer carrier. The nanomaterial is well soluble in water and sufficiently stable (no decomposition was observed upon dry storage at 4°C for 4 months). The study of its biological properties is in progress.



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P10

SPECTROSCOPIC MARKERS OF PHENOTHIAZINE DRUG ADSORPTION ON MESOPOROUS ANATASE TiO_2

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During the last two decades, the exceptional pharmacological properties of phenothiazines (PTZ) have drawn great interest on the study of these compounds. Phenothiazines are widely used as antidepressants to manage and treat various psychoneurologic disorders such as schizophrenia, bipolar disorder, and acute psychosis. The phenothiazine drugs also play a very important part in chemotherapy. PTZ ($C_{12}H_9NS$) (Fig. 1) is a heterocyclic compound that contains ring nitrogen and sulfur atoms that easily exhibit oxidative properties.

Fig. 1. Phenothiazine $C_{12}H_9NS$ molecular structure. Color coding: grey-carbon, white hydrogen, blue-nitrigen, and yesllow-sulphur atoms.

The non-polar nature of PTZ molecule limits its water solubility which makes it difficult to formulate solid materials and constitutes a major drawback in drug clinical applications. Recent advances in nanotechnology demonstrated high application potential of titanium dioxide nanoparticles (TiO_2 NPs), with their high antimicrobial activity, chemical stability, low toxicity, and high biocompatibility, as controlled drug delivery system. Most of these applications are based on the surface chemistry of titanium dioxide because of unique importance of interactions between the organic species and TiO_2 surfaces. Due to PTZ molecular structure with electrons lone pair on the N atoms and π electrons of the aromatic rings, it acts as good electron donor to an empty *d* orbital of TiO_2. Additionally, the –CN and –SC groups are able to interact with hydroxyl groups on a semiconducting oxide surface providing an effective bonding of PTZ molecule with TiO_2 surface. Earlier we report on simple mechanochemical method to fabricate PTZ-TiO_2 nanocomposites for optoelectronic applications [1-2], however, the analysis of the mechanism of molecular interaction of PTZ with the TiO_2 surface has not been fully explored yet and still is an urgent task. In this study, we focused on the understanding of the adsorption process of phenothiazine (PTZ) drug on mesoporous anatase TiO_2 from ethanol and chlorophorm solutions using FTIR (Bruker IFS-88, 400-4000 cm^{-1}) and FT-Raman (FRA-106 attachment, Nd:YAG laser, λ_{ex}=1.064 μm, 2 cm^{-1} resolution) and PL (Edinburgh Instruments FLS1000) spectroscopy. Possible mechanisms of the drug adsorption that involve bonding to active sites on TiO_2 pore surface and electrostatic interaction with Ti^+ cations are discussed.

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P11

COMPARISON OF BSA FLUORESCENCE IN SALINE AND PHOSPHATE BUFFER SOLUTIONS UNDER GAMMA-IRRADIATION

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In a previous study [1], we analyzed the morphological patterns formed during the desiccation of bovine serum albumin solutions (0.5 mg/ml of BSA in 20 mM NaCl) and how gamma irradiation affects these patterns. Spectral analysis of the irradiated solutions revealed a dose-dependent decrease in fluorescence intensity. To further understand the role of the solvent composition — specifically, the presence or absence of a pH-stabilizing buffer — in these fluorescence changes, we compared our results with those reported by M. H. Gaber [2], who examined BSA fluorescence under similar irradiation conditions, but used a significantly higher protein concentration (4 mg/ml BSA) in 10 mM phosphate buffer.

Direct comparison shows a substantial divergence between these two data sets. However, literature suggests that higher BSA concentrations require proportionally higher radiation doses to produce equivalent fluorescence quenching [3]. After dividing the values of Gaber's doses by 8 (reflecting the eightfold concentration difference), we observed that the relative maxima of fluorescence (normalized to the respective non-irradiated controls) from both studies exhibit nearly collinear trends on the logarithmic dose scale within the 50–2000 Gy range.

These results indicate that BSA concentration is the dominant parameter governing the observed differences in fluorescence response to gamma irradiation, while the effect of solvent composition — in this case, saline versus phosphate buffer — appears to be negligible under the studied conditions. This suggests that saline may serve as a viable alternative to buffered solutions in the studies of BSA fluorescence under irradiation.

It can also be noted that in the work [3] the changes in the fluorescence of human serum albumin (HSA) were observed above a dose of 200 Gy, and in our diameter measurements via dynamic light scattering, the diameter of the protein increased markedly after 200 Gy. It can be hypothesized that, starting with this dose, the destruction of the internal tryptophan in BSA and HSA begins, while at smaller doses radiation affects mainly only the external tryptophan in BSA.

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P12

ASSESSMENT OF TRYPTOPHAN CONTENT IN THE BLOOD OROPHARYNGEAL CANCER PATIENTS AFTER COVID-19. A SIMPLE METHOD ANALYSIS.

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Metabolic disorders one of the common factors that lead to complications during COVID-19. Among other the tryptophan and its metabolite play a significant role. Since the production of serotonin is limited by tryptophan molecule which can also give negative dynamic during illness especially in older people [1]. And vice versa a diet rich in tryptophan promotes improvement in depressive states, therapy of autism, cognitive function, multiple sclerosis, inflammatory bowel disease, and so forth [2]. Moreover the tryptophan one of the most easily and research molecule that convenient as fluorescence marker.

The work examined the blood plasma of 17 patients with oropharyngeal cancer after suffering from COVID-19. A mixture of plasmas from three healthy people was used as a control. Precipitation of high-molecular proteins and peptides was carried out by adding an equal volume of 10% perchloric acid and centrifugation. After that, the blood plasma samples were additionally dissolved in phosphate buffer and have measured. The measurement results obtained by fluorescence spectrometer in range from 280 to 550 nm have a maximum under 360 nm, with excitation at a wavelength of 280 nm. The tryptophan content in blood plasma was determined, a calibration curve was first constructed based on the fluorescence of a tryptophan solution at known concentrations.

The experimental data on the content of free tryptophan in the blood plasma of cancer patients show a significant difference compared to control although these data do not have a pronounced correlation and may be either less or more than the control values. This may be a consequence of the different effects of two pathological processes.

The data obtained in this work indicate the feasibility of prolonged determination of the content of free tryptophan in the blood plasma of cancer patients who have suffered COVID-19 or have been exposed to other viral diseases.

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P13

DESIGN OF NOVEL MOLECULES WITH ANTI-COVID-19 ACTIVITY: FROM COMPUTER SIMULATIONS TO ORGANIC SYNTHESIS

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This abstract presents a series of studies focused on the design of organic compounds with potential anti-COVID-19 activity. The primary targets of our research were the main protease (Mpro) and the papain-like protease (PLpro) of SARS-CoV-2 — key viral enzymes responsible for processing polyproteins. Inhibition of these proteases effectively blocks viral replication.

Our approach to developing new drug candidates integrates several methodologies: chemoinformatics tools for generating virtual libraries of potential structures [1,2]; machine learning techniques for constructing models of biological activity [3]; and molecular modeling, including molecular dynamics simulations, to investigate the binding interactions of potential ligands with the target enzymes [4]. The possibilities of a number of structures as promising protease inhibitors have been analyzed in this work. Among them, a library of such structures was generated using an evolutionary algorithm on the basis of the working substance of the well-known drug nirmatrelvir (Pfizer). Eight new structures showing significant binding to the corresponding protein were found using the docking procedure [1].

A proprietary library of chemical compounds, comprising approximately 80,000 molecules of various classes and structural features, was comprehensively analyzed. The main focus of the study was the identification of ligands with potential dual antiviral and anti-inflammatory activity. For the in silico screening, we employed molecular targets that reflect the proposed mechanism of action of the well-known drug cepharanthine against COVID-19. Docking simulations were carried out against the receptor-binding domain of the SARS-CoV-2 spike glycoprotein in complex with its receptor, human ACE2, to identify promising candidate compounds. Receptor-focused docking was also performed using additional macromolecular targets relevant to the inhibition of key viral replication pathways and the reduction of inflammation in affected tissues. Several compounds were identified as promising candidates for subsequent in vitro evaluation. Among them is the structure shown in Fig. 1, which was synthesized during the course of the project.

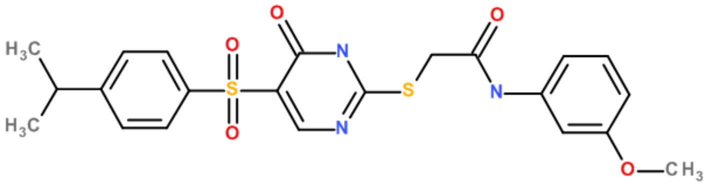

Fig. 1. One of the promising dual-action molecules identified in this study

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P14

THE DISTINCTIVE FEATURES OF THE INFRARED VIBRATIONAL SPECTRA OF 2'-DEOXYADENOSINE AND ADENOSINE MOLECULES ISOLATED IN Ar MATRICES

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The conditions necessary for the emergence of life on planets are one of the most interesting mysteries of science. Some modern research provides compelling evidence for the possibility of extraterrestrial origin of some DNA/RNA building blocks of life [1]. The study of biological molecules under extreme conditions in the laboratory can be a source of useful information for fundamental astrophysical and astrochemical research, as well as for practical aspects of human space exploration. Nucleosides as the main building blocks of DNA and RNA [2] are of great interest for understanding life on the molecular level. To date, information on the behavior of canonical nucleosides under extreme conditions is quite limited [3-5]. Therefore, in this study an attempt was made to compare the vibrational spectra of two building blocks of DNA and RNA obtained under matrix isolation conditions.

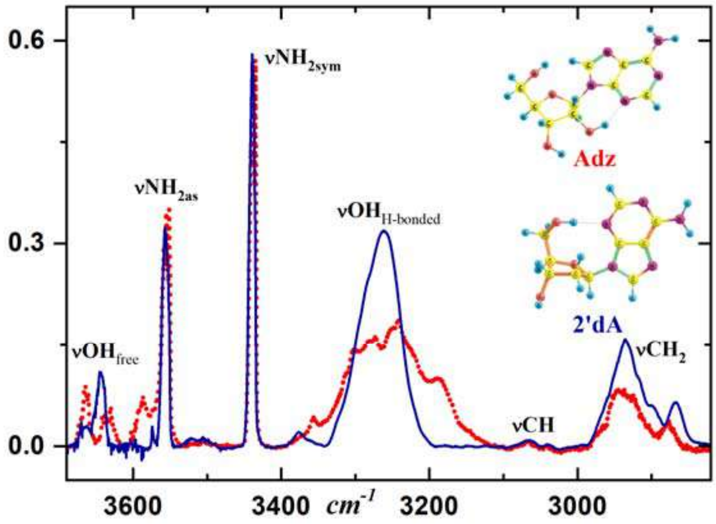

Fig. 1. FTIR spectra of 2'-deoxyadenosine (2'dA) and adenosine (Adz) molecules in the νOH(NH, CH) stretching vibration region (3690-2820 cm^{-1}): Nucleoside molecules were isolated in the Ar matrices at T= 8 K (matrix to sample ratio = 700:1).

We have previously demonstrated that 2'-deoxyadenosine and adenosine retain thermal stability during sublimation in a vacuum at temperatures of 450–465 K [5]. The most complete information about the conformations of nucleoside molecules fixed in matrices is provided by the region of OH(NH) stretching vibrations involved in intramolecular hydrogen bonds (Fig. 1).

The absorption bands of NH_2 vibrations coincide very well (in terms of frequencies and intensities) for these molecules (Fig. 1). Spectral bands of stretching vibrations of free and hydrogen-bonded OH groups (Fig. 1) in combination with quantum chemical calculations make it possible to estimate the population of *anti*- and *syn*-conformers in the inert Ar matrices [4, 5]. It was found that UV irradiation has a significant effect on the conformational equilibrium and stability of nucleosides isolated in the Ar matrix and this effect was discussed.

Acknowledgments: National Academy of Sciences of Ukraine (Grant No. 0123U100628), Polish Academy of Sciences and Institute of Low Temperature Physics and Structural Studies of PAS.

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P15

RAMAN SPECTROSCOPY OF CARBON NANOTUBES WRAPPED WITH SINGLE- OR DOUBLE-STRANDED DNA OR SURROUNDED BY N-METHYLPYRROLIDONE MOLECULES: COMPARISON OF D AND G BANDS

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Due to exceptional electrical conductivity, high surface area, and sensitivity to local chemical environments, single-walled carbon nanotubes (SWNTs) offer a highly effective platform for biosensing based on electrical properties. SWNTs can form percolated networks or thin films. These networks create interconnected pathways for charge transport, which makes them perspective for label-free electronic biosensing. A target molecule that binds to the functionalized SWNT via the probe causes a change in the charge distribution or local dielectric environment, which can be detected as a shift in electrical resistance, current, capacity, or in the Raman spectrum. Raman spectra of nanotubes are extremely sensitive to changes in the external environment, which manifest themselves in changes in the position, shape, and intensity of characteristic bands of nanotubes.

In this work, the vibrational structure of SWNTs wrapped with single- or double-stranded DNA (*ss*DNA/*ds*DNA) or surrounded by N-methylpyrrolidone (NMP) molecules is studied by Raman spectroscopy. Nanotubes were sprayed from aqueous (with DNA) or NMP suspensions on quarts substrates. Raman spectra were recorded in the range of 1000-1700 cm^{-1} in which bands assigned to a tangential (G) and defect (D) modes are observed. It was found that Raman spectra of nanotubes obtained from nanotube suspensions with NMP or with biopolymers showed a difference, which is associated with different nanotube surrounding and with different nanotube-DNA and nanotube-NMP interactions. In contrast to NMP, dsDNA and ssDNA isolate nanotubes effectively from one another and prevent their aggregation into bundles, and exhibit some selectivity in adsorption onto nanotubes of different chirality.

It was found that minimal differences were observed between the spectra of SWNTs:*ss*DNA and SWNTs:*ds*DNA. In contrast, the band assigned to D mode of the SWNTs:NMP spectrum is more intensive and wider than that band in spectra of SWNTs:*ss*DNA and SWNTs:*ds*DNA samples. It was revealed that the width of the band assigned to the D mode of the SWNTs:NMP spectrum is greatly wider than the width of this band in other samples, and its total intensity is about twice as large as that in the other samples. In addition, the band in the SWNTs:NMP spectrum is red-shifted by 2 cm^{-1} compared with the D band of SWNTs covered by DNA. It is supposed that the main influence on the spectral position of the band and its width in the Raman spectra of SWNTs can be caused by bundling, charge transfer with adsorbed compound, different dielectric constant of the environment, and stress from the adsorbed molecules. Note that NMP exhibits weaker donor-acceptor properties and does not induce noticeable compression of the nanotube structure, so the bundling of nanotubes can mainly influence the D-band in the Raman spectrum.

As observed, the peak positions of high frequency component of G mode (G) are nearly identical across all samples. However, the G-band width in the SWNTs:NMP sample is significantly (~1.4 times) broader compared to those from the DNA-prepared samples. Among the samples of DNA-wrapped nanotubes, the G-band of SWNTs:*ds*DNA is slightly broader than that of SWNTs:*ss*DNA. In contrast, the G-bands for SWNT samples with ssDNA and dsDNA closely match, but their position and intensity show a noticeable difference from the G-bands of the SWNTs:NMP network. Influence of a combination of such factors as bundling, charge transfer, change of dielectric constants, and stress induced by adsorbed molecules on the shift of the band peak, increase in intensity, broadening of bands in the Raman spectrum of SWNTS is discussed.

Acknowledgments: This work was supported by the National Academy of Sciences of Ukraine (Grant 0123U100628).

P16

PECULIARITIES OF THE ELECTROPHYSICAL PROPERTIES OF ALBUMIN MACROMOLECULES IN AQUEOUS SOLUTIONS OF SODIUM CHLORIDE

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The research is devoted to the analysis of the results of modeling the electrophysical properties of the zeta potential of human serum albumin in aqueous solutions as a function of sodium chloride and albumin concentrations, macromolecular radius, and pH of the aqueous solutions. Numerous papers have been devoted to the study of the physical properties of aqueous albumin solutions, but a holistic picture of the relationship between the structure and properties of the albumin macromolecule with changes in the parameters of aqueous solutions is currently absent.

In [1], we constructed an effective cell model of the zeta potential of the human serum albumin macromolecule in aqueous sodium chloride solutions, which takes into account the change in salt concentration and pH of the aqueous environment. Within the framework of the cell model, it was established that the zeta potential of albumin is a function of the radius of the macromolecules, the thickness of the Stern layer, and the cell radius in the case when the diffuse electric layers of neighboring albumin macromolecules overlap [1].

Analysis of the results of modeling the electrophysical properties of aqueous-salt solutions of albumin using a cellular approach shows that the zeta potential value depends on the following key factors [1]:

- Sodium chloride concentration. Zeta potential decreases with increasing sodium chloride concentration.
- Albumin concentration. Zeta potential increases significantly with decreasing albumin concentration. However, at the same time, with increasing albumin concentration, the effect of salt on zeta potential becomes less significant, and vice versa: with increasing salt concentration, the effect of albumin concentration becomes less noticeable.
- Macromolecular radius. As the radius of albumin in solution increases, the zeta potential decreases at all albumin concentrations. However, as the radius of albumin decreases and the salt concentration increases, the change in zeta potential becomes less and less significant.

Further study in [2] of the dependence of the zeta potential of albumin macromolecules on the pH of their aqueous solution revealed its similarity to the behavior of the magnetization of paramagnets as a function of magnetic field. The nature of the dependence of the zeta potential of albumin macromolecules on the pH of their aqueous sodium chloride solutions was determined on the basis of the equation of the magnetization of paramagnets. It was shown that near the singular point of 42°C the behavior of the zeta potential as a function of pH has a linear character, which coincides with the area of application of the Landau theory.

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P17

3D MODELS OF PROTEINS AND PUTATIVE G-QUADRUPLEXES IN PORCINE CIRCOVIRUS TYPE 3 SINGLE-STRANDED CIRCULAR DNA

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3D models of biopolymers predicted by artificial intelligence AlphaFold 3 have the same accuracy as their structures determined by experimental methods. Recently, porcine circovirus type 3 (PCV-3) with single-stranded circular DNA genome was detected for the first time in Ukraine [1]. In this work, 3D models of proteins (replicase and capsid) for the two evolutionarily most distant PCV-3 isolates were obtained by AlphaFold 3. In addition, 4 conservative G-quadruplexes (G4s) formed by three G-tetrads (one of which is shown in Fig. 1) were identified. The 100% identity of the G4 motifs for more than 1010 PCV-3 isolates with complete genome from the GenBank database was confirmed by the BLAST software for nucleotide sequences alignment. Structural comparison of the spatial organization of proteins (replicase and capsid) for two PCV-3 isolates has shown that the number of β-sheets of their capsid proteins differs by 1.7 times.

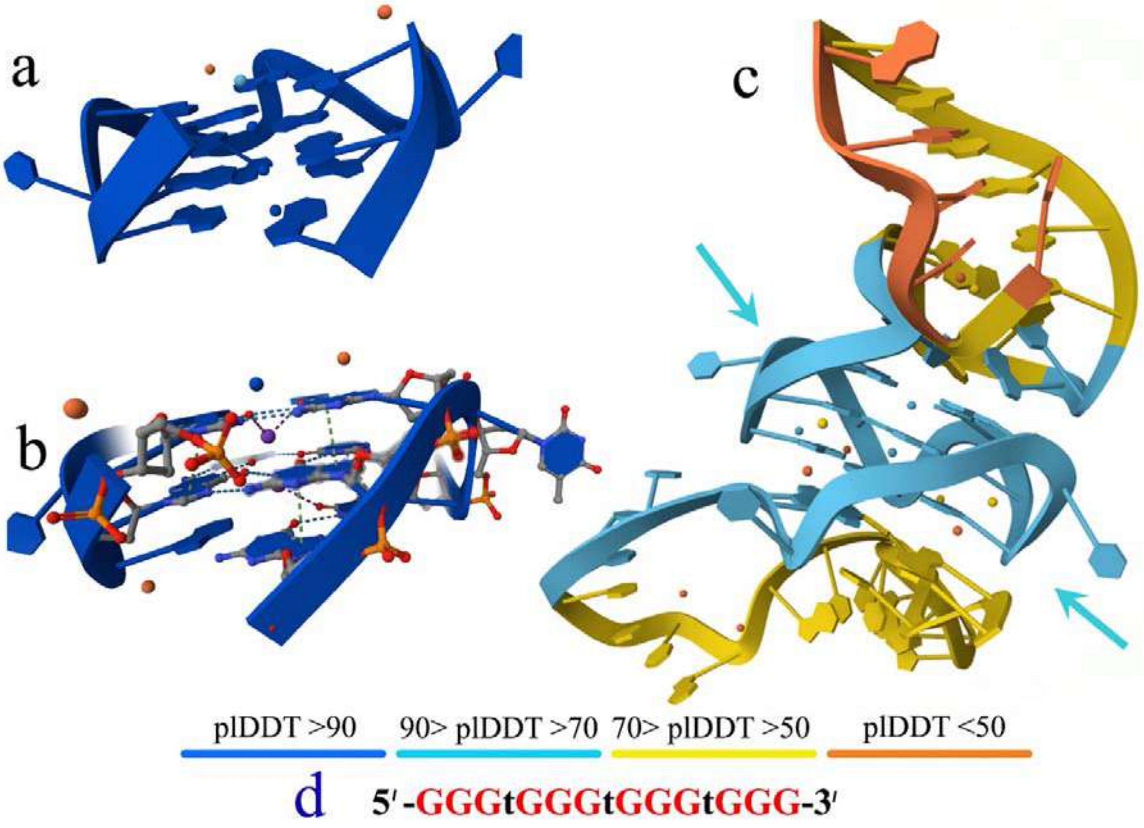

Fig. 1. 3D models of G-quadruplexes formed by three G-tetrads in single-stranded DNA of PP067099 isolate of the PCV-3 for a fragment of 15 nucleotides (nt) at positions 1164-1178 for 8 Na+ (**a**, **b**) and 57 nt. at positions 1144-1200 for 20 Na+ (**c**; arrows indicate G4) in the intergenic region. (**a**, **b**) – plDDT > 90, (**c**) – 90 > plDDT > 70. (**d**) – G4 motif. The dotted line shows hydrogen bonds between complementary nucleotides in the tetrad and stacking interactions between nucleotides of parallel tetrads (**b**). The parameter plDDT indicates the quality of the 3D model on a scale from 0 to 100.

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P18

CONFIRMATION OF PERFECT G-QUADRUPLEXES IN MYCOBACTERIA TUBERCULOSIS BY ALPHAFOLD 3 ARTIFICIAL INTELLIGENCE

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G-quadruplexes (G4s) are non-canonical structures formed in guanidine-rich sequences of RNA and DNA molecules, stabilized by stacking interactions of planar G-tetrads and monovalent metal ions. In this work, from a number of putative perfect G-quadruplexes formed by four G-tetrads in the sense strand of *Mycobacterium tuberculosis* (MTB) H37Rv DNA, those G4s were identified, the 3D models of which were confirmed by the AlphaFold 3 artificial intelligence (AI).

QGRS Mapper software was used for search of putative perfect G4s. 3D models of G4s were built by the AlphaFold 3 AI [1] for 10 K+ ions. For a reliability of the 3D model prediction in AlphaFold 3 the pIDDT parameter was used. A pIDDT value for a high level of model confidence should be over 90 on a scale from 0 to 100.

At the first stage, 11 putative conserved G-quadruplexes of four G-tetrads were found in the DNA sense strand of MTB H37Rv with complete genome (one of which is shown in Fig. 1 and has 100% identity to 629 *M. tuberculosis* isolates according to the BLAST multiple alignment in GenBank), the G-score of which ranged from 97 to 108.

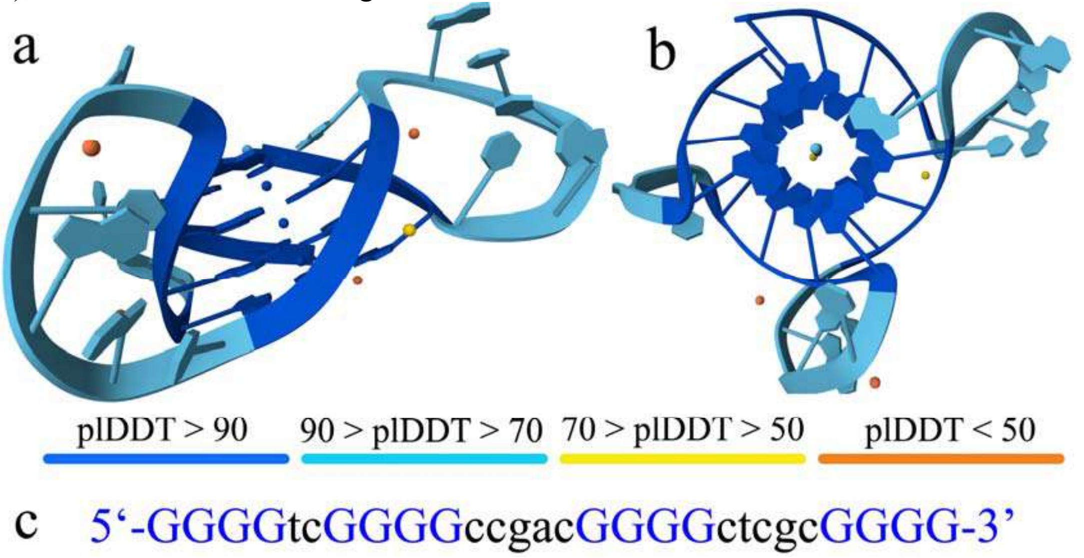

Fig. 1. G-quadruplex (plDDT>90) is formed by four G-tetrads at position 1091957-1091984 of the *rpsI* gene of DNA sense strand of the *Mycobacterium tuberculosis* H37Rv isolate: side view **(a)** and top view **(b)**; conservative motif of the putative G-quadruplex **(c)**.

At the second stage, instead of experimental testing of the identified G4s in the MTB genome, AlphaFold 3 was used for their 3D model precise prediction. For two determined G4s plDDT was more than 90, for the other two G4s plDDT was ranged from 70 to 90, for six G4s – 70 > plDDT > 50, for one G4 – plDDT < 50. As a control of the confidence of these models, the parameters of the 3D model of G4 the formation of which was experimentally confirmed in the *mexC* gene of the gram-positive bacterium *Pseudomonas aeruginosa* by NMR spectroscopy (70 > plDDT > 50) were used.

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P19

HYBRID POLY(N-ISOPROPYLACRYLAMIDE) HYDROGELS PHYSICALLY CROSS-LINKED BY ACID ACTIVATED LAPONITE ®

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The hybrid stimuli-responsive hydrogels represent significant interest in different areas related with biomedical application for intelligent drug delivery, treatment of diseases and in wound dressing. These hydrogels (also called "smart" or "intelligent") have attracted significant interest in areas related with different biomedical, pharmaceutical, bioengineering, extraction and separation, and agricultural applications [1].

The objective of the current study was investigation of the behavior of the hybrid poly(N-isopropylacrylamide) hydrogels physically cross-linked by acid activated synthetic hectorite Laponite ® (Lap) platelets. The nitrogen adsorption based on application of BET and *t*-plot techniques were used for estimation of the contribution of small nanopores, micropores and external pores in surface area. The behavior of the swelling degree and differential scanning calorimetry (DSC) thermograms for different pNIPAAm hydrogels filled with Lap/LapA platelets was discussed. Observed swelling behaviour of pNIPAAm-based hydrogels may reflect details of interactions between segments of pNIPAAm chains with Lap/LapA platelets. In absence of platelets the swelling degree was minimal as compared with physically cross-linked samples containing Lap or LapA. With increase of the temperature the swelling degree decreased and became very low in the vicinity of lower critical solution temperature (LCST) located at $T \approx 33$-34 °C for all samples. The effects of incorporation of platelets on behavior of the swelling degree are discussed. DSC measurements were done in the temperature range around the gel-sol transition ($T=28$-45 °C) in both for heating and cooling circles. Broad endothermic (heating) peaks for all hydrogels were observed near 34.8 °C and reflect the collapse of the network structure. The enthalpies of the phase transition ΔH were quite different for studied samples that reflect the changes in interactions of the pNIPAAm networks with Lap/LapA platelets.

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P20

HBA1C PREDICTION FROM BLOOD FTIR-ATR SPECTRA USING CURVE FITTING AND AUTOML

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This work presents an interpretable methodology for predicting glycated hemoglobin (HbA1c) levels through curve fitting analysis of Fourier-transform infrared (FTIR) spectra from dry whole blood samples. The approach focuses on deconvolution of the spectrum using pseudo-Voigt functions to identify spectral signatures through the identification of peak markers for glycation-related biomarkers. Preprocessing involved Savitzky-Golay smoothing (5-point window, 3rd-order polynomial), rubberband baseline correction using the BoxSERS module, and normalization against the Amide I peak intensity (1640–1680 cm^{-1}) to standardize spectral comparisons.

Peak detection was performed on second-derivative spectra, retaining only peaks present in ≥10% of the 673 clinical samples (250 healthy, 78 prediabetic, 345 diabetic; HbA1c 3,57–14%). Spectral deconvolution employed pseudo-Voigt profiles. Five key parameters were extracted per peak: position, height, full width at half maximum (FWHM), normalized area, and mixing parameter (η). These parameters served as input features for H2O AutoML modeling, with the dataset split into 80% training and 20% testing sets.

Model development revealed that peak height parameters yielded superior predictive performance compared to area, FWHM, or positional shifts. Model performance on the test data: $R^2=0{,}586$. A 7-fold cross-validation strategy ensured robustness, while ensemble and deep learning models were excluded to prioritize interpretability. SHAP (SHapley Additive exPlanations) analysis of the top 10 H_2O AutoML models identified 20 consistently significant peaks linked to HbA1c.

The most significant peak was observed at 1574 cm^{-1}. While primarily attributed to C-N-H bending vibrations (amino groups), in the infrared spectra of fatty acids, this peak can also correspond to antisymmetric carboxylate vibrations. Additionally, a closely related peak at 1570 cm^{-1} is commonly associated with C=C stretching vibrations in fatty acids. Interestingly, a decrease in the absorption value at 1574 cm^{-1} correlates with an increase in predicted HbA1c levels, and vice versa. Similar trends (decreased absorption with increased HbA1c) are observed for the absorption peak at 1402 cm^{-1}, which reflects C–H bending vibrations in double bonds characteristic of unsaturated fatty acids. In contrast, an increase in absorption at 1366 cm^{-1}, corresponding to aldehydic C–H bending vibrations, is associated with higher HbA1c levels, potentially indicating increased oxidative processes. The model also showed a strong association between high HbA1c levels and increased absorption at 1011 cm^{-1}. This region corresponds to sugar moieties in glycosylated proteins (C-O glycosylation) and, as noted in the literature, is considered unique to glycated proteins, caused by C-O or C-N glycosidic bonds. Additionally, high absorption at 1030 cm^{-1}, associated with phosphorylated monosaccharides such as glucose and fructose, also correlates with increased HbA1c levels. Notably, an increase in the number of β-turns in protein secondary structure, indicated by higher absorption at 1678 cm^{-1} and 1673 cm^{-1} (Amide I), is related to a decrease in HbA1c levels. These observations align well with studies of changes in the representation of erythrocyte membrane protein secondary structures when blood glucose levels rise.

The curve fitting approach combined with the AutoML demonstrated high biochemical interpretability, directly linking spectral features to pathophysiological processes like protein glycation and lipid oxidation. Critically, the consistency of top predictive peaks across multiple models underscores their biological relevance to HbA1c quantification.

P21

CARBON NANOPARTICLES AS BIOMOLECULAR SENSORS

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Carbon nanostructures are attracting significant attention as promising platforms for biomolecular sensing due to their unique electronic and surface properties [1]. In this work, we investigate their sensitivity to amino acid residues and molecular dyes as model molecules. Using squaraine dyes containing oxygen and nitrogen heteroatoms in their *pi*-conjugated chromophores as examples, it is shown that the experimental spectra of squaraine dye films deposited on carbon nanostructures with different carbon hybridization states exhibit a transformation of the electronic structure upon interaction [2].

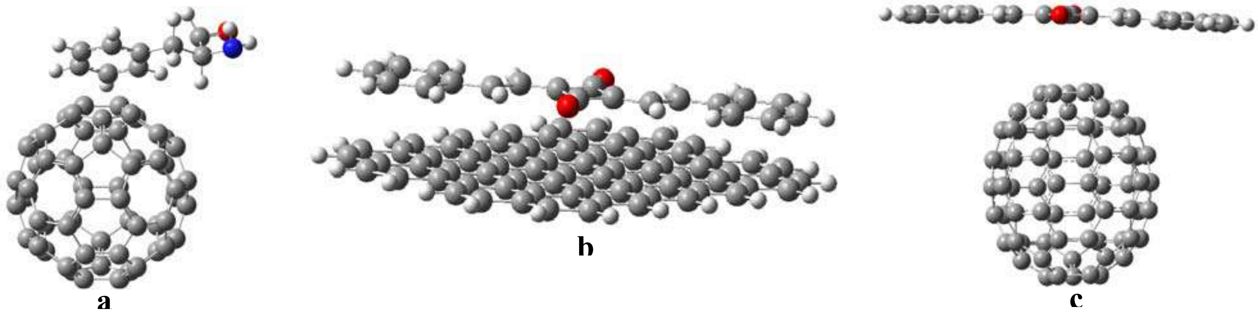

Fig. 1. Geometry of complexes: a – C_{60} fullerene – phenylalanine, with its benzene ring positioned above the benzene ring of the fullerene; b – squaraine dye – graphene; c – C_{70} fullerene – squaraine dye, oriented perpendicularly to the longer radius of the fullerene.

This process is accompanied by band gap modulation, as evidenced by absorption spectral shifts toward shorter wavelengths (up to 680 nm for fullerenes and 667 nm for carbon nanotubes compared to pure dye films). Quantum-chemical calculations confirm the formation of stable donor–acceptor complexes, with the highest binding energy observed for squaraine dyes interacting with a graphene sheet (–151 kJ/mol)[3], followed by C70 fullerene complexes in different localizations (–78 kJ/mol and –70.8 kJ/mol). The stability of these complexes arises from charge redistribution, dipole moment formation, HOMO–LUMO level alignment, and *pi–pi* stacking interactions. Furthermore, the interaction between dyes and carbon nanostructures induces orbital hybridization, leading to the emergence of new molecular orbitals simultaneously localized on both components, as well as shifts in HOMO–LUMO transitions relevant to the phototherapeutic window (1.4–4.6%). These results demonstrate the sensitivity of carbon nanostructures to dye molecules and confirm their potential as effective nanosensors for biomolecular detection. Amino acid residues, among which phenylalanine represents the simplest *pi*-conjugated amino acid, exhibit transformations of structural characteristics that define their properties.

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P22

DRYING OF AQUEOUS SESSILE DROPLETS OF COLLOIDAL SUSPENSIONS ON BASE OF NANOPLATELES OF LAPONITE RD® WITH ADDITIVES OF POLY(ETHYLENE OXIDE)

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The drying of colloidal dispersion droplets is central to applications in coating technologies, printing, and the fabrication of functional nanostructures [1]. The sessile droplet techniques are very important in many practical applications related with to microprinting of the sensors and electronic components, creation of functional coatings and films, and producing the tools for biomedical diagnostics. Among the most widely recognised patterns formed during evaporation is the "coffee" ring effect, where suspended particles accumulate at the droplet edge due to capillary flows driven by non-uniform evaporation.

This work studies the drying of aqueous sessile droplets of colloidal suspensions based on nanoplatelets of Laponite RD® (Lap) with additives of poly(ethylene oxide) (PEO). The drying experiments were done on glass substrate. The effects of water soluble PEO on the drying kinetics and morphology of the dried deposits were discussed. Observed data were explained by strong interactions between Lap platelets and PEO chains, and gel-network formation. Note that Lap + PEO systems are widely used for preparation of hydrogels with thermo-responsive sol-gel transition, transparent hydrogels and films for biomedical applications, as well as shake-gel aqueous mixtures [2]. The adsorption mechanism of PEO on the Lap surface includes interaction between the surface silanol (SiOH) groups and the ether oxygen of the macromolecule via hydrogen bonding. Behavior of ζ-potential of Lap platelets at different contents of Lap and PEO is also discussed. Observed effects were explained accounting for the structure of adsorption layer of PEO surrounding the Lap platelets. In concentrated suspensions of Lap (≥2.0 wt. %) the addition of PEO strongly influences the spatial distribution of Lap particles. The effects of bridging of Lap particles by PEO become more evident for high values of molecular mass.

Acknowledgments: The authors are very grateful to support by the funding of the National Academy of Sciences of Ukraine, Projects # 0125U000300 and # 0123U104433.

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P23

GREEN SYNTHESIS OF SILVER NANOPARTICLES USING *DIOSPYROS VIRGINIANA* FRUIT EXTRACTS

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The green synthesis of silver nanoparticles (AgNPs) is based on using components of natural origin (in particular, plant extracts and compounds, synthesized by microorganisms). It has significant advantages over chemical and physical synthesis because it avoids the use of toxic agents, it is characterized by simplicity, cost-effectiveness, and environmental sustainability. The study of the process of metal NPs green synthesis has recently received considerable attention because of the possible NPs practical application, in particular, in medicine. Extracts from various plant species are used now for NPs green synthesis. Presence of compounds with reducing activity in the extracts is an important prerequisite when choosing plants for use in this synthesis. In addition, the extracts used should also contain compounds that act as stabilizing agents. Thanks to them, it is possible to avoid using additional chemical compounds to stabilize NP solutions.

In this work, we compared the possibility of using of the extracts from the fruits of different *Diospyros virginiana* cultivars to obtain silver nanoparticles. The fruits of cvs Polyarna, Zobor, and Raketa were extracted by 70% EtOH. The activity of the extracts was studied by their ability to reduce Fe^{3+} to Fe^{2+}. The extracts were mixed with 1mM $AgNO_3$ solution and heated on water bath during 1 h at 80°C. Obtained AgNPs were visualized by TEM analyses (JEM-1400 microscope with accelerating voltage of 80 kV).

Extracts from the fruits of the three plant varieties differed in their reducing activity. In particular, the extract from the Raketa cv had such activity 12-20 times higher than the activity of extracts from Zobor and Polyarna cvs. The NPs solutions remained stable without precipitation during the entire observation period (2 months). According to TEM data AgNPs samples differed in NPs size: nanoparticles obtained from the Raketa cv were the smallest (less than 50 nm, Fig.1).

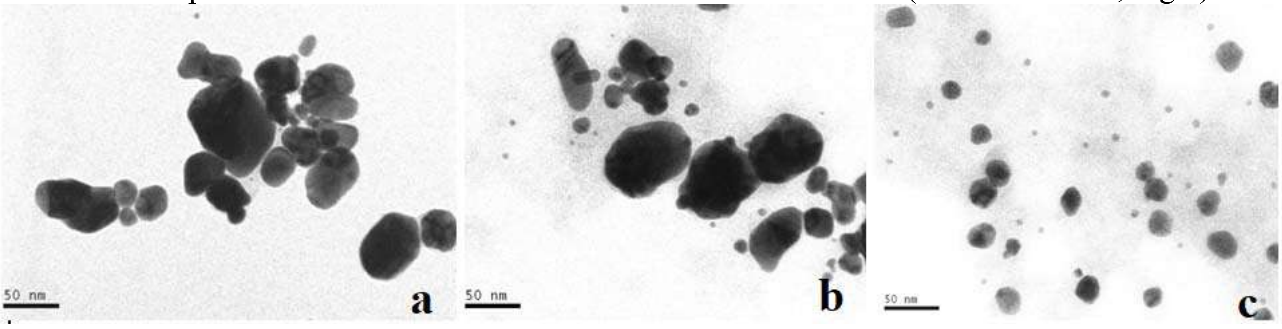

Fig. 1. TEM images of AgNPs synthesized by *Diospyros virginiana* cvs Polyarna (a), Zobor (b), and Raketa (c) extracts. Scale bars: 50 nm.

It can be assumed that such differences are associated with the variations in chemical composition of the extracts and different reducing activity: the greater this activity, the smaller the average size of the obtained nanoparticles.

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P24

FERROMAGNETIC NANOPARTICLES OF IRON/COBALT AND IRON/MANGANESE OXIDES IN AQUEOUS SOLUTIONS OF SURFACTANTS

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Nanoparticles of iron/cobalt and iron/manganese oxides in the form of stable suspensions are used in the development and manufacture of nanotracers, which are used to check the mixing processes of animal feeds, which are in both solid and liquid states, the coding of liquid additives and the efficiency of their uniform distribution in prepared premixes and compound feeds [1, 2]. Suspensions of nanotracer nanoparticles must be stable, and feed mixtures must be homogeneous. Since feeds are multicomponent mixtures, a statistical approach is used to assess the distribution of particles in the mixture and, thus, determine the quality of their mixing [3, 4]. Nanotracers, which are used as markers for the analysis of feed mixing, contain information about the type and specific feature of agricultural products and its genetic composition [5].

This work presents methods for obtaining ferromagnetic nanotracers based on iron/cobalt and iron/manganese oxides and studying their ability to form stable solutions of aqueous suspensions in the presence of surfactants.

The work presents step-by-step methods for obtaining ferrofluids based on iron/cobalt and iron/manganese oxides and their subsequent dispersion in aqueous solutions of surfactants. The manganese and cobalt content in the obtained stable aqueous suspensions was determined by the colorimetric method. To determine the sizes of nanotracers, an innovative statistical approach NTA (Nanoparticle Tracking Analysis) or nanoparticle trajectory analysis was used, which allows studying and visualizing the size and concentration of nanoparticles in a solution by tracking the Brownian motion of an individual nanoparticle using a microscope in its field of view [6]. According to the results of NTA research and its software, the trajectory of each of the nanotracer particles was detected and tracked, and their displacements along the coordinate axes were calculated. The diffusion coefficients (D_t) of nanoparticles were determined and analyzed.

Laboratory studies were conducted on the addition of a liquid nanotracer mixed with an enzyme to animal feed and the content of cobalt and manganese oxides in the extracted ferromagnetic tracer nanoparticles was analyzed.

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P25

METASURFACE BASED NANOBIOSENSORS: COMPARATIVE ANALYSIS OF ALL-DIELECTRIC, METAL-DIELECTRIC AND GRAPHENE METASURFACE MODEL STRUCTURES

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The development of innovative nanobiosensors of various designs for numerous biomedical applications is one of the fastest-growing areas in modern nanoscience and nanotechnology. Nanobiophysics focuses on studying the physical effects and mechanisms that provide sensitivity in nanosensory structures to biologically significant or medical diagnostic parameters of biological samples. Among the promising new materials used in nanobiosensors as sensing elements, metasurfaces exhibit unique optical and electronic properties along with high tunability, allowing the precise control over the sensors working characteristics. Based on our previous experimental findings from microwave dielectrometry measurements and recent numerical modeling results, we proposed several model sensor structures based on metasurfaces with different designs for potential biomedical applications [1-4].

In this report, we present a comparative analysis of the physical characteristics and application prospects of the biosensors developed, which are based on all-dielectric [2], metal-dielectric [3], and graphene strips containing [3] metasurfaces. In our long-term modeling study, performed using COMSOL software, we conducted computational modeling of the design and operational parameters of the metasurfaces with different compositions [2-4]. We also tested the applicability of the biosensors to determine the concentrations of biologically significant proteins, such as Human Serum Albumin, Bovine Serum Albumin and IgG, in liquid samples. Our numerical modeling utilized data from experimental studies on the complex permittivity of the protein solutions, obtained with the microwave dielectrometry setup developed earlier [1].

We present optimized structures of the developed biosensors based on all-dielectric and metal-dielectric metasurfaces, as well as metasurfaces with graphene strips. We compare the sensitivity of these sensors to changes in protein concentrations in the tested aqueous solutions. The advantages and disadvantages of sensors based on different sensing elements are discussed.

We believe that the results obtained from this research can be utilized in the production of the designed biosensors and their subsequent biological testing.

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P26

A DITHIZONE METHOD FOR DETERMINING ZINC IN ZINC-BASED NANOSTRUCTURED BIOMATERIALS

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Nanostructured materials have been suggested to be used as a source of dietary zinc for livestock animals. Importantly, Zn-based nanomaterials have been proposed as a potential alternative source of dietary zinc for animals, science their unique properties, which are mediated by nanostructures, can increase zinc's bioavailability, resulting in faster absorption in the gut and rapid distribution between the tissues [1]. However, the limitations of their widespread introduction into livestock and poultry farming are caused by the possible toxic effect, which is due to their physicochemical characteristics (route of administration, dosage, etc.).

In our previous works, we have shown that the synthesized nanostructured zinc carbonate hydroxide (ZnCH)$Zn_5(CO_3)(OH)_6$ (ZnCH) microflakes have low toxicity and can be used in veterinary medicine [2,3].

In this study, to understand the degree of bioavailability of Zn-based nanomaterials, research was conducted to determine the rate of zinc release from nanostructure materials under different conditions, in this case, in different physiological pH of animal's esophagus. For this purpose, a method for determining zinc through the formation of a complex with diphenylthiocarbazone (dithizone H2Dz) by optical absorption spectroscopy has been developed. The rate of zinc release from ZnCH microflakes has been shown by model systems to be influenced by pH values from 2.1 (stomach) to 7.3 (rectal cat).

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P27

DFT STUDY OF TEGAFUR COMPLEXES WITH MoS_2: STRUCTURE, INTERACTION ENERGIES AND VIBRATIONAL SPECTRA

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We investigated complexes of anticancer drug tegafur with pristine MoS_2 as well with MoS_2 having point defects. Tegafur (5-fluoro-1-(oxolan-2-yl)-pyrimidine-2,4-dione or 1-(oxolan-2-yl)-5-fluorouracil) is a chemotherapeutic prodrug of 5-fluorouracil. Tegafur is metabolized to 5-fluorouracil by the CYP2A6 enzyme. First, we located all possible conformers of tegafur using the DFT/B3LYP/aug-cc-pVDZ level of theory. A total of three conformers of tegafur were found. Structure of the most stable conformer is shown in Fig. 1. This conformer is characterized by the trans arrangement of the oxygen atom of the oxolane fragment and the O2’ atom of the pyrimidine fragment. The other two conformers differ from the most stable one by the conformation of the 5-membered oxolane ring or by the rotation of the oxolane fragment around the N1-C bond relative to the pyrimidine fragment. Next, we calculated the structure of the complexes formed by the most stable conformer of tegafur and the fragment MoS_2 (27 molybdenum atoms and 54 sulfur atoms). The calculations were carried out using the density functional M06-2X. Five complexes with the pristine MoS_2 fragment were found in which the tegafur molecule interacts with the MoS_2 surface formed by sulfur atoms (stacked complexes). Four other complexes were also found in which the tegafur molecule is located at the edge of the MoS_2 fragment. For these complexes we performed the NBO (Natural Bond Orbital) analysis, which showed the formation of coordination covalent bonds between the tegafur atoms and the edge molybdenum atoms in these bonded complexes. Calculations showed significant differences in the interaction energies between stacked and bonded complexes. In the stacked complexes, the interaction energy is approximately in the range from -10 to -12 kcal/mol, while in the bonded complexes it reaches -72 kcal/mol. This difference is explained by relatively weak van der Waals interactions in the stacked complexes and significantly stronger interactions in the complexes with covalent bonds. Taking into account the aqueous environment (PCM approach) leads to a significant weakening of the interaction in all complexes. The interaction energy in stacked complexes decreases to approximately -3 kcal/mol, and in bound complexes to -20 kcal/mol.

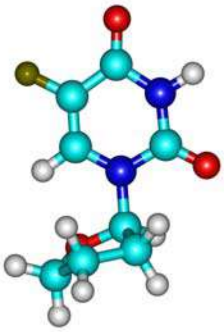
Fig. 1. Structure of tegafur.

In addition, we studied tegafur complexes with the MoS_2 surface that have point defects of two types: the first is the substitution of a surface sulfur atom by a molybdenum atom (denoted as Mo_S), the second is a vacancy of two adjacent surface sulfur atom (denoted as V_{2S}). Six complexes for MoS_2 with Mo_S defect and four complexes for MoS_2 with the V_{2S} defect were found. The presence of the mentioned defects leads to the formation of covalent bonds with the tegafur molecule located on the surface of the fragment. As a result, the interaction with the surface increases to -60 kcal/mol.

We also analyzed calculated vibrational spectra of all studied complexes and located spectral (IR and Raman) markers of tegafur interaction with MoS_2.

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P28

FABRICATION AND CHARACTERIZATION OF ELECTROSPUN PMMA NANOFIBERS LOADED WITH LEVOFLOXACIN OR CHLORAMPHENICOL

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The electrospinning technique for nanofiber production attracts significant attention of nanoscience researchers owing to the wide spectrum of applications of products from the nanofibers including biomedical applications such as wound dressing, drug delivery, tissue engineering, and regenerative medicine. Specifically, electrospun nanofibers loaded with antimicrobial drugs or nanoparticles exhibit strong bactericidal and other antimicrobial activity [1]. Their distinctive features include a high surface area-to-volume ratio, adjustable porosity, flexibility, and some other unique mechanical and physicochemical properties.

In this work, we fabricated polymer mats formed by polymethylmethacrylate (PMMA) nanofibers loaded with antibiotics levofloxacin (LV) or chloramphenicol (CAM). The obtained mats were characterized by microscopic method, UV-visible absorption spectroscopy, and laser desorption/ionization (LDI) mass spectrometry. We also analyzed the release kinetics of the drugs from the mats and studied their antibacterial properties. The diameter of the obtained electrospun nanofibers was determined as about 2 μm. The release of the antibiotics from the nanofibrous mat when soaked in an aqueous solution was studied using UV-Vis spectroscopy and LDI mass spectrometry. These observations showed that 50% of LV amount released from the mat within the first 10 minutes, and the following 20% - within the next 3 hours. In contrast, the release time of CAM was significantly longer: only 10% of the CAM amount released from the mat within the first 5 hours, and the next 5% required 45 hours to be released to the solution. The overall release fraction for CAM was only 35%, which took about 650 hours. The reasons for such significantly slow dynamic of process of the COM release from PMMA mats are discussed in our report. The antibacterial properties of the antibiotic-loaded nanofiber mats were studied against Gram-positive and Gram-negative bacteria. The study showed that mats loaded with LV as well as mats with COM demonstrated high efficacy against the studied bacteria, except for CAM loaded mats effect on bacteria strain P. aeruginosa 9027 against which the mats with CAM showed lower antimicrobial activity.

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P29

ELECTROPHYSICAL PROPERTIES OF AQUEOUS COLLOIDAL SOLUTIONS OF FULLERENE $C_{60}@\{H_2O\}_n$

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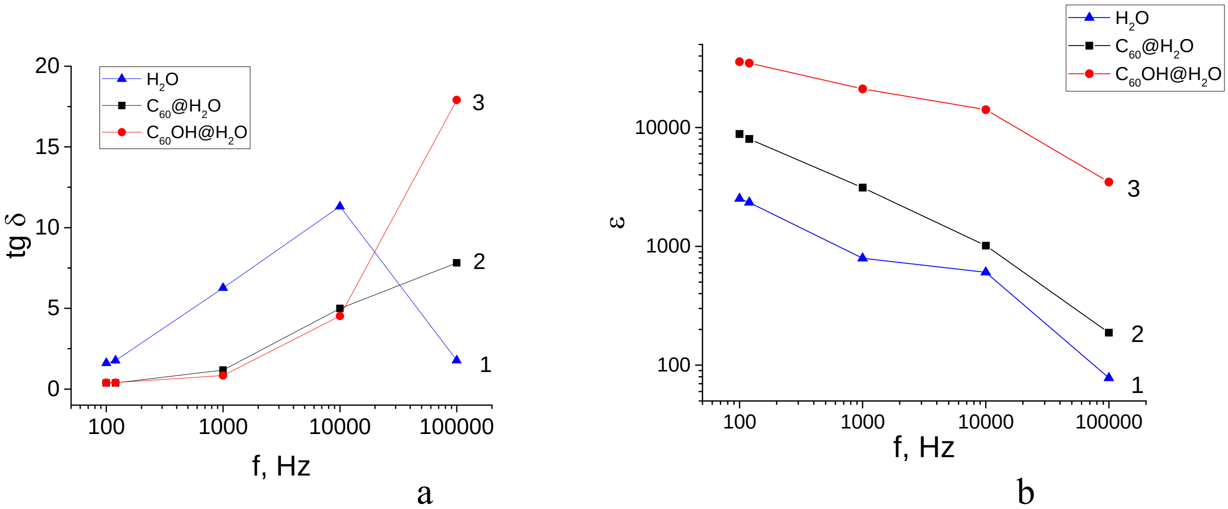
The dielectric loss tangent δ and permittivity ε of aqueous colloidal solutions of fullerene $C_{60}@\{H_2O\}_n$ obtained using the cryogenic vacuum-sublimation technique were studied [1]. The solid phase of the $C_{60}@\{H_2O\}_n$ mixture was obtained by joint condensation of water vapor and fullerene C_{60} on a cooled substrate. Upon heating the solid phase to room temperature and melting $C_{60}@\{H_2O\}_n$, a stable light-yellow colloidal aqueous solution was obtained. Measurements of the permittivity and dielectric losses were performed for different concentrations of C60 molecules in the solution in the frequency range of 100-10^4 Hz. The measurements showed that the dielectric loss tangent of the colloidal solution of $C_{60}@\{H_2O\}_n$ is significantly higher than that of ordinary water, and has a maximum shifted to higher frequencies. Presumably, this phenomenon is due to the formation of metastable spherical layers of water molecules around the fullerene molecules due to donor-acceptor bonds between the water molecules and the C_{60} surface [2]. The permittivity of the $C_{60}@\{H_2O\}_n$ solution also turned out to be higher in comparison to pure water, which is apparently explained by the processes of polarization of water molecules H_2O by fullerene molecules. Functionalization of C_{60} molecules with polar –OH groups under conditions of higher substrate temperature leads to charge redistribution in the $C_{60}@\{H_2O\}_n$ – H_2O system, polarization of water molecules, and formation of a space charge around $C_{60}@\{H_2O\}_n$, which increases dielectric losses, especially at high frequencies. The proposed technique can be used as an express test for determining the presence of C_{60} molecules in an aqueous solution.



a b

Fig. 1. Frequency dependences of the dielectric loss tangent δ (a), dielectric constant ε (b) of aqueous colloidal solutions of fullerene $C_{60}@\{H_2O\}_n$ (■ – sample 2, obtained by melting $C_{60}@\{H_2O\}_n$, condensed at a substrate temperature T1 = 90 K; ● – sample 3, obtained by melting $C_{60}@\{H_2O\}_n$, condensed at a substrate temperature T2 = 223 K) and control water sample 1 (▲).

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P30

EFFECT OF COLLOIDAL METAL NANOPARTICLES AND LOW-INTENSITY LASER LIGHT ON THE SYNTHESIS OF PHENOLIC COMPOUNDS AND ANTIOXIDANT ACTIVITY BY MEDICINAL MACROMYCETES

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Recent studies have highlighted the use of photoactivated nanoparticles (NPs), demonstrating significant interest and potential importance in this area. When exposed to light under specific conditions, metal nanoparticles can exhibit catalytic properties in various biochemical reactions.

Analysis of the obtained results on the influence of colloidal solutions of metal NPs and the complex action of NPs and laser irradiation on the synthesis of phenolic compounds in the mycelial mass of macromycetes allowed us to establish the features of their influence. Depending on the type of fungus and the characteristics of metal NPs, a wide range of values of the content of phenolic compounds was observed from 22.97±0.3 to 97.31±0.3 mg of gallic acid equivalents (GAEs) per gram of dry mass. The highest levels of phenolic compounds were recorded in ethanol extracts of the mycelial mass of *Inonotus obliquus* and *Lentinus officinalis*. For *I. obliquus*, the highest content of phenolic compounds ‒ 98.24±0.2 mg GAEs/g of dry mass was observed after treatment of the inoculum with photoinduced Mg NPs. For *L. officinalis*, the highest indicator ‒ 97.31±3.7 mg GAEs/g of dry mass was achieved when using photoinduced Ag NPs. The lowest content of phenolic compounds was observed in methanol extracts of mycelial mass of *Hericium erinaceus* with FeNPs without irradiation – 22.97±0.3 mg GAEs/g of dry mass.

Certain patterns of the influence of NPs and photoinduced NPs have been established. In particular, for *H. erinaceus* and *L. officinalis*, the highest values of the content of phenolic compounds were observed under the influence of AgNPs, and their concentration increased under irradiation with blue laser light. For L. edodes and *Pleurotus eryngii*, the synthesis of phenolic compounds was influenced by FeNPs and MgNPs, but the concentration of phenols in the extracts of the mycelial mass of *L. edodes* did not differ statistically. Photoinduced FeNPs and MgNPs also increased the synthesis of phenolic compounds in the mycelium.

Considering that metal NPs and photoinduced NPs promoted the synthesis of phenolic compounds in mycelial masses, we conducted a study of the antioxidant activity of alcoholic extracts of mycelial masses of the studied species of edible and medicinal macromycetes.

The results of the study of ethanolic and methanolic extracts of the mycelial mass of our model objects showed high values of free radical scavenging relative to DPPH after the effect of NPs and photoinduced NPs on the inoculum of fungi. The highest values of free radical scavenging were recorded for samples obtained as a result of the treatment of the inoculum of I. obliquus and L. officinalis with colloidal solutions of photoinduced AgNPs and FeNPs. The lowest values were found for methanolic extracts of H. erinaceus, L. edodes with MgNPs without irradiation.

Thus, the results of our research allow us to state the possibility of implementing effective mycobiotechnologies using colloidal solutions of metal NPs and low-intensity laser irradiation. It was established that the treatment of the seed inoculum with colloidal solutions of metal NPs and short-term irradiation with low-intensity laser light increases biosynthetic activity, namely the synthesis of phenolic compounds and affects the increase in antioxidant activity of strains.

P31

QUANTUM POINT-CONTACT SENSORS

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The possibility to study a person's emotional state using a non-invasive express method is of great interest both for the development of modern science and for solving a wide range of applied problems, particularly in the field of public safety. For instance, in 2019 the U.S. Air Force sponsored a comprehensive study aimed at assessing stress states of the human body based on the analysis of breath and sweat [1].

Our work is focused on developing the method for human emotional states analysis through the examination of breath using unique physical objects as the quantum point-contact sensor. In this study, Yanson point contacts based on the metal-organic compound Cu–TCNQ were used as the gas sensor element. Previously, we demonstrated the broad potential of such quantum point-contact gas sensors for the diagnosis of various metabolic states of the human body, including various hormonal conditions [2]. Of particular interest are studies aimed at serotonin and cortisol detection [3], hormones that are directly connected to specific emotional states [4]. These findings served as the starting point for the current research.

Quantum point-contact sensors were obtained using combined electrochemical deposition from a saturated solution of TCNQ in acetonitrile onto a textolite substrate foiled by copper. Prior to deposition, TCNQ was purified using vacuum zone sublimation, carried out with specially designed laboratory equipment.

The study involved 30 volunteers. During the experiments, response curves of the point-contact sensor to the action of breath of each participant were recorded before and after emotional stimulation. Analysis of the corresponding breath profiles revealed consistent patterns of change in the sensor response parameters that were universal across all subjects. These observations correlate strongly with data obtained in our previous studies, indicating a clear relationship between hormonal and emotional states detectable through breath analysis. This result demonstrates the significant potential of Cu–TCNQ quantum point-contact sensors for diagnosing a wide spectrum of human physiological states.

Thus, in this work we propose a method for investigating human emotional states by breath analysis in real time regime. This approach shows great perspectives for practical applications in the field of public safety, which is confirmed by the international interest in this area [1].

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P32

ELECTRIC CHARGE TRANSFER IN MOLYBDENUM DISULFIDE MoS_2 NANOPOWDER OVER WIDE TEMPERATURE RANGE OF 95–350 K

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The work is devoted to the study of charge transfer in MoS_2 nanopowder over a wide temperature range. Resistance curve derivative analysis (RCDA method) of the temperature dependence of electrical resistance revealed that three conductivity mechanisms can be found in the studied temperature range. The temperature intervals were established where the mechanisms manifest themselves in their pure form (Fig. 1). It was found that at temperatures above 315 K, intrinsic conductivity occurs due to thermal excitation of electrons from the valence band to the conduction band. The temperature range of 230–275 K corresponds to the impurity ionization. The sulfur vacancies act as donor impurity centers. At temperatures below 180 K, charge transfer occurs due to the 3D Mott variable range hopping conduction mechanism. Between the temperature ranges where the mechanisms manifest themselves in their pure form, there are fairly wide transition temperature ranges where the action of the mechanisms is superimposed. The established mechanisms made it possible to obtain information about the band structure in the studied MoS_2 nanopowder, as well as the characteristics of the impurity level that provides impurity conductivity. It was found that the band gap for the nanopowder is approximately 1.7 eV, which is higher than in the bulk material (1.2 eV) [1]. It was shown that the distance from the donor level induced by sulfur vacancies to the bottom of the conduction band is about 280 meV. The density of localized states near the Fermi levels is about $1 \cdot 10^{16}$ cm^{-3} eV^{-1}. The characteristic decay length of the wave function (localization length) of a localized charge carrier is about 4 nm. The *o* value is in good agreement with the published data (2–3 nm) of the Bohr radius for the sulfur vacancy in molybdenum disulfide [2].

These data are important for biotechnological applications MoS2 nanoparticles, allowing planning of strategies for using these materials.

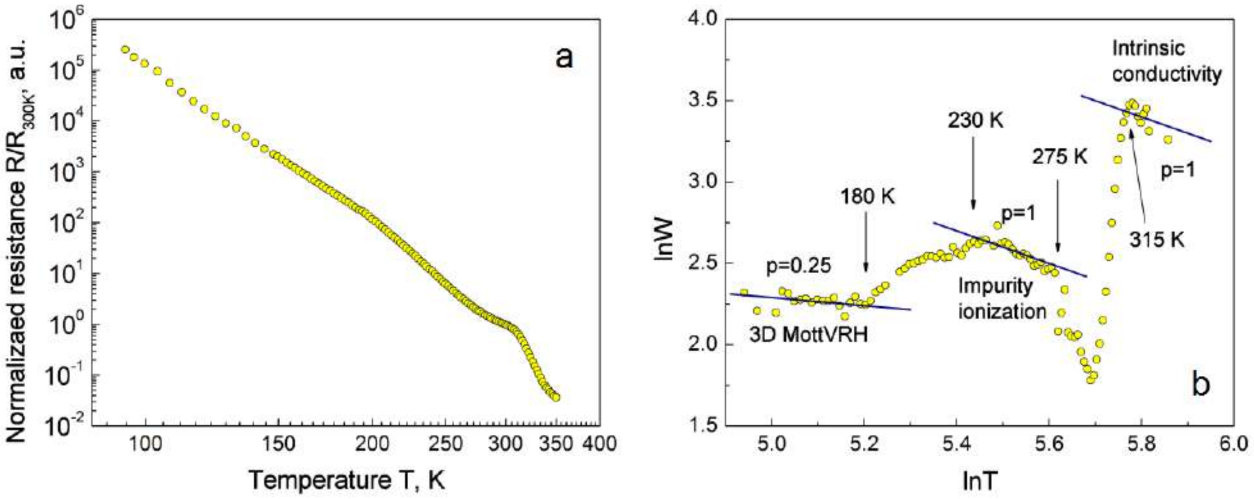

Fig. 1. (a) Temperature dependence of electrical resistance of MoS_2 nanopowder. The data are normalized to resistance at temperature 300 K.

(b) Temperature dependence of logarithmic derivative W ($W=-\partial lnR/\partial lnT$) on lnW *vs* lnT plot. Straight sections with a negative slope correspond to conduction mechanisms that can be detected in pure form.

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P33

ANALYSIS OF THE HEAT CAPACITY OF FLUOROSUBSTITUTED ALIPHATIC ALCOHOLS USING AN ARTIFICIAL NEURAL NETWORK

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Thermodynamic coefficients of individual liquids allow us to analyze the energy of intermolecular interactions, to relate microscopic and macroscopic state parameters of the system to changes in the molecular structure of the liquid. Comparison of the thermodynamic properties of liquids within one homologous series and the substitution series obtained by replacing hydrogen atoms with fluorine atoms in their molecules allows us to analyze the features of the mechanisms of molecular processes that occur in fluorosubstituted liquids.

Analysis of literature sources showed that the best studied fluorosubstituted alcohols (such as 2,2,2-trifluoroethan-1-ol and 1,1,1,3,3,3-hexafluoropropan-2-ol) have found wide use in the chemical industry and biochemical engineering as specific solvents. Fluorosubstituted alcohols continue to master new areas of use – they are used in nanobiotechnology for stabilizing peptides, for biomodification of enzymes, for changing the structure of protein macromolecules, for modifying the lipid membranes, etc [1]. However, despite the wide use of fluorosubstituted alcohols in various industries, their thermodynamic properties still remain poorly studied.

Using the principle of corresponding states, a comparative analysis of the temperature dependences of the isobaric heat capacity of aliphatic alcohols and their fluorosubstituted analogues in a wide temperature range along the liquid-vapor coexistence curve was carried out. The authors used data for aliphatic alcohols (within the homologous series from ethan-1-ol to nonan-1-ol), their perfluorosubstituted analogues (within the homologous series from trifluoroethan-1-ol to heptadecafluorononan-1-ol), presented in modern experimental databases and databases simulated by artificial neural networks [2, 3]. Experimental data on the temperature dependences of the isobaric heat capacity for perfluoroalcohols are practically absent in the literature today, so for perfluoroalcohols simulations by artificial neural networks were used [2, 3]. The relative deviation between simulated heat capacity data for aliphatic alcohols and similar data obtained experimentally increases from 1% for ethan-1-ol to 4% for nonan-1-ol.

It is shown that the homologous series of aliphatic alcohols and their fluorosubstituted analogues have differences in normalized caloric properties. It is shown that in a wide temperature range along the liquid-vapor coexistence curve, the normalized isobaric heat capacity of fluorosubstituted alcohols is almost twice as high as the corresponding value for aliphatic alcohols, which the authors associate with a decrease in the number of hydrogen bonds in fluorosubstituted alcohols compared to aliphatic alcohols.

Unlike aliphatic alcohols, for their fluorosubstituted analogues, the second derivative of the heat capacity with respect to temperature along the liquid-vapor coexistence curve is opposite in sign, indicating the dynamics of hydrogen bond breaking upon fluorosubstitution in aliphatic alcohols.

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P34

MOLECULAR SPECTROSCOPY AS A POWER TOOL IN STUDYING THE PORPHYRIN–DNA INTERACTION

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The porphyrins are macrocyclic compounds with unique spectroscopic and photophysical properties. They are widely used as photosensitizers in anticancer photodynamic therapy, probes for studying the structure and dynamics of nucleic acids, anti-viral and antimicrobial agents, and carriers of antisense oligonucleotides for their delivery, stabilizers of G-quadruplexes of telomeric DNA etc. The interest in studying porphyrin-DNA interaction is caused by the great potential of the data obtained for biomedical application, nanotechnology, and molecular electronics.

In this work we discuss the application of various spectroscopic techniques (absorption spectroscopy, polarized fluorescence, thermal denaturation with absorption and fluorescence registration, fluorimetric titration, resonance Raman spectroscopy and resonance light scattering) to study the binding of cationic *meso*-porphyrins, pheophorbide derivatives and their conjugates with phenazine dyes (Fig. 1) to nucleic acids of different primary and secondary structure, including single-stranded, double-stranded and quadruplex ones [1–8].

Using the spectroscopic methods, the binding modes of the porphyrins to nucleic acids were identified, the thermodynamic parameters of binding were obtained, the formation of porphyrin aggregates on the surface of the biopolymer was revealed, and their size was determined.

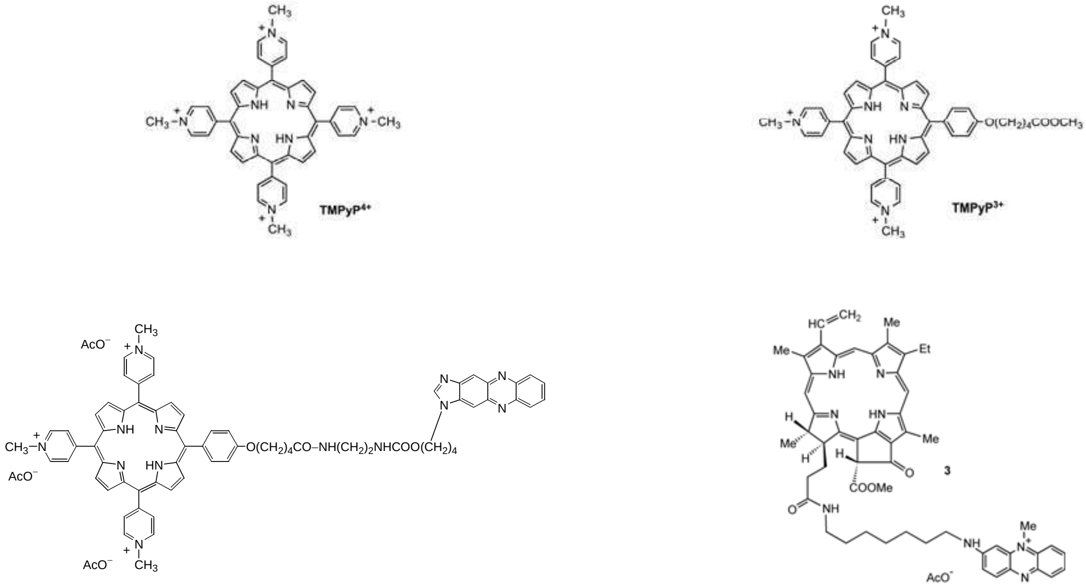

Fig. 1. Examples of molecular structures of the porphyrins and porphyrin-phenazine conjugates.

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P35

PHYSICOCHEMICAL PROPERTIES OF CHIRAL BIOMOLECULAR NANOSYSTEMS: CLUSTEROLUMINESCENCE, AIE, AND CISS

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Chirality is a fundamental property of molecules that governs their ability to engage in asymmetric interactions, particularly in biological, catalytic, and optical processes. It plays a key role in physicochemical phenomena such as clusteroluminescence (CL), aggregation-induced emission (AIE), and chirality-induced spin selectivity (CISS). This work explores the interplay between chirality and optical effects, including AICD/AACD, CPL, and AIE, which emerge due to the aggregation of chiral or achiral molecules [1–3].

Studies demonstrate that clusteroluminescence in non-conjugated systems may arise from dense molecular packing and n–π* orbital overlap, especially in polypeptides and amino acids [2,3]. Racemic polypeptides exhibit stronger luminescence than their homochiral counterparts due to conformational changes [1]. Meanwhile, AICD (aggregation-induced circular dichroism) and AACD (aggregation-annihilated CD) effects show that aggregation can enhance or suppress chiral optical activity depending on system geometry [1,4,5].

Clusteroluminogenic polymers, particularly those incorporating amino acid residues or chiral structural motifs, demonstrate how supramolecular chirality can modulate their luminescence behavior, enabling targeted applications in chiral sensing, bioimaging, and theranostics [4].

Of particular interest is the CISS effect, observed in systems with fluorescent probes bound to magnetic surfaces or in chiral sensors, where spin transport depends on molecular chirality [5]. The CISS phenomenon arises from spin-selective interactions between chiral molecules and electrons, leading to asymmetric charge transport depending on the relative alignment of electron spin and molecular geometry. This effect is also sensitive to external magnetic fields, which modulate electron spin orientation and thus affect electron transfer efficiency. Chiral molecules provide a structural framework for the spin-dependent transmission of electrons, and theoretical models incorporate spin-orbit interactions and quantum interference to explain these effects. The CISS mechanism has practical implications for DNA-based sensors, catalysis, and the development of spintronic devices [6].

An example of the interrelation between AIE and chirality can be found in nanoparticles-based photosensitizers that exhibit enhanced luminescence upon aggregation [7]. When such nanoparticles are functionalized with chiral molecules or assembled in chiral configurations, their emission properties become sensitive to the supramolecular chirality of the system. This allows for the design of photoactive nanomaterials that combine efficient AIE behavior with selective chiral recognition, which enables their use in enantioselective sensing and light-activated therapy.

Overall, these results highlight the critical role of chirality in tuning photophysical properties, paving the way for CPL-active, AIE-efficient, and CISS-sensitive systems based on controlled self-assembly.

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P36

INTERACTIONS IN COMPOSITES OF METHYLENE BLUE DYE WITH MoS_2 AND C60 FULLERENE CHARACTERIZED BY LASER DESORPTION/IONIZATION MASS SPECTROMETRY

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Among a variety of nanocomposites, in the present work we studied a combination of methylene blue (MB) dye with molybdenum disulfide MoS_2 and fullerene C_{60}. The unification of several biologically active components is currently tested for the combined therapy of cancer with the expectation of a synergistic effect of different mechanisms of action: separately, MB is used for photodynamic therapy, while MoS_2 is promising for photothermal therapy. Biological effects of C_{60} are also a subject of intense research. This determines the importance of studying molecular processes, possible covalent and noncovalent interactions in composites of these substances.

Two-component ($MB + MoS_2$), ($C_{60} + MoS_2$), ($MB + C_{60}$), and three-component ($MB + MoS_2 + C_{60}$) systems were prepared by ultrasound treatment of aqueous mixtures of the components. A method of choice for studying intermolecular interactions in the multi-component systems is laser desorption/ ionization (LDI) mass spectrometry.

Earlier, we have established correlations between the aggregation state and intermolecular interactions of the MB dye with characteristic features of its mass spectra [1, 2], which we were guided by in our present studies. In brief, it was established that in the case of monomeric adsorption of MB^+ cations on inert substrates, such as carbon nanotubes [1], an abundant signal of MB^+ cation is recorded in the desorption mass spectra. In the case of MB dimerization or aggregation, a redox reaction occurs, resulting in the formation of the $[MB + H]^+$ reduction product [2], readily detected in the mass spectra.

In the positive ion LDI mass spectra of binary ($MB + MoS_2$) nanocomposite, an abundant signal of MB^+ cation was recorded, which pointed to monomeric adsorption of the MB^+ cation at the partially negative MoS_2 surface. Similarly to the case with carbon nanotubes [1], noncovalent electrostatic interactions took place. In the LDI mass spectra of the binary ($MB + C_{60}$) system, substantial "damage" of MB^+ was observed: there was a set of peak groups corresponding to sequential loss of four methyl $–CH_3$ groups present in the MB^+ structure. In the higher mass range, there was a set of peak groups which may be tentatively attributed to MB dimer and species related to loss and addition of CH_3 groups. Obviously, these transformations were caused by redox interactions of MB^+ with C_{60}. This effect of C_{60} was preserved in the triple ($MB + MoS_2 + C_{60}$) composite: a similar set of MB^+ fragments formed due to $–CH_3$ loss was registered along with the peaks characteristic of C_{60} and MoS_2. The products of MB^+ polymerization, however, were not observed obviously because of the relatively low content of MB^+ at the MoS_2 surface.

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P37

THE EFFECT OF AMINO ACIDS ON THE DEGRADATION AND OXIDATION OF POROUS SILICON IN AN AQUEOUS MEDIUM

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Nanoporous silicon has unique physicochemical properties, simple manufacturing technology and good biocompatibility. Therefore, this material, like other siliceous materials, is promising for biomedical applications, such as biosensors, bioimaging and drug delivery [1-3]. Such applications require control of the degradation rate of silicon nanoparticles, which can be achieved by changing the porosity and pore size, as well as by functionalizing the surface with various compounds. It was proposed to use amino acids to modify the surface charges of silicon and silicon oxide nanoparticles [2]. Their advantages are biocompatibility and low toxicity. In this work, the effect of amino acids on the degradation and oxidation of porous silicon in an aqueous medium was studied using photoluminescence (PL) of porous silicon (PS).

Nanoporous silicon samples were formed by anodizing of p- type (100) silicon. The porosity of the samples was 70%. The PS surface was treated with amino acid solutions, then dried in air under room conditions The structure of the PS layer was studied using scanning electron microscopy. The change in the chemical composition of the PS surface was investigated using IR spectra.

It was shown that amino acids with non-polar radicals such as glycine, alanine, valine, proline and phenylalanine contribute to the effective oxidation and degradation of PS. It was also shown that the presence of amino acids leads to changes in the PL of PS. The behavior of PL is well explained within the quantum-size model in terms of decrease in the size of the emitting silicon nanocrystallites as a result of the interaction with the aqueous solutions [3]. Degradation and oxidation of the PS are assumed to be the immediate cause of the decrease in the nanocrystallite sizes.

The enhanced degradation of PS can be associated with the ability of amino groups to act as nucleophiles and stimulate the reaction of silicon with water molecules. Oxidation of PS probably also occurs by active oxygen species, the formation of which is stimulated by porous silicon in solutions of amino acids, and especially glycine. The results obtained in the work allow us to assess the influence of the studied amino acids on the processes of interaction between PS and the aqueous medium and to take it into account when using PS as a drug carrier.

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P38

BIOPHYSICAL PROPERTIES OF GAMMA-IRRADIATED MODEL BIOMEMBRANES CONTAINING CYTOCHROME C

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Natural cell membranes are capable of instantaneous cooperative structural rearrangements in response to external physical stimuli, thereby modulating the susceptibility of cells to environmental influences. Nevertheless, under conditions of extreme environmental stress, cellular membranes require effective protective mechanisms against such impacts. Analysis of the dynamics of post-radiation changes in various cell types indicates that the primary determinant of differences in radiosensitivity lies not in the extent or character of the damage itself, but in the cell's ability to overcome it, i.e., to activate intrinsic self-protective mechanisms. For instance, the radioresistance of erythrocytes is largely attributed to the presence of hemoglobin molecules. It is well established that the specific radiation behavior of heme-containing proteins is determined by the porphyrin group within their structure, which functions as an energy trap. To date, studies of the radioprotective properties of heme-containing proteins remain inconclusive and continue to be a subject of experimental investigation and scientific debate. The application of artificial protein–lipid membranes, as simplified models of natural biomembranes, enables the exploration of radioprotective properties and biological efficiency of heme-containing proteins, as well as elucidation of their role in radiation-induced modifications of biomembranes.

Using fluorescence spectroscopy, we investigated model lipid membranes composed of phosphatidylcholine (PC), as well as protein–lipid complexes formed from PC liposomes with cytochrome **c** supplementation, which were subsequently exposed to ionizing γ-radiation at doses of 100, 250, and 1000 Gy. Fluorescence analyses of model biomembranes with ANS, MBA, and pyrene probes provided an assessment of radiation-induced damage across the lipid bilayer. Examination of PC liposomes irradiated at 1000 Gy revealed radiation-induced alterations in membrane surface properties, manifested by increased polarity in the microenvironment of the ANS probe. Additional structural changes at the bilayer phase boundary were observed, resulting in an expansion of the hydrophobic region and an increase in sorption sites for the MBA probe. Furthermore, a reduction in pyrene excimerization was detected, indicating decreased lateral diffusion within the hydrophobic core of the bilayer. This effect reflects increased structural rigidity of fatty-acid chains induced by ionizing radiation. By contrast, fluorescence studies of irradiated membrane – cytochrome **c** complexes did not demonstrate significant differences in ANS and MBA probe fluorescence parameters or in pyrene excimerization, relative to non-irradiated controls.

The porphyrin group within heme proteins, under radiation exposure, is capable of trapping free electrons as well as radiolysis products, including hydrated electrons, hydroxyl radicals, and hydrogen radicals. Our experimental results suggest that, during irradiation of model protein–lipid complexes, heme-containing proteins can attenuate the final radiobiological effect. This finding supports the hypothesis of a radioprotective function of cytochrome c under ionizing radiation in model protein–lipid membranes.

P39

INTERACTION CHARACTERISTICS OF HEMOGLOBIN MOLECULES WITH ORGANOSELENIUM COMPOUNDS

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Selenium is an essential element present in eukaryotic organisms in the composition of proteins and selenium-containing compounds. Selenium proteins with known functions are oxidoreductase enzymes, while other selenium proteins participate in thyroid hormone metabolism. Selenium-containing compounds are characterized by powerful antioxidant, anti-inflammatory, and antiviral effects. The toxicity of selenium limits the possibilities of using selenium preparations as effective antioxidants. To overcome the toxicity of inorganic forms of selenium, new organic selenium-containing compounds are being synthesized. Among the many synthesized organic selenium derivatives, heterocyclic compounds occupy a special place. The highest biological activity is demonstrated by five-membered selenium-containing heterocycles, which exhibit antimicrobial, antiviral, antitumor, and antiallergic effects.

The investigated organic complex 5-cyano-2-methyl-6-(methylselanyl)-4-(thiophen-2-yl)-1,4-dihydropyridine-3-carboxamide (S5) contains a selenium atom bonded to a heterocycle and a methyl group. This structure determines the chemical properties of the compound and its interaction features with model biomembranes and macromolecules. The interaction of the organoselenium complex with human hemoglobin molecules was studied. The spectral characteristics of the hemoglobin macromolecule solution in the Soret band are determined by the properties and structural state of the protein's heme group. Spectral changes in hemoglobin molecules in the presence of selenium complexes S5 at concentrations of 9, 12, 15, and 18 μM were associated with a decrease in light absorption by the protein (λ_{max} = 402 nm) in response to the increasing selenium concentration. It is assumed that the decrease in hemoglobin absorption in the Soret band is due to conformational changes in the protein molecule at the heme group level, initiated by the selenium complex S5.

Conformational changes in the hemoglobin molecule induced by the selenium complex occur not only in the heme group but also in other regions of the macromolecule. Using tryptophan fluorescence quenching, it was established that the nonpolar area of the protein globule undergoes rearrangement, while the molecular surface remains unaffected by S5. Neutral acrylamide and the ionic quencher I^- were used as fluorescence quenchers. The effectiveness of acrylamide quenching depends on the polarity of the environment of aromatic residues and the diffusion rate of the quencher inside the protein molecule. It was found that the quenching constant of protein fluorescence by acrylamide increases with the growing concentration of S5 in the solution, indicating an increase in the structural mobility of the nonpolar volume of the protein globule.

Structural changes in the heme group and the nonpolar regions of hemoglobin molecules induced by the selenium complex S5 affect the efficiency of protein-lipid interactions in the hemoglobin-liposomal membrane system. The obtained kinetic dependencies of hemoglobin binding to model membranes and the calculated kinetic parameters of the fast and slow phases of molecular interaction indicate a decrease in the efficiency of protein-lipid complex formation in response to increasing selenium concentration.

The studied organic selenium-containing compound, when interacting with hemoglobin molecules, integrates into the hydrophobic region of the macromolecule and causes changes in its spatial configuration.

P40

SOME ASPECTS OF OPTICAL SPECTROSCOPY OF DRUGS BASED ON INDOLE DERIVATIVES

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Indole is a well-known heteroaromatic compound consisting of the fused benzene and pyrrole rings. Compounds containing the indole fragment form the great class of biologically active substances that possess a broad range of biomedical activities (such as anti-pathogenic, anticancer, anti-inflammatory, etc). One of the natural amino acids – tryptophan – is an indole derivative. The naturally occurring alkaloid – Tryptanthrin – can easily bind and stabilize the telomeric G-quadruplex (G4) DNA. Due to this unique feature Tryptanthrin and its metal complexes demonstrate the antitumor properties and other types of biological activity [1,2]. As it was shown by us [3], the attachment of some groups to heteroaromatic *pi*-electron system can cause dramatic changes of optical spectra. Now our presentation is aimed to manifest some aspects of optical spectroscopy investigations (mainly at low temperatures) of indole (Ind), tryptophan (Trp) and tetracyclic drugs Tryptanthrin (Try) and indoloquinazoline (IQX).

Optical absorption (at room temperature), fluorescence (at room temperature and T=78K) and phosphorescence (at T=78K) of the solutions of Ind, Trp, Try and IQX in different solvents were investigated under different excitation wavelengths. Positions of the first excited singlet (S_1) and triplet (T_1) energy levels of these compounds were estimated. The spectral manifestation of the solvent effect on the studied compounds properties was obtained. As expected, the main centre of optical absorption, fluorescence and phosphorescence of Trp is Ind *pi*-electron system. Optical absorption spectra of Try and IQX contain several bands and one of them is associated with the absorption of Ind *pi*-electron system. In the fluorescence (under both temperatures) and phosphorescence of Try two optical centers have been fixed, one of them being associated with emission of Ind fragment of Try *pi*-electron system. In contrast to Try, in the fluorescence (under both temperatures) and phosphorescence of IQX only one optical center has been fixed, and it is not the emission of Ind *pi*-electron system.

The obtained results will be the basis for future studies on the interaction of these compounds with biomolecular targets, such as duplex and quadruplex DNA

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P41

BINDING OF NATIVE DNA TO MoS_2 NANOFLAKES: EXPERIMENTAL AND THEORETICAL STUDIES

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Currently, the study of the optical and physicochemical properties of 2D materials is of great interest. Such materials include MoS_2, which is currently considered as a promising candidate for use in the field of nanobiosensing (for the development of sensitive nanobiosensors) and nanomedicine (as a theranostic agent) [1].

In the present work, we study whether native DNA would bind to MoS_2 flakes (FLs) at relatively low ionic force (10^{-3} M Na^+, pH7) using experimental (differential UV spectroscopy and thermal denaturation method) and theoretical (DFT) methods. Based on analysis of the TEM image which showed the adsorption of DNA on MoS_2 FLs and the observation of an increase in the thermal stability of DNA and a decrease in the hyperchromic coefficient at binding with MoS_2 FLs in the thermal denaturation measurements we concluded about the binding of the biopolymer with MoS_2 nanoflakes at these conditions. It was observed, first of all, that the melting curve of DNA in the nanoassemblies has S-like form that indicates keeping the duplex structure of DNA at the conjugation. Observed changes in these DNA characteristics (an increase in melting temperature and a decrease of hyperchromic coefficient) were explained by the electrostatic interaction of the negatively charged oxygen atoms of the phosphate groups of DNA with the MoS_2 FLs.

Consideration of possible complexes of a nucleotide fragment (ribosephosphate group) with MoS_2 nanolayer employing the DFT method showed the forming of the coordination bonds of this nucleotide fragment with Mo atoms located at the edge of the MoS_2 nanolayer and with point structural defects of MoS_2 surface containing the S vacancy. This observation allows us to propose a mechanism of binding of native DNA to MoS_2 FLs, in which their conjugation begins with point contacts of DNA phosphate groups with Mo atoms (at the edge or/and in defects) through the formation of the coordination bond. The results indicate a huge impact of defects and edge atoms of MoS_2 FLs on their biofunctionalization.

The biocompatible MoS_2 FLs are model objects for the development of drug-related products based on transition-metal dichalcogenides. For example, such products can find application in photodynamic therapy, where separation and size control of the acting nanoassemblies are necessary. The results obtained in the present study can also be used to fabricate various hygiene products, as well as products for use in medicine and pharmacology.

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P42

IMPACT OF SUBSTITUENTS ON THERMAL RECYCLIZATION OF 2-IMINOCOUMARINS: EXPERIMENTAL, COMPUTATIONAL AND THEORETICAL INSIGHTS

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Coumarin derivatives have garnered a significant interest and found diverse applications last decades. Particularly, they are considered as effective medicines possessing antimicrobial, antituberculosis and antioxidant activity [1, 2], as well as anti-Alzheimer's agents [3]. A unique and efficient pathway of obtaining these compounds is recyclization reaction [4-6]. This reaction occurs *via* heating up to a certain temperature ($T_{\max}$) which was reported to be influenced significantly by substituents. Meanwhile, there is a clear lack of systematic study of this issue.

To this end, a set of 2-(2-benzoylhydrazineylidene)-2H-chromene-3-carboxamide derivatives was synthesized, differed both in electrophilicity and position of the substituents, which formed 3-(1,3,4-oxadiazol-2-yl)-coumarin derivatives [7] by the recyclization reaction. It was established that exploiting *n*-BuOH as a solvent for the recyclization is optimal due to the best results in yield and purity with reasonable full conversion time, relatively high operational temperature as well as correspondence to the principles of green chemistry. Thermogravimetry analysis (TGA) revealed a significant shift of the recyclization temperature ($\Delta T_{\max}$) depending on the substituent nature. The values of $\Delta T_{\max}$ ranged within *ca.* 100 K and were both positive and negative relative to the unsubstituted compound. Additionally, activation energy of recyclization was determined for the unsubstituted compound by means of TGA.

Quantum-chemical calculations at 6-31G (d) level of theory as well as the approach [8] using PM3(d,p), allowed us to elucidate certain important features of the reaction. In particular, changes in polarity of the double bonds involved in the reaction was shown, which is obviously related to substituents' electrophilicity and position. Then, one of the recyclization stages, E-Z isomerization, was pointed as a rate-limiting step of the reaction. The developed mathematical model based on linear elastic theory supposed that some moieties of 2-iminocoumarins could contact each other during their rotation around the corresponding C=C bond resulting to certain elastic deformations. This theoretical insight is in line with the results of quantum-chemical calculations. The model has analytically justified the shape of the relation between the rotation angle and the energetic cost of rotation, which was obtained by means of the calculations. Actually, it strictly confirms indirect impact of substituents on intramolecular events occurring distantly from their localization.

Generally, such combined experimental, quantum-chemistry and theoretical insight appeared to be fruitful for exploring the substituent impact and may see increased application in the future.

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P43

NEMATIC LIQUID CRYSTALS DOPED WITH RESORCINOL: SUPRAMOLECULAR ARRANGEMENT AND POTENTIAL BIOMEDICAL APPLICATION

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Drug delivery systems based on nanostructurized materials, such as liquid crystals (LC), possess a number of unique features and seem prospective for transdermal application [1,2]. In particular, they emerge as multifunctional anisotropic scaffolds capable of reacting to temperature, light, electric or magnetic fields [2]. These systems are mostly configured as a kind of ordered solvent for an active component (drug molecule), where no specific intermolecular interactions are anticipated. However, accounting for possibilities of such interactions paves the way for developing a novel type of LC-based drug delivery systems, where an active component itself is a structure-governing factor.

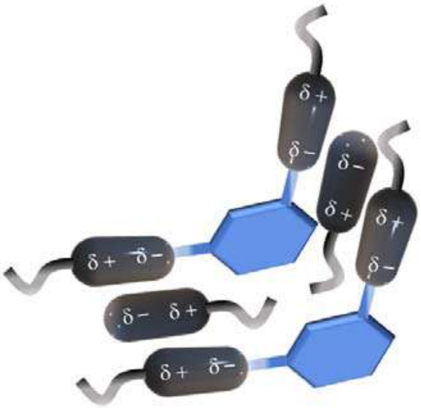

Fig. 1. A possible molecular arrangement in 5CB+RES systems. 5CB molecules are schematically presented as sticks with flexible moieties, RES molecules are presented as rigid hexagons. Partial charges localization in 5CB molecules is marked as δ– and δ+ [3]

Recently, we examined a system composed of a nematic LC medium of 4-pentyl-4'-cyanobiphenyl (5CB) and an antimicrobial drug resorcinol (RES). As it was evidenced by differential scanning calorimetry (DSC), introduction of RES into 5CB matrix caused anomalous increase in the nematic-to-isotropic phase transition (up to ~15 °C), which directly pointed to specific intermolecular interactions in the system. This finding has been strictly supported by FTIR data, which revealed 5CB-RES hydrogen bonding [3].

The maximal enhancement in nematic ordering corresponded to 5CB : RES 3 : 1 molar ratio was another unusual feature of the system [3]. This ratio is non-stoichiometric, so one can suppose extensive rearrangement of LC structure rather than formation of intermolecular complexes of a certain composition. One of several considered examples of such rearranged structures is presented in Fig. 1. Quantum-chemical calculations using semi-empirical PM3 method with added one polarization function on heavy atoms and one polarization function on hydrogen atoms have been involved to approve and characterize the structures. Toxicity and antimicrobial activity of 5CB, RES as well as their 3 : 1 mixture were also determined.

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P44

FEATURES OF LASER DESORPTION/IONIZATION MASS SPECTRA OF EXFOLIATED $MoSe_2$ AND WS_2 NANOMATERIALS

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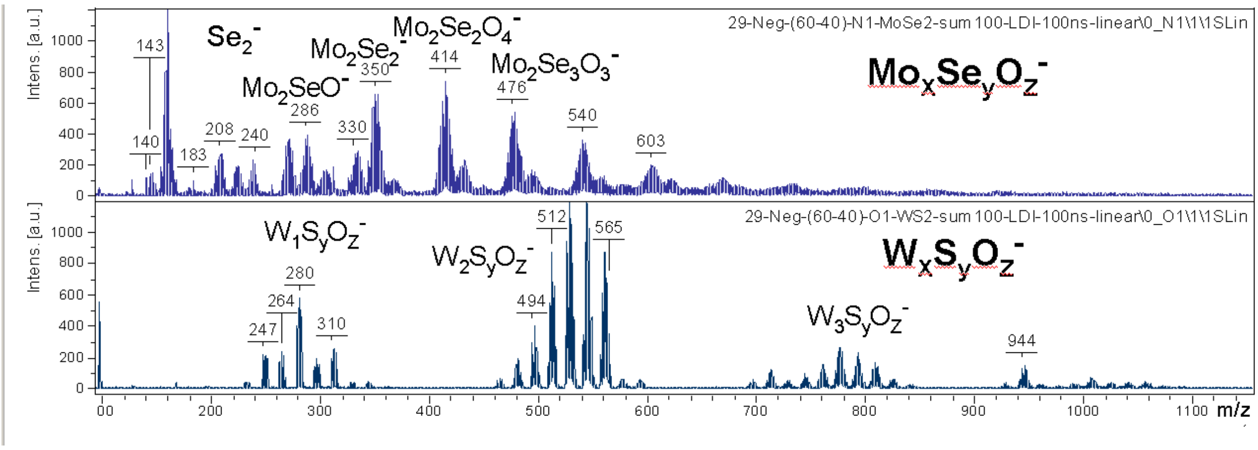
Inorganic nanomaterials *per se* are actively tested for various biomedical applications. To evaluate the properties of these materials, suitable experimental methods must be applied. Among mass spectrometric techniques, the desorption methods such as laser desorption/ionization (LDI), are the most informative for testing inorganic solids.

2D nanomaterials produced by exfoliation of transition metal dichalcogenides (TMD) are promising for photothermal therapy and drug delivery. While mass spectrometric characteristics of a TMD representative MoS_2 are already established [1], there is a lack of data on $MoSe_2$ and WS_2, which we replenish in the current work. The primary complication in interpreting the TMD spectra is caused by the polyisotopic nature of the Mo, W, Se, and S elements. Further, clusters of atoms are usually sputtered under LDI from inorganic solids.

Negative ion LDI mass spectra of nanosheets obtained by ultrasound exfoliation of $MoSe_2$ and WS_2. are presented in the following figure:



There are three groups of peaks in the LDI mass spectrum of WS_2, which belong to isotopic peaks envelopes of $W_xS_yO_z^-$ clusters containing one, two, and three atoms of W. Such a pattern is similar to the $Mo_xS_yO_z^-$ distribution characteristic of MoS_2 [1]. Substitution of sulfur for selenium in $MoSe_2$ causes changes in the composition of the sputtered $Mo_xSe_yO_z^-$ clusters: a series of clusters containing two Mo atoms dominates the spectrum.

Composites of $MoSe_2$ and WS_2 with biologically active methylene blue dye and oligomers of ethylene glycol were prepared by sonication and probed by LDI. It was shown that these compounds do not undergo any modification in their interactions with the TMD.

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P45

RADIATION MODIFICATION OF THE PROPERTIES OF PEG–PVA-BASED HYDROGELS IN THE PRESENCE OF SILVER NANOPARTICLES

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Hydrogels based on polyethylene glycol (PEG) and polyvinyl alcohol (PVA) are biocompatible and tunable, which makes them attractive for a broad spectrum of biomedical uses. The incorporation of silver nanoparticles (AgNPs) not only provides clear antibacterial activity but also affects the stability and durability of the polymer structure. Ionizing radiation can be applied both as an effective method of sterilization and as a tool for targeted structural modification of these hydrogels.

In this work, PEG–PVA films were prepared with and without silver nanoparticles and then irradiated with doses of up to 1000 Gy. Their structural and optical features were studied using SEM, UV–Vis absorption, FTIR, and Raman spectroscopy. SEM images showed a uniform distribution of silver nanoparticles and distinct morphology, while UV–Vis spectra revealed a pronounced plasmon resonance peak of silver at 420 nm. FTIR analysis demonstrated clear rearrangements of chemical bonds under irradiation, and Raman spectroscopy indicated enhanced vibrational responses in the films containing silver, reflecting stronger polymer–nanoparticle interactions.

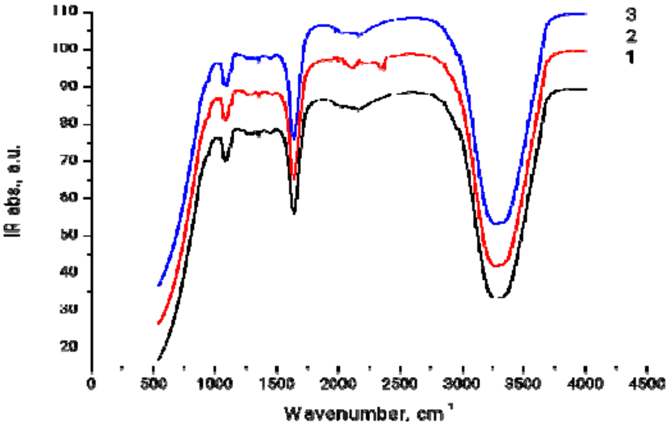

Fig. 1. IR absorption spectra of hydrogel films in the initial state (1) and after irradiation with doses of 70 and 1000 Gy (2,3).

The results show that high-dose irradiation substantially modifies the structure of PEG–PVA hydrogels. At the same time, the addition of silver nanoparticles stabilizes the polymer matrix and brings both antibacterial and unique optical properties. These findings suggest that such materials are highly promising for the creation of next-generation boluses in radiotherapy, capable not only of adapting the dose distribution with precision but also of delivering chemotherapeutic agents locally and providing simultaneous antiseptic protection.

Round Table

PL7 (RT1)

NANOBIOPHYSICS AT THE B.VERKIN INSTITUTE FOR LOW TEMPERATURE PHYSICS AND ENGINEERING OF THE NATIONAL ACADEMY OF SCIENCES OF UKRAINE: A HISTORICAL REVIEW

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The beginning of the new century was marked by the emergence of new fields in physics related to the production and study of nanomaterials, revolutionizing technology. Among these, leading positions were occupied by new carbon nanomaterials, including fullerenes, nanotubes, and graphene, which possess unique physical properties and great potential in the fields of nanotechnology and bionanotechnology. During this period, a new direction in physics emerged: nanobiophysics, a new branch of science that operates at the interface of physics, biology, chemistry, materials science, nanotechnology, and medicine.

Research in nanobiophysics at the Department of Molecular Biophysics began in 1995 with the first preparation of an aqueous suspension of fullerene, marking the start of extensive studies on fullerene–biomolecule interactions in Ukraine and abroad. This work was later expanded to the fabrication and investigation of photopolymerized fullerene films. A novel method for producing such films was developed, based on simultaneous film deposition and UV irradiation. These films were further explored as thin membranes for gas separation, demonstrating notable selectivity ratios for O_2:N_2 and for He:CH_4.

In 2002, systematic studies of the physical properties of single-walled carbon nanotubes (SWCNTs) and their nanobiohybrids were initiated. Particularly significant advances were made in hybrids of carbon nanotubes with DNA. The physical mechanisms underlying the formation of these nanostructures were identified, along with factors governing their stability, evolution, and response to external conditions. It was demonstrated that single-stranded DNA wraps around nanotubes not only due to its intrinsic helical structure but also because this conformation maximizes binding energy between nucleobases and the carbon surface. Comparative studies of homopolynucleotides revealed that more ordered polynucleotides exhibit stronger interactions with nanotubes, ensuring higher hybrid stability. Interaction energies for all canonical nucleobases with nanotubes and graphene and their structures were determined, enabling construction of a stability series consistent across both systems. These results are very important for establishing the stability of nanohybrids created by a nanotube with different types of DNA. An unusual phenomenon of multilayer wrapping of single-stranded DNA around SWCNT induced by ultrasound was experimentally discovered. The formation of hybrids with double-stranded (native) DNA was also experimentally investigated, and a physical model was proposed. These findings carry practical importance for DNA-based nanosensors and nanomedicine. For the first time, the luminescence of films of semiconductor nanotubes surrounded by a DNA polymer was experimentally observed and studied. The effect of hypochromism, i.e., the effect of weakening the intensity of light absorption by carbon nanotubes in the UV region, arising from π–π interactions between nanotubes and DNA bases, was discovered and explained. The self-assembly of SWCNTs coated with anionic biopolymer due to binding with cationic porphyrins was experimentally observed and studied. Exciton energy transfer between isolated semiconducting carbon nanotubes within these complexes was identified, and an appropriate model was proposed. For the first time, a significant increase in the luminescence intensity of semiconductor SWCNTs forming hybrids with biomolecules in aqueous suspensions and films was detected when defects on the surface of the nanotubes were repaired by an amino acid or an antioxidant molecules. Molecular interfaces have been developed for the efficient immobilization of enzymes on nanotube or graphene surfaces used in biosensors. For the first time, the fundamental steps of self-assembly in complexes of carbon nanotubes with the cationic dye methylene blue were elucidated, highlighting their potential for nanodevice fabrication.

In addition to fundamental research, considerable attention is paid to the development of ways of practical application of the obtained results. Thus, it was shown that several of the studied nanobiosystems can be used as biosensors, for example, for glucose, lactic acid and cysteine, using the luminescence of nanotubes or conductivity through the nanotube network. It was found that a composite film of carbon semiconductor nanotubes and a polymer can be used to create a bolometer for detecting light in the IR region.

Since 2015, extensive research has focused on graphene nanostructures and their interactions with complex biomolecules, including DNA, enzymes, and drug molecules. These studies revealed several new phenomena, such as the structural disordering of single- and double-stranded polynucleotides adsorbed onto graphene oxide (GO), accompanied by characteristic changes in their electronic and vibrational spectra. The interactions were shown to arise primarily from π–π stacking between nucleobases and the graphene surface, further stabilized by hydrogen bonding with oxygen-containing groups of GO. Such mechanisms underlie the design of nanobiostructures through non-covalent functionalization and self-assembly, opening up potential for biosensing and drug delivery applications. Importantly, GO-based nanohybrids with anticancer drugs (e.g., 5-fluorouracil and 5-chlorouracil) were prepared and studied, demonstrating GO suitability as nanoplatforms for targeted therapy. Additional findings included GO-induced stabilization of A-motif duplexes from two single-strands of poly(rA) at neutral pH. Simulations showed that for a positively charged graphene surface, a noticeable contribution to the total energy of interaction with an oligonucleotide is provided by the Coulomb attraction between them. It was found that the interaction of nucleobase with weakly oxidized graphene is the largest in comparison with graphene or with significantly oxidized graphene. It was revealed that the interaction of cationic porphyrin TMPyP4 with graphene is accompanied by distortion of the flat porphyrin core and some twisting of the side rings. Structural and energy characteristics of a number of complexes of organic and biological molecules with graphene materials were obtained, which show their high adsorption properties. It makes them promising for the creation of effective materials for cleaning the environment from toxic pollutants.

In recent years, the department’s research has focused on the design of composite nanomaterials incorporating carbon nanotubes, graphene oxide, reduced graphene oxide, transition metal dichalcogenides, silver nanoparticles, and titanium dioxide. Particular attention has been given to their complexes with biological systems and the investigation of their physical (spectral, conductive, structural) and biophysical properties. Current efforts are directed toward the development of multimodal nanoplatforms based on 2D nanomaterials and their integration into polymer nanofibers for the fabrication of antibacterial coatings and wound-healing membranes. A combination of advanced experimental techniques, including spectroscopy, mass spectrometry, and electron microscopy, along with quantum mechanical calculations and computer modeling, is employed to elucidate the underlying mechanisms. This research lies at the forefront of modern nanoscience, with significant implications for biology and medicine.

More than 100 articles in international journals and 2 monographs have been published on the topic of nanobiophysics: "Photophysics of Carbon Nanotubes Interfaced with Organic and Inorganic Materials" Springer-Verlag London 2012, and "Nanobiophysics: Fundamentals and Applications" Pan Stanford Publishing Pte Ltd., Singapore; 2015. Scientists of the department are the initiators and organizers of the international conference "Nanobiophysics: Fundamental and Applied Aspects".

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RT2

BIOPHYSICISTS OF KHARKIV UNIVERSITY AND THE ADVANCE OF BIOPHYSICS

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Biophysics has a long and distinguished tradition at V.N. Karazin Kharkiv National University, where pioneering studies in applied physics, biology, and medicine have converged to form a vibrant school of scientific thought. From the mid-20th century, Kharkiv researchers have made seminal contributions to membrane biophysics, radiation biophysics, and the study of biomolecular interactions, establishing the University as one of the leading centers of biophysical research in Eastern Europe. The PhD program (the program for obtaining a candidate of science degree, equivalent of PhD) in biophysics was launched in Kharkiv University in 1936 while the Department of Molecular and Cellular Biophysics was established in 1978.

The Kharkiv University biophysical community has historically combined rigorous physical approaches with pressing biomedical challenges. Early works on the effects of ionizing radiation on biological systems provided fundamental insights into DNA damage and repair. In parallel, studies of cell membranes and transport phenomena opened pathways to understanding electrophysiological processes and the molecular basis of cellular signaling. These foundational achievements not only advanced fundamental science but also laid the groundwork for practical applications in education, pharmacology, and biotechnology.

The strength of this tradition is reflected in the outstanding contributions of Kharkiv University professors. Docent Lev Stiopin made a profound contribution to bioelectrodynamics and quantum biophysics; he laid the basis for the dielectric measurements of biofluids. Professor Boris Yemets introduced ESR and NMR approaches for biological applications, developing a concept of the behavior of tiny gas-phase bubbles in liquids. Senior researcher Oleg Nikolov has pioneered research in radiation biophysics; he also established a direction of medical instrument making at the department and was behind microwave dielectric measurements, ESR, and NMR facilities in Kharkiv University and in the city of Kharkiv. Professor Victor Lemeshko is widely recognized for his studies on energy conversion in biological membranes and the mechanisms of mitochondrial function, advancing our understanding of bioenergetics and oxidative stress. Professor Anatolii Paranich has pioneered research in pharmacological and environmental biophysics and cellular responses to ionizing radiation, laying a foundation for radiation medicine and radiobiological safety. Docent Sergiy Gatash has contributed significantly to mathematical biophysics, blood cells biophysics and the development of experimental approaches to study platelet aggregation, RBC sedimentation and microwave dielectric measurements, bridging theoretical modeling with experimental data in modern biophysics. Collectively, their research achievements represent milestones that continue to inspire younger generations of scientists.

Equally important is the contribution of Karazin biophysicists to education and academic development. Their efforts were instrumental in the establishment of new interdisciplinary specialties such as biomedical electronics and medical physics, which integrated physical sciences with modern healthcare needs. Docent Ella Romodanova played a decisive role in shaping the curriculum for biomedical electronics in bridging it with medical education, ensuring that students gained both physical and clinical perspectives. Docent Sergiy Gatash, Professor Galyna Gorbenko and Professor Volodymyr Tovstiak contributed greatly to the development of medical physics at Karazin and introduced this specialty to Ukraine, creating a curriculum that combined advanced physical principles with practical applications in diagnostic imaging and therapy. Visionary steps of Kharkiv University biophysicists also supported the revival of the School of Medicine at Karazin University, ensuring continuity between fundamental biophysical research and its clinical applications. By shaping new curricula and training programs, Kharkiv biophysicists have nurtured a generation of specialists capable of bridging physics, engineering, and medicine, thus broadening the international impact of the University.

The achievements of Docents Larysa Sichevska, Olga Gorobchenko, and Tetyana Ovsiannikova have also been essential in strengthening both research and teaching at the Department of Biophysics. Larysa Sichevska has significantly advanced studies in radiation biophysics, molecular cell biophysics, and biophysical methods of biomolecule characterization, while also contributing to the development of laboratory courses that train students in experimental rigor. Olga Gorobchenko is widely recognized for her research on protein–ligand interactions, radiation biophysics, and microwave dielectric measurements of biomolecular liquids, work that not only advances fundamental knowledge but also informs applied biomedicine. Tetyana Ovsiannikova has made key contributions in the area of cellular biophysics, effects of external physical factors on biological objects, and experimental methods for studying membrane processes, while being deeply engaged in mentoring and academic program design. Together, their contributions strengthen the bridge between research excellence and the cultivation of new generations of biophysicists.

Inspired and chaperoned by the prominent Ukrainian biophysicist and then Head of the Department, Professor Volodymyr Maleev journal “Biophysical Bulletin” was established in 1998. The efforts of two generations of the Department faculty and staff keep this journal a launching pad for thriving careers of young biophysicists and open open-access platform for displaying research in biophysics and related fields. The Biophysical department of Kharkiv University hosts the Kharkiv branch of the Ukrainian Biophysical Society brought to life more than 40 years ago by outstanding scientists and the trademarks of Ukrainian biophysics - professors Yurii Blagoii and Volodymyr Maleev. A series of citywide biophysical workshops under the umbrella of the Kharkiv Branch of the Ukrainian Biophysical Society is always a place to present and discuss submitted for defense Ph.D. and Dr.Sci. theses and share recent achievements of biophysical labs from Kharkiv, Ukraine, and abroad.

Today, the biophysicists of Kharkiv University continue to expand these traditions in new directions. Research in nanobiophysics, membrane-active peptides, targeted drug delivery, and the development of nanostructured platforms for antimicrobial peptides reflects the University’s commitment to addressing modern biomedical challenges. At the same time, the Department is strongly engaged in structural and functional studies of proteins and membranes, red blood cell and platelet physiology, and the biophysical mechanisms of cell microvesiculation. These efforts are supported by the integration of advanced techniques, including microfluidics, surface-sensitive spectroscopy, mathematical modelling, and light scattering.

An increasingly important aspect of this development is international collaboration. In recent years, biophysicists of V.N. Karazin Kharkiv National University have strengthened their partnerships with European universities through joint research projects, Erasmus+ mobility, and summer internships for students. These initiatives not only enrich scientific exchange but also help young researchers gain exposure to cutting-edge methods and build lasting academic ties. The community also maintains strong connections with graduates and alumni of Karazin University worldwide, who contribute to global science and serve as ambassadors of Kharkiv biophysics.

Despite the challenges of recent years, including the ongoing war in Ukraine, Kharkiv biophysicists have shown remarkable resilience and dedication. Laboratories continue to function, students and faculty remain engaged in teaching and research, and international collaborations are actively pursued. This determination underlines not only scientific strength but also human courage — ensuring that Kharkiv remains a vital part of the global biophysical community.

Together, these achievements — from pioneering research and curriculum development to international partnerships and alumni contributions — form the identity of the “Kharkiv School of Biophysics”. It is a community bound by scientific rigor, innovation, and resilience, shaping not only Ukrainian science but also contributing meaningfully to the progress of global biophysics.

RT3

HOW THE BIOPHYSICS IN IRE STARTED AND PROGRESSED: ACCORDING TO THE MEMOIRS BY V. YA. MALEEV

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A brief account of the idea behind the establishment of the Department of Biological Physics at the Institute of Radiophysics and Electronics of the NAS of Ukraine, its early research, and the first results in molecular biophysics based on the memoirs of Prof. V.Ya. Maleev [1].

The idea of establishing a Department of Biological Physics at the Institute for Radiophysics and Electronics of the National Academy of Sciences of Ukraine (IRE NASU) belonged to Volodymyr Maleev, Doctor of Physical and Mathematical Sciences, Professor, laureate of State Prize of Ukraine in Science and Technology, and the founder of biophysics as a scientific field within academic institutions of a physical profile in Ukraine.

As early as the beginning of the 1960s, Maleev, then only a Candidate of Physical and Mathematical Sciences, despite his young age (slightly over 30), foresaw the potential of applying physical methods and approaches to solving certain biological problems, primarily at the molecular level. Thanks to his initiative, and with the support of O.Ya. Usikov, Director of IRE, and B.E. Paton, President of the Academy of Sciences of Ukraine, a new scientific direction – biophysics – was launched, and the Biophysical Department was established within institutions of a physical profile, a pioneering decision at the time.

President of the Academy of Sciences of USSR M.V. Keldysh and V. Ya. Maleev at the seminar in IRE, 1964

The first years of the department's work were devoted to the search for effective radiophysical and spectroscopic methods for studying the structure, stability, and dynamics of biopolymers – proteins and nucleic acids – in an aqueous environment. Under the leadership of V.Ya. Maleev, the young team developed experimental approaches for analyzing DNA conformations, taking into account its hydration (dielectrometry in the millimeter range, infrared spectroscopy of wet films, piezogravimetry, and differential scanning microcalorimetry of biopolymer–water systems).

Already in its early years, the department achieved world-class results: it was demonstrated that the methods developed there opened fundamentally new possibilities for studying the structural organization of nucleic acids, revealing the patterns of their interactions with ligands, as well as providing quantitative evaluations of processes that had previously remained beyond the reach of experimental science. These achievements laid the foundation for the international recognition of the Kharkiv school of molecular biophysics and set the stage for the field's further development in Ukraine.

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RT4

TRIBUTE TO ACADEMICIAN B.I. VERKIN – THE FOUNDER OF THE BIOPHYSICAL AND BIOMEDICAL RESEARCH AT THE INSTITUTE FOR LOW TEMPERATURE PHYSICS AND ENGINEERING

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Outstanding contribution of academician Boris Ieremievich Verkin (1919-1990) to physical sciences is well documented in the memoirs of his colleagues [1], who stood at the origins of the Institute for Low Temperature Physics and Engineering founding together with B.I. in 1960. Along with basic physical research, B.I. Verkin had contributed to biophysics [2], cryobiology, and applied biomedicine [3]. He had founded the Chair of molecular and applied biophysics at Kharkov University to train future scientists in this field.

It is believed that research in "biological physics" was inspired worldwide after the deciphering of the structure of DNA molecule by a physical experimental technique in 1953. However, this confirmation of existence of "material carrier of heredity" was of special significance for science in the Former Soviet Union where genetics at those times was branded and prosecuted as "a bourgeois idealistic pseudoscience". To start research in the area related to DNA and genetics at that time required civic courage and heroism - I want to especially emphasize this page of activity of Boris Ieremievich.

B.I. Verkin main idea of biophysical studies of DNA was to establish physical parameters of the molecules of nucleic acids and their components, with hope to apply low temperature research experience to search superconductivity of DNA. A set of physical experimental techniques for DNA studies was developed in biophysical departments founded by him at the ILPTE. In particular, low temperature matrix isolation spectroscopic technique was created by Yu.P. Blagoi and his team. Together with I.K. Yanson, L.F. Sukhodub, A.B. Teplitsky pioneering techniques of soft field ionization and low temperature mass spectrometry were elaborated; the results obtained by these novel techniques were summarized in the monograph "Interaction of biomolecules: new experimental approaches and methods" [2]. Some of these experimental data were included into the NIST of USA database and were used by developers of semi-empirical quantum chemical methods as the empirical parameters of nucleic acids components.

Along with basic research, B.I. Verkin developed design and production of cryogenic biomedical equipment at the Engineering bureau of the ILTPE [3], including cryosurgery [4]. He promoted implementation of cryogenic techniques to food storage in the framework of the state food supply program [5].

Currently, the new generation of biophysicists, educated by B.I. Verkin, continues to elaborate new directions in biophysics, such as nanobiophysics.

This work was supported by the NAS of Ukraine Grant N0123U100628.

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4. B.I. Verkin et al. Cryosurgery in stomatology. – Kiev: Naukova Dumka, 1984.
5. B.I. Verkin, D.N. Bolshutkin, Yu.N Sklovsky. Novaya "professiya" azota. (*New "profession" of nitrogen*). – Kharkov: Prapor, 1985.

RT5

CONTRIBUTION OF PROFESSOR BLAGOI Yu.P. TO MOLECULAR BIOPHYSICS OF NUCLEIC ACIDS

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In the memories of his colleagues and apprentices, Yurii Pavlovich Blagoi (1929 – 2018) is remembered as an outstanding scientist, physicist and biophysicist, and simply an excellent person. He was a member of a cohort of active scientists who ensured the development of the Kharkiv scientific school of molecular biophysics, which received recognition in Ukraine and abroad.

Blagoi's entire scientific career (1960 – 2018) is closely connected with the Institute for Low Temperature Physics and Engineering (ILTPE). Together with B.I. Verkin, Blagoi stood at the origins of the creation of the biophysical direction at the ILTPE. From 1962 to 2000 he was the head of the Department of Molecular Biophysics, which he had created. Maintaining the link between fundamental science and education, in 1980-1985 he headed the Department of Molecular and Applied Biophysics at Kharkov University, and afterward taught for many years as a professor in this department. His lecture courses on the physics of biopolymers were attended by about 600 students from more than 20 countries around the world. Among his students are more than 20 candidates of sciences and 2 doctors of sciences, who are actively working both in scientific organizations of Ukraine and in leading world laboratories.

Blagoi Yu.P. was a member of the editorial boards of Ukrainian scientific journals “Biophysical Bulletin” and “Problems of Cryobiology”. He was among the founders of the Ukrainian Biophysical Society and organizers of a series of scientific conferences on “Spectroscopy of Biopolymers” and summer schools on “Biophysics of Nucleic Acids”. In 2008, Yurii Pavlovich, as part of a team of colleagues, received the State Prize of Ukraine in the field of science and technology for the cycle of works "Fundamental physical properties of biopolymers that determine their functioning."

Yurii Pavlovich's wide range of scientific interests included various aspects of molecular physics and biophysics: structural and spectral characteristics of nucleic acids and their components in solutions and low-temperature matrices, intermolecular interactions of biomolecules, DNA-metal ions interactions [1], and application of cryogenic methods of cryo-grinding and freeze-drying of pharmaceutical raw materials.

Here we gave only a formal list of Professor Blagoi’s achievements reflected in publications [2-4]. Warm recollections about Yurii Pavlovich's personality and the experience of scientific collaboration will be presented in the informal session discussion.

Acknowledgements: This work was supported by the National Academy of Sciences of Ukraine (Grant 0123U100628).

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RT6

IN MEMORIAM:
Yu.V. MALYUKIN, THE FOUNDER OF NANOBIOPHYSICS IN THE INSTITUTE FOR SCINTILLATION MATERIALS OF STC “INSTITUTE FOR SINGLE CRYSTALS”

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On June 7, 2020, our Institute suffered an irreparable loss: Professor **Yuriy Viktorovych Malyukin**, Corresponding Member of the National Academy of Sciences of Ukraine and an outstanding leader in fundamental science, passed away at the age of 63. He was full of energy, ideas, and creative plans until his very last days.

Prof. Malyukin was widely recognized in Ukraine and abroad as one of the pioneers in the rapidly developing field of nanostructured materials. His early works on impurity centers in oxyorthosilicate crystals and related materials laid the foundation for novel approaches to modifying scintillation properties, particularly in crystals doped with cerium ions. Another of his major scientific contributions was in the study of excitonic dynamics in organic nanoclusters (J-aggregates), a promising class of materials with applications as fluorescent probes and artificial photosynthetic antenna complexes.

Perhaps his most remarkable achievement, which allows us to regard him as one of the founders of modern nanobiophysics, was the creation and study of a new class of luminescent, redox-active nanomaterials for biological and medical applications. His enthusiasm was boundless when he spoke about these nanoparticles and their unique properties to biologists and medical researchers. Thanks to his conviction in their potential, close collaborations were established with leading biomedical institutions in Ukraine and with pharmaceutical companies. These joint efforts revealed extraordinary properties of redox-active nanomaterials, including radioprotective effects, antitumor activity, wound-healing potential, and positive impacts on aging.

Prof. Malyukin’s legacy continues through the work of his students and colleagues. Among their recent achievements is the development of the dietary supplement VAGAREVITA™, based on redox-active nanoparticles, an exceptional case where fundamental physical and physico-chemical studies of rare-earth orthovanadates were transformed not only into dissertations and publications but also into the large-scale production of a promising health product.

Over the course of his career, Prof. Malyukin authored or co-authored more than 400 scientific papers, 15 patents, and 3 monographs. Under his supervision, 18 PhD and 5 doctoral dissertations were defended. His school of science is distinguished by its strength and continuity: among his students are 8 Laureates of the President of Ukraine Prize for Young Scientists, 4 Laureates of the Verkhovna Rada of Ukraine Prize for talented young scientists, and 1 Laureate of the State Prize of Ukraine in Science and Technology.

The cherished memory of Yuriy Viktorovych Malyukin will forever remain in the hearts of all who knew and worked with him. For his students, colleagues, and future generations of scientists, he will remain an enduring example of true devotion to science, creative thought, inspiring leadership, tireless energy, and service to both science and the Motherland.

RT7

TRIBUTE TO PROFESSOR O.M. OGURTSOV

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AUTHOR INDEX

Наукове видання

9-та Міжнародна конференція

Нанобіофізика: фундаментальні та прикладні аспекти
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