Newsletter of the Science & Technology Wing Embassy of India Moscow

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JULY — AUGUST 2020

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SCIENTIFIC ARTICLES & NEWS

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SCIENTIFIC ARTICLES & NEWS

1. MIPT BIOINFORMATICIANS FIND WAY TO PERSONALIZE DRUG PRESCRIPTION AGAINST STOMACH CANCER

https://xn--m1afn.xn--p1ai/en/news/en-media/mipt-bioinformaticians-find-way-to-personalize-drug-prescription-against-stomach-cancer/

Researchers from the Moscow Institute of Physics and Technology and their colleagues have developed the first technique for personalizing stomach cancer therapy based on RNA sequencing of tumor cells. The study, supported by the Russian Science Foundation, was published in *Cold Spring Harbor Molecular Case Studies*.

Credit: Depositphotos

Stomach cancer is the fifth-deadliest oncological disease. It is seldom diagnosed in the early stages, which complicates treatment. There are several treatment options available that rely on chemotherapy and therapeutic antibodies. However, patient response is often unpredictable, so personalized therapies with drug prescriptions tailored to individual cases are required.

Problematic recurrent tumors of the stomach are treated with therapeutic antibodies. They block the receptors on the surface of cells that are responsible for receiving growth-promoting signals. Without them, cell division stops and the tumor does not increase in size. Preventing the growth of blood vessels is particularly important, because they supply nutrients and oxygen to the tumor. Ramucirumab is a therapeutic antibody used to disrupt the growth of blood vessels in tumor tissue. The efficacy of this drug varies widely from patient to patient.

MIPT bioinformaticians and their colleagues from medical research centers and the industry have proposed that a patient's data on the gene expression levels in cancer be used to evaluate ramucirumab efficacy in each individual case.

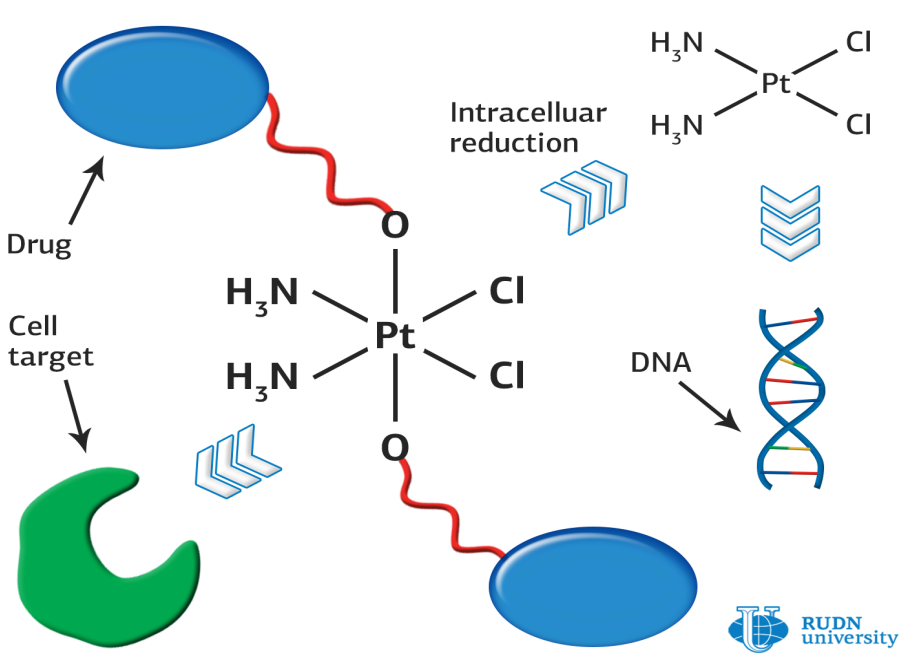
"This is virtually the first published case of successful [ramucirumab] prescription to patients with gastric cancer, which was not random but rather informed by the analysis of the molecular markers we track based on RNA sequencing," said Maxim Sorokin, a senior researcher at the MIPT Laboratory for Translational Genomic Bioinformatics and the head of the Bioinformatics Department at Oncobox.
Combined with information technology, modern molecular biology methods enable researchers to collect qualitative data on the expression of every gene in a cell. By analyzing these data, it is possible to find the key to diagnosing oncological diseases and predicting the efficacy of their treatment.

The study reported in this story was co-authored by researchers from MIPT, Sechenov University, Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry of RAS, Blokhin National Medical Research Center of Oncology, Vitamed Clinical Center, Vladimirsky Moscow Regional Research Clinical Institute, and Oncobox.

2. A RUDN UNIVERSITY CHEMIST CREATED ANTI-TUMOUR COMPOUNDS THAT ARE UP TO 80 TIMES MORE EFFECTIVE THAN THEIR COUNTERPARTS

http://eng.rudn.ru/media/news/science/a-rudn-university-chemist-created-anti-tumour-compounds-that-are-up-to-80-times-more-effective-than-their-counterparts/

A chemist from RUDN University has created platinum complex compounds that are superior in activity to cisplatin, the drug for the treatment of tumour diseases. The new compounds turned out to be also less toxic to healthy cells.



Platinum-based anticancer drugs — cisplatin, oxaliplatin, and carboplatin — are used for chemotherapy in about half of cancer cases. They penetrate cells and interact with DNA molecules. The process is fatal for rapidly dividing cancer cells because the drugs prevent the duplication of DNA molecules, which is necessary for successful division. Since cancer cells divide rapidly, they are the first to

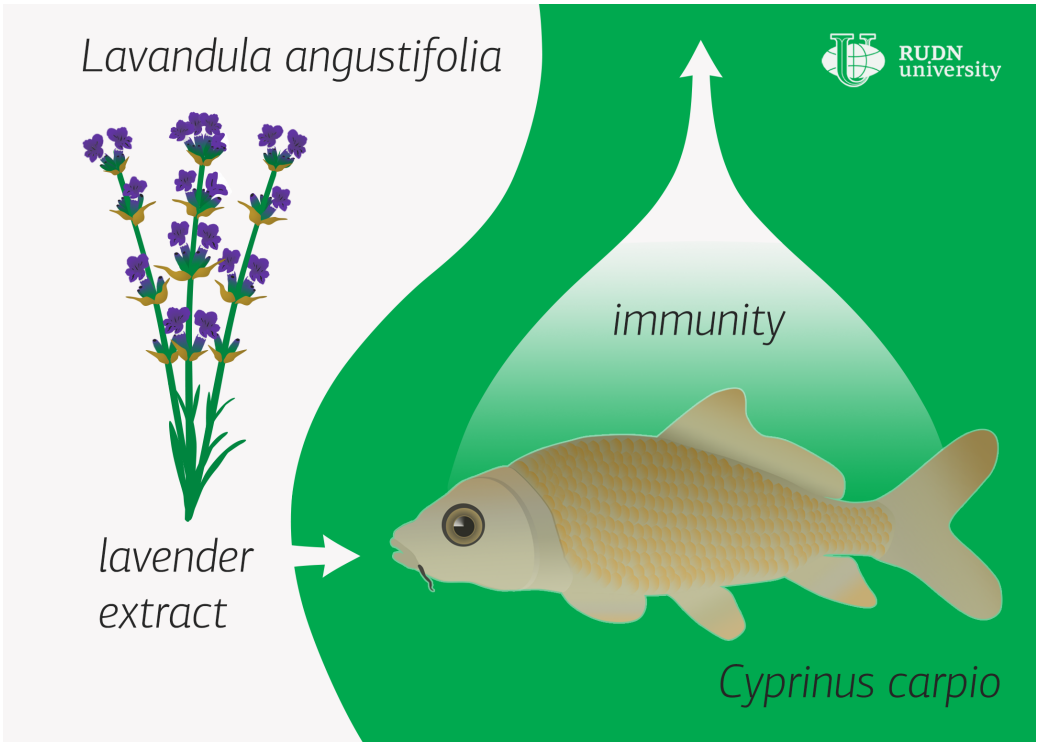
be affected. Still, platinum derivatives have certain disadvantages: low stability under physiological conditions and high toxicity.

To create new drugs, a strategy that involves the development of hybrid molecules is often used in modern chemistry. Such substances consist of two or more active fragments that are linked by a linker into one molecule. They usually have a double action, characteristic of each of the fragments.

A chemist from RUDN University, candidate of biological sciences Kirill Kirsanov, created a series of new drugs: hybrids of cisplatin, lonidamine, and bexarotene. Lonidamine itself has an anti-tumour effect due to its ability to suppress energy metabolism in cancer cells. In combination with radiation therapy, it is used to treat brain tumours. Bexarotene is used for the treatment of lung cancer and breast cancer, as it inhibits the growth of tumour cells of hematopoietic and squamous origin.
A derivative of cisplatin with bexarotene turned out to be the most promising. A combination of succinic acid and ethylenediamine was used as a linker. In tests conducted on four tumour cell lines, the hybrid drug was 80 times more active than bexaroten and 20 times higher on average than cisplatin, and the new drug was 80 times more active than cisplatin on MCF7D cell line. Based on the resulting leading compound, new and more effective anti-tumour medications can be developed.

3. RUDN UNIVERSITY BIOLOGIST DISCOVER THAT LAVENDER ENHANCES THE IMMUNITY OF CARP BIOLOGIST. MORTEZA YOUSEFI HAS FOUND THAT LAVENDER EXTRACT ADDED TO THE FOOD REDUCES STRESS AND IMPROVES IMMUNITY IN CARP IN FISH FARMS.

http://eng.rudn.ru/media/news/science/rudn-university-biologist-discovered-that-lavender-enhances-the-immunity-of-carp/



A significant part of fish in fish farms dies due to illnesses provoked by stress during transportation, sorting, and other operations. The use of antibiotics for the treatment and prevention of infections in fish is not only costly, but also leads to bacterial strains resistant to antibiotics to develop. Therefore, the use of herbal preparations is of particular value as a means of maintaining the health of fish.

Professor Yousefi of RUDN University and his colleagues decided to check whether inclusion of narrow-leaved lavender extract (Lavandula angustifolia) to the feed of common carp (Cyprinus carpio) can enhance the immunity of the fish.

It had already been known that the components of narrow-leaved lavender extract, cineole and linalool, have anti-inflammatory, antioxidant, and anti-stress effects. The biologists assumed that these substances can help fish cope with the negative effects of the stress hormone cortisol.

Youssefi and his colleagues divided the fish into four groups. For 70 days, the fish in the first group received a diet which contained 0.5% of lavender extract, 1% in the second group, and 1.5% in the third one. The fourth group was the control, in which the carps did not receive lavender extract at all. After that, veterinarians subjected the fish to three hours of stress: the water level in the aquarium was reduced by 90%. Before and after the stress test, the authors studied a number of indicators that directly or indirectly reflect the effects of stress in fish.

After 70 days, the fish that received 1% and 1.5% lavender extract additives demonstrated positive changes such as a significant increase in the concentration of soluble and cell-mediated factors of innate immunity, i.e. plasma globulins, immunoglobulins, white blood cells, as well as increased activity of plasma lysozyme and the alternative pathway complement. In the same two experimental groups, gene expression of a number of pro-inflammatory proteins was lower than that in the control group. Lavender did not significantly affect fish growth.

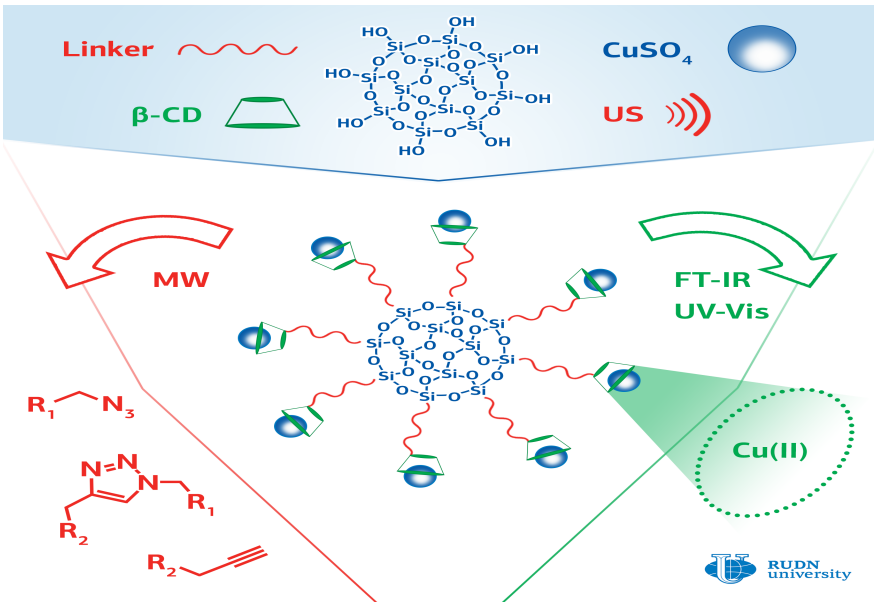
Professor Yousefi and his colleagues have found that levels of stress markers in the blood, cortisol and glucose, increased significantly after fish in each group experienced stress. But the more lavender extract fish received, the lower these indicators were. Moreover, fish from lavender extract receiving groups showed another beneficial difference from the control group: a higher level of catalase and superoxiddismutase enzymes in the blood. This indicates that their antioxidant defense systems were in better state than those in the fish in control group.

The inclusion of lavender extract to the feed of common carp is recommended in an amount of 1.0-1.5% to suppress stress, inflammation, and oxidative stress and to enhance the immune response in fish, the scientists from RUDN University concluded.

4. A RUDN UNIVERSITY CHEMIST CREATED NEW CATALYST FOR CLICK REACTIONS

http://eng.rudn.ru/media/news/science/rudn-university-chemist-created-new-catalysts-for-click-reactions/

A chemist from RUDN University has created a series of catalysts for click chemistry. These reactions are widely used in the synthesis of biologically active substances, as well as in biological and medical research. New catalysts produce a yield of 99%. They are based on cyclodextrin and copper ions.



Click chemistry methods are used to synthesize libraries of substances with high chemical diversity, which is important when developing new drugs. These reactions are necessary for introduction of labels (for example, fluorescent ones) into biological macromolecules, proteins, and DNA molecules. This is used in biological and medical research.

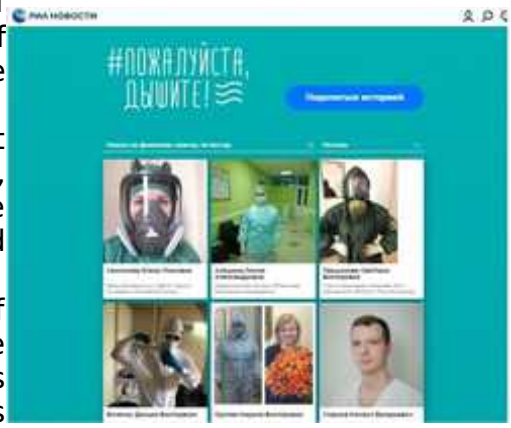
The most commonly used click chemistry reaction is the addition of a substance that contains a carbon-carbon triple bond (alkine) to a compound containing a fragment with three nitrogen atoms in a row (azide). The classic version of the reaction involves the use of copper in oxidation state (I) as a catalyst. For this, ions of copper (II) and an excess of a reducing agent are introduced into the reaction, or copper (I) is used and the reaction is conducted with protection against oxygen, which imposes certain restrictions on the application of this reaction.

A chemist from RUDN University Rafael Luque and his colleagues have developed a series of catalysts with copper ions attached to the surface of silica gel particles using cyclic cyclodextrin oligosaccharide. Cyclodextrin consists of seven glucose molecules closed in a cycle. Inside the cycle there is a container that can hold the copper ion and increase its catalytic activity. Ultrasound irradiation was used to facilitate the binding of cyclodextrin to the surface of silica gel.

The effectiveness of the created catalysts was evaluated on a model reaction of phenylacetylene with benzylazide. The researchers managed to achieve a yield of the reaction product of more than 99%. The yield with copper (II) acetate was 14%, and in the case of copper (II) sulfate, the reaction did not occur at all. The method for producing the catalyst is simple, safe for the environment, and cheap; its use does not require to add reducing agents or oxygen-free conditions. The catalysts can find application in the pharmaceutical industry and in biomedical research.

5. NATIONAL ACTION "PLEASE BREATHE!" WILL BECOME UNLIMITED

https://minzdrav.gov.ru/news/2020/06/29/14323-vsenarodnaya-aktsiya-pozhaluysta-dyshite-stanet-bessrochnoy



The media group “Russia Today”, the organizer of the “Please Breathe!" Campaign in support of Russian doctors and volunteers, decided to make the action perpetual.
“The significance of the medical profession does not depend on the beginning and end of pandemics, therefore, we believe it is right not to limit the duration of our“ Please Breathe! ”dates, ”said Dmitry Kiselev, general director of MIA Russia Today.
In late May, Russia Today MIA, with the support of the Russian Ministry of Health, launched an online campaign, Please Breathe! In which it collects stories about doctors, medical workers, employees of hospitals and hospitals, and volunteers throughout Russia into a single thematic portal on the ria website.ru
Since the start of the asset, the action has already over four hundred stories from all over Russia. Those who want to talk about their heroes - doctors and volunteers can fill out a form on the portal. Promotion rules are also listed on the portal. The action is a sign of immeasurable human gratitude and a desire to preserve the memory of those who daily risk their lives to save the lives of others. It was initiated by the Russia Today MIA with the support of the Ministry of Health of the Russian Federation and the Moscow Department of Health, the Volunteer-Medik Water and Health Center, the Association of Volunteer Centers, and the ANO National Priorities /stopkoronavirus.ru website. VGTRK became the general partner of the action.

6. SCIENTISTS FOUND A WAY TO IDENTIFY DISEASES BY BLOOD SERUM

https://english.spbstu.ru/media/news/nauka_i_innovatsii/scientists-found-way-identify-diseases-blood-serum/

Researchers of Peter the Great St. Petersburg Polytechnic University (SPbPU) in collaboration with colleagues from Tsinghua University (China) developed a new dynamic light scattering method to determine the sizes of circulating immune complexes in blood serum. The results of the study were published in the first quartile Biology Journal, MDPI Publishing House. Scientists mentioned, that this method is fast, contactless, safe and cheap. That why it could be used in blood screening studies, for example, as part of regular medical examinations.

The scientific group of the Higher School of Applied Physics and Space Technologies SPbPU investigated how the immune complexes are formed in blood serum. The immune complexes are molecular aggregates, which consist of antigens, antibodies, and proteins of the immune system. The size and concentration of such immune complexes indicate the state of the immune system. Normally a certain concentration of the immune complexes presents in blood serum, high concentration of immune complexes is formed due to the pathological condition.

The international scientific group investigated the blood serum of donors with various pathologies, such as autoimmune diseases, cancer, diabetes mellitus, etc.

According to scientists the increased (compared with the average) size of the immune complexes indicates the presence of diseases, and by itself can have a potentially negative effect on the state of the body. A high concentration of the newly formed immune complexes can disrupt the functioning of the immune system. These complexes can clog microcapillaries, or accumulate in the tissues, causing chronic inflammatory processes.

"*We found out, that the infection in the body leads to the formation of a large number of the immune complexes in the blood,"*said Elina Nepomnyashchaya, an employee of the Laboratory for Laser Photometry and Spectroscopy of St. Petersburg Polytechnic University.

Elena Velichko, Head of the Laboratory of Laser Photometry and Spectroscopy SPbPU, notes: *"Our method is quite fast, it doesn't require the use of specific expensive antigens. Its work is based on the interaction of laser radiation with serum or plasma proteins. Using the developed method, we were able to trace the activation path of the immune system in the blood. Our results can be used in pharmacology for drug testing and in the modern preventive diagnosis of immune diseases."*

The research is carried out jointly with medical institutions of St. Petersburg (Russia). In future, the scientific group plans to conduct research with the fellow biologists to determine how different substances affect the activation of the immune system.
Subsequently, scientists plan to study the disorders of the immune system due to cancer. Researchers hope to "teach" the immunity to recognize the cancer cells and to recover.

7. DIFFERENTIAL SCANNING CALORIMETRY TO QUANTIFY PROTEIN-LIGAND BINDING

https://kpfu.ru/eng/news-eng/scanning-calorimetry-protein-ligand-binding.html

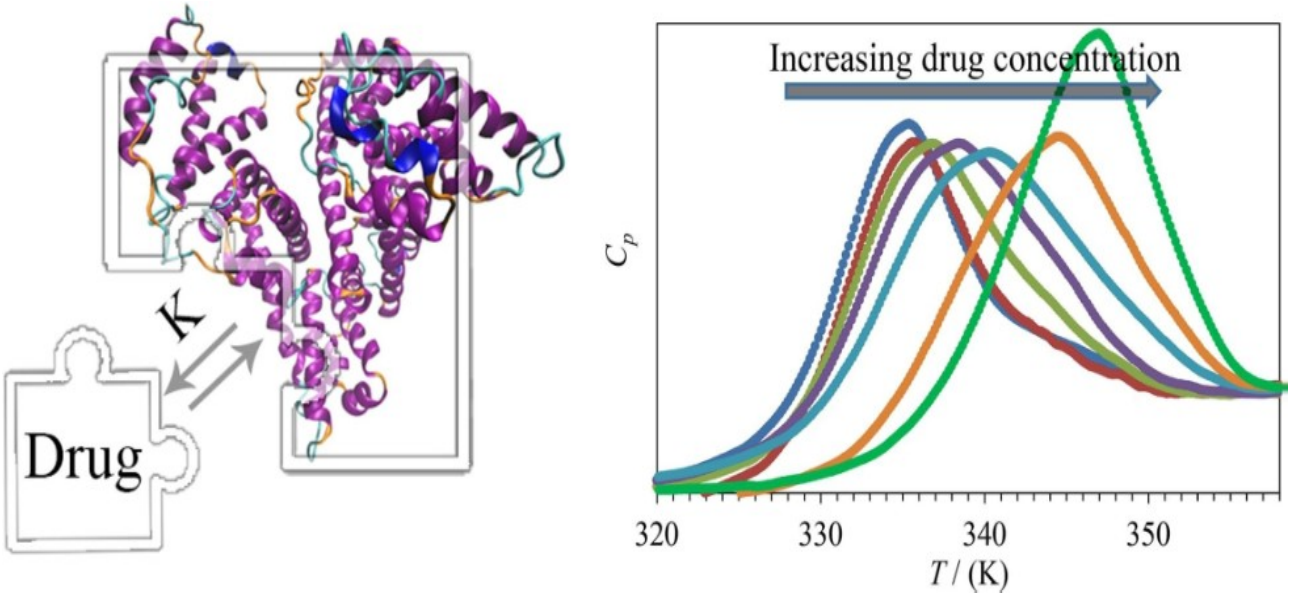


Figure: Graphical abstract

A paper appeared in International Journal of Pharmaceutics.

A team of researchers from Kazan Federal University, Russia, led by Dr. Igor Sedov, reported an application of capillary differential scanning calorimetry technique for the study of the binding of albumin, a plasma transport protein, with different drug ligands.

The processes of binding of various biologically active ligands to proteins can be quantitatively characterized by the values of thermodynamic binding constants, which determine the ratio between the concentrations of free and bound ligand. Accurate determination of these quantities is not an easy task. Presently, a fairly sensitive and robust isothermal titration calorimetry method is most commonly used; however, it does not allow to study the processes with very high binding constants or separate binding steps.

The differential scanning calorimetry (DSC) method, based on monitoring changes in the heat capacity of a heated sample, is widely used to study protein denaturation. A shift of the denaturation peak to higher temperatures in the presence of a ligand is a sign of protein-ligand binding. However, the relationship between the shift magnitude and the binding constant cannot be described by a simple mathematical formula. Therefore, only a few attempts were made to use DSC thermograms for the quantitative ligand binding studies. The authors of the paper developed a program that takes into account the denaturation and ligand binding equilibria and allows one to predict the DSC curve from the known binding constants and protein and ligand

concentrations. Then the values of the constants can be optimized to provide the best fit of the calculated curves to the experimental ones.

The application of this approach to albumin is complicated by the mechanism of denaturation of this protein, which is usually considered to be two-stage. However, the authors showed that the two-state model of protein denaturation used in the program gives the results consistent with other experimental methods. Moreover, the analysis of DSC thermograms helps measure very high binding constants, as well as weak binding constants with the second molecule of a ligand, and the stoichiometry of a complex at the large excess of ligand, when simultaneous binding to several centers, including those with low affinity, occurs.

Albumin is the main transport protein in blood plasma and can bind to a wide variety of molecules. Albumin has a two-domain structure with at least two high-affinity and several low-affinity binding sites. The binding affinity of drugs to plasma proteins influences the fraction of the free drug in plasma, which, in turn, is one of the major factors governing drug permeability through physiological barriers. Only unbound drugs can cross these barriers. As an example, the studied strong albumin binders – naproxen and ibuprofen – have limited brain bioavailability due to low permeability through the blood–brain barrier. On the other hand, slowly metabolized drugs with weak plasma binding have increased clearance, which may result in lower efficacy. The binding constant values can give the idea about the fraction of an unbound drug in blood plasma, while the knowledge of sequential binding constants is important for the studies of competition between drugs and other substrates or between two different drugs for albumin binding centers. In the case when the strongest binding center is occupied by another molecule, the unbound fraction of the drug will be determined by its affinity to the other binding sites. The interest in albumin binding also arises from the prospective use of drug delivery systems based on albumin nanoparticles.
The DSC-based method has potential applications to a wide range of proteins and bioactive ligands and can be useful in drug development and protein science. This work was supported by the Russian Science Foundation (grant 19-73-00209).

8. EXPERIMENT CONFIRMS LIQUIDS SHOW PROPERTIES OF SOLID BODIES AT MICROSCOPIC SCALES

https://kpfu.ru/eng/news-eng/experiment-confirms-liquids-show-properties.html

An international paper went out in Physical Review B.

The collaborators are Kazan Federal University, Vereschagin Institute of High Pressure Physics (Russian Academy of Sciences), Queen Mary University of London, Imperial College London, Rutherford Appleton Laboratory, Wuhan University of Technology, and Sichuan University.

Co-author, Chair of the Department of Computational Physics of Kazan Federal University Anatolii Mokshin explains, “The key difference between the liquid state of matter and the solid state is the presence of shear stiffness in solids. In other words, solids can retain their shape in contrast to liquids and gases, which take the shape of the vessels in which they are placed. Together with our foreign colleagues, we found out that such an understanding is not entirely correct. We were able to obtain experimental confirmation of the presence of shear stiffness in a liquid. And this means that on a spatial scale comparable to the size of molecules and atoms, a liquid exhibits elasticity and rigidity, like a solid. This is very surprising. In particular, a liquid

at these extremely small scales will respond to external deformation influences like an ordinary solid. The results are obtained for the case of gallium melt. However, they are true for any fluid."

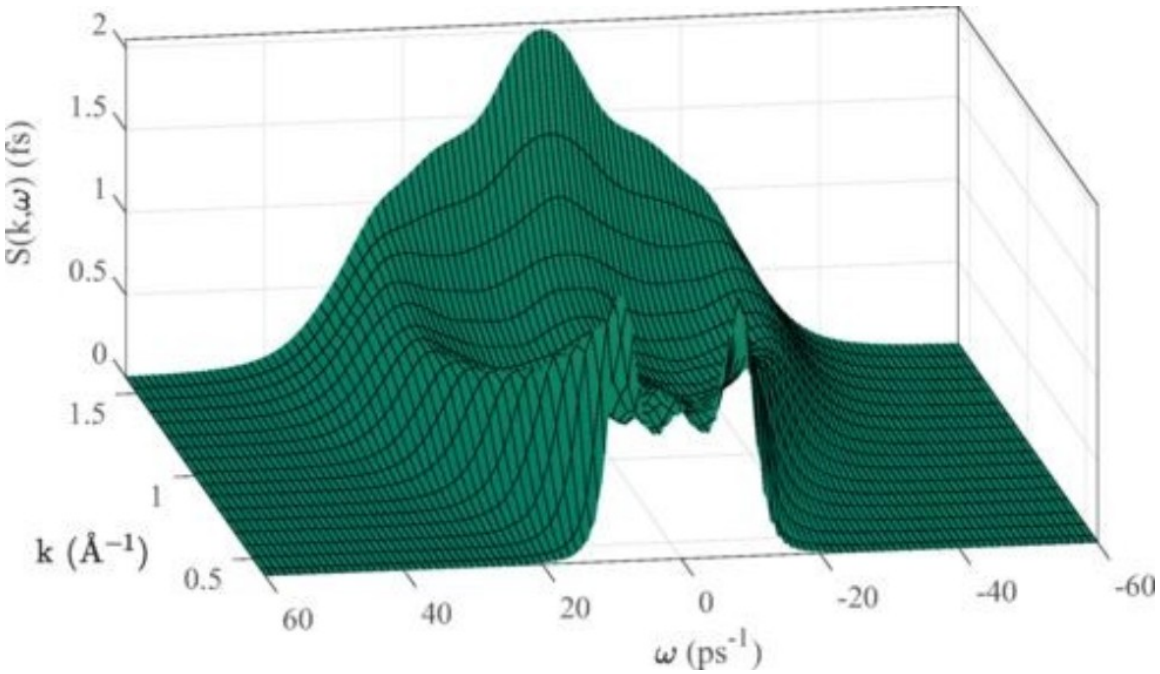


Figure: Dynamic structure factor of liquid gallium calculated from molecular dynamics simulations

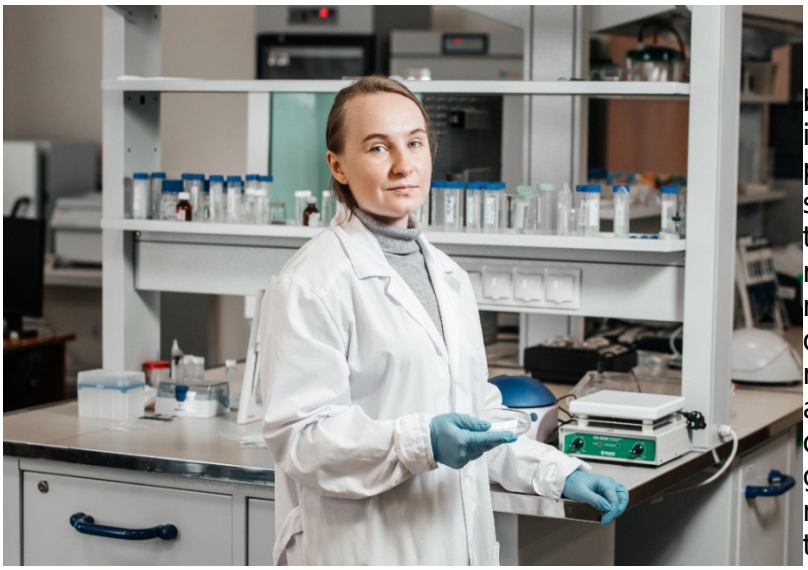
The uniqueness of this work, according to the interviewee, is that for the first time a comprehensive study was carried out, including experiments on inelastic neutron scattering, large-scale molecular dynamics calculations performed by the Kazan University computer cluster and the supercomputer of the Interdepartmental Supercomputer Center of the Russian Academy of Sciences, and a theoretical explanation in the framework of the original self-consistent relaxation theory of the liquid state.

"New data are important for understanding a number of fundamental scientific questions related to liquid state physics. They must be taken into account when designing nanodevices, nanostructures and metamaterials. Firstly, it is now possible to more accurately evaluate the physical parameters of liquids near the solidification temperature and the conditions (temperature and pressure) under which nanostructures can be constructed. Secondly, new possibilities have appeared for controlling liquids confined by nanometer-sized structures. One of the branches of modern physics, nanofluidics, is studying these issues," concludes Mokshin.

9. TPU IMPROVES MATERIALS FOR ORGAN REGENERATION

https://news.tpu.ru/en/news/2020/06/25/36399/

Researchers of Tomsk Polytechnic University proposed a method for improving implants for organ regeneration. New technology can expand the potential of tissue engineering. The results were published in the Surface & Coatings Technology. The detailed information about the research was published by RIA Novosti.



One of the areas of modern biomedicine is the improvement of materials to produce scaffolds. These scaffolds are used as the basis to grow new tissues in regenerative medicine or as a material for targeted drug delivery. The scaffolds with necessary cells or medicines are implanted into the organ damaged areas, where they gradually dissolve, being replaced by the body's own tissues.

Despite the fact that modern scaffolds are completely biocompatible and have good mechanical properties, their application is still limited due to the hydrophobic properties of their materials. Thus, they do not get wet while interacting with water molecules.

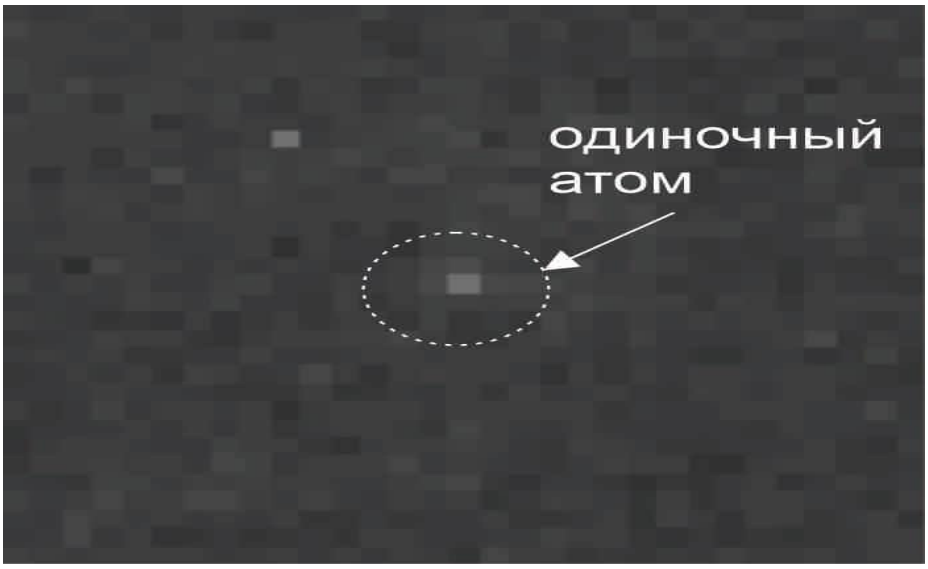
"*This property worsens the attachment of cells and their division and also increases the scaffold decomposition period in the body.*"

Anna Lipovka, a member of the research group, PhD student of the TPU Research School of Chemistry & Applied Biomedical Sciences, says.
The most effective method to increase scaffold hydrophilicity is plasma treatment. However, after a few days, the effect weakens and gradually disappears, worsening the scaffold survival rate.
To improve th properties, TPU team supplemented the plasma surface treatment by applying a thin film of graphene oxide. This nanomaterial has high hydrophilicity, which does not degrade over time.
Comparative tests demonstrated that the processed material retains the necessary hydrophilicity for a sufficiently long time. It is a major achievement in the development of safe implantable materials, which are in great demand by modern reconstructive surgery in the treatment of cardiovascular, oncological and a number of other diseases.

The TPU team plans to study the interaction of new scaffolds with living cells and tissues during implantation. In addition, Imperial College London (UK) and TPU to use laser processing to create an electrically conductive layer that enables monitoring the state of the scaffold in the body.

10. SCIENTISTS OF RZHANOV INSTITUTE OF SEMICONDUCTOR PHYSICS AND NSTU NETI CAPTURED A SINGLE RUBIDIUM ATOM IN AN OPTICAL TRAP FOR A LONG TIME AND PHOTOGRAPHED IT

https://en.nstu.ru/news/news/scientists-of-rzhanov-institute-of-semiconductor-physics-and-nstu-neti-captured-a-single-rubidium-at/



This is one of the necessary steps in creating a domestic quantum computer.

Scientists of Rzhanov Institute of Semiconductor Physics SB RAS, Novosibirsk State University and Novosibirsk State Technical University NETI succeeded in holding a single rubidium atom in an optical tweezers for forty seconds. The scientists registered the atom in the trap by a much cheaper video camera than is usually used for such research, the image being obtained with a long-focus lens. The details of the experiment are presented in the journal "Quantum Electronics".

Single atoms can act as qubits, i.e. elements for storing and transmitting information in quantum computers. These computers are believed to employ accelerated machine learning methods, calculate the behavior of multicomponent systems thus enabling new materials creation, test medications at the molecular level and quickly decode modern data encryption systems.

Trapping a single atom in an optical tweezers or, as it is also called, a dipole trap is the first step to creating an array of qubits and conducting quantum calculations. The array contains many atoms, with each one being held by "its own" optical tweezers. Accordingly, the task is not only to capture atoms, but also to register them correctly.

The electronic states of cold atoms can exist for a few seconds, which is quite a long time in the context of quantum computing; therefore, such atoms are convenient to be used as qubits. About 20 research groups in the world are working with single cold atoms, with two of them in Russia: at Rzhanov Institute of Semiconductor Physics SB RAS and at Lomonosov Moscow State University.

"We solved a complex problem consisting of several tasks: first, we needed to cool the atoms (that is, reduce their speed), this is done using laser beams: the flow of photons

from the laser is absorbed by the atoms and slows them down. Secondly, a single atom must be trapped. This is also performed by laser beam with a very precise focus of several microns: it is the typical size of the spot for holding an atom. And thirdly, we needed to photograph an atom: in a short time of a hundred milliseconds we "registered" infrared photons which the atom emits while trapped, about 1000 photons per second (this is a very small amount and a household video camera will not register them). The conditions of our experiment require that the captured atoms are registered in a short time. Thus they can be used as qubits," explains Ilya Beterov, Senior Researcher at Rzhanov Institute of Semiconductor Physics SB RAS, Associate Professor of the Optical Information Technologies Department, NSTU NETI.

Foreign research groups use highly sensitive scientific EMCCD video cameras with electronic multiplication for registering, but they are expensive.They cost about five million rubles and have not been delivered to Russia since 2015. Novosibirsk physicists worked with a scientific sCMOS video camera of the previous generation which is significantly cheaper (it cost about six hundred thousand rubles).

The scientists were able to achieve impressive results: they reliably registered an atom with a minimum exposure time of 50 milliseconds. This is typical of experiments conducted by researchers in France, Germany, Korea, and other countries using more advanced EMCCD cameras. In recent experiments, the longest time during which Novosibirsk scientists observed a single atom was 40 seconds.

"We had to place the lens of the optical tweezers as far away from the cloud of cold atoms as possible, so that they did not interact with the glass, the dielectric surface. This process can negatively influence the further two-qubit quantum operations experiments. This is why we used a long-focus lens, but as a result, it was more difficult to register the photons emitted by the atom as a smaller number of them gets into the lens when it is far from the atom. In addition, a single atom's emission is rather low, so all of it had to be focused on a single pixel of the camera's matrix. However, it later turned out that if we just try to register a single atom, we see almost nothing against the background of the video camera noise, because the tweezers laser removes the atoms from resonance with the illuminating radiation. In order to solve this problem, we turned off the dipole trap for a very short time, no more than one millionth of a second. During this time a single atom does not have time to leave the trap. We repeated this for several thousand cycles, accumulating the signal during the time when the dipole laser is turned off," adds Ilya Beterov.

According to the researcher's observations, the work of the Novosibirsk team is the first to implement the simultaneous use of a long-focus lens and a sCMOS video camera, and the result may be of interest not only to Russian physicists.

"Foreign research groups can also be underfinanced, and this is important for everyone that a significantly cheaper video camera shows an acceptable result for the experiment," says Ilya Beterov.

The next step of Novosibirsk scientists is to learn how to perform high precision one-cubit operations and turn to two-cubit operations. That is, to put it simply, to "collect" the logical elements of a quantum computer of cold atoms changing the electronic states of the atom and controlling them.

The research is supported by the Russian Science Foundation (Project No. 18-12-00313), as well as by Russian Foundation for Advanced Research Projects.

For the reference: since 2018, Rzhanov Institute of Semiconductor Physics SB RAS has been a member of the scientific consortium whose work is aimed at the development of quantum technologies and in particular at the creation of a domestic quantum computer. The consortium was based at Lomonosov Moscow State University and includes leading universities and research institutes, such as Saint Petersburg State University, Bauman Moscow State Technical University, National Research Nuclear University "MEPhI", the Institute of Solid State Physics RAS, Valiev Institute of Physics and Technology RAS, Prokhorov General Physics Institute RAS, and others.

11. NOVOSIBIRSK SCIENTISTS HAVE DEVELOPED THE WORLD'S FIRST "SMART" PROGRAM FOR VOICE DIAGNOSTICS OF LARYNGEAL DISEASES AND DEPRESSION

https://en.nstu.ru/news/news/novosibirsk-scientists-have-developed-the-world-s-first-smart-program-for-voice-diagnostics-of-laryn/

In early May, specialists of NSTU NETI together with colleagues from NSPU and the phoniatric center developed the world's first system that can diagnose long-term psychoemotional abnormalities often masked by the patient's voice. The system also helps to determine the early stages of the tumors development in the vocal apparatus. In addition to medicine, the system can be used in teaching, social work, security and identification systems.

Scientists from the Novosibirsk State Technical University NETI came to conclusion that psychoemotional disorders can be diagnosed by analyzing sound waves. After years of research, they found that the voice changes were related to psychoemotional disorders. The patented technique allows accurate detecting abnormalities by digital audio processing.

Previuosly, the attempts to create similar voice diagnostics systems were also made abroad. In Russia, such developments were conducted mainly for military purposes.

The scientists of Radio Engineering and Electronics Faculty created the device whose unique feature is the algorithm of the voice signal digital processing. This algorithm finds a correlation between voice changes and psychoemotional disorders of the speaker.

Novosibirsk scientists have confirmed the hypothesis that human speech changes depending on the type of disorder. Thanks to tests conducted on children of the primary school group, experts found a variable in a specially created mathematical model that is responsible for the correlation of the voice with the psychoemotional state. According to scientists, the number of disorders is now growing among both children and adults. This can be anxiety, depression, aggression, or autoagression.

The device performs analysis using an algorithm based on acoustic analysis of the audio signal. A set of test phrases is recorded on a microphone and digitized by a high-resolution sound card. This is how the sound wave is converted into a digital signal. Then the program processes this wave: the algorithm calculates the parameters of high-frequency and low-frequency vibrations, sound power, and builds a curve. The obtained parameters of the studied voice are compared with the reference sample. Based on the differences obtained, the person's psychoemotional state is determined. The system will be easy to use: it only needs a microphone, a specialized audio card and a computer with the software.

"To explain how the program works, let me give you an example. Let's assume that there is a sound parameter X, which in a normal person has a value of 0.2—0.3, and in a person with a clear psychoemotional disorder, it equal 5. From this we can conclude that a person has certain symptoms, for example, autoaggression. This is the correlation we were looking for. Finally we have found it" says Daria Borovikova, a co-author of the development, a young scientist at Radio Engineering and Electronics Faculty.

In addition to psychoemotional diseases, the program can also detect functional disorders of the voice, which can later lead to constant organic changes in the larynx: laryngitis, chorditis, knots and polyps of the vocal chords, laryngeal papillomatosis and other diseases. According to scientists, functional disorders are more difficult to diagnose than organic ones, which can be seen using laryngoscopes and endoscopes. However, they also pose a threat. Such disorders are usually associated with improper use of the vocal apparatus. They often occur in children who begin to incorrectly engage in vocalism at an early age. It is the long incorrect sound reproduction that leads to inflammations.

Previously, psychological disorders and functional disorders in the patient's voice were detected by a specialist exclusively "by ear". The results of such diagnostics were subjective and depended on a particular doctor's competence. "The objective detection of abnormalities in the voice of a patient is a very complex and challenging task. Contacting highly qualified specialists is not always possible. Detection of functional disorders in the voice at early stages allows preventing the diseases," said Olga Fetisova, a leading specialist of the regional consulting and diagnostic phoniatric center, a speech therapist of the highest qualification category.

Other developments based on the use of voice analysis technologies nearly always involved the use of sensors that had to be fixed on the patient's neck. The disadvantage of such methods is the need for contact between the doctor and the patient. It may be impossible, for example, in conditions of self-isolation. Most of the

methods have vulnerabilities related to signal processing technology. The voice analysis system developed by NSTU NETI scientists is devoid of these disadvantages and aims at the remote signal characteristics recognition as well as tracing the changes in the signal.

Another area of the digital voice processing system application may be the sphere of security and military affairs. With additional research, the program will be able to make an examination of the voice in the terrorists and criminals phone conversations. It can also become an additional element in the lie detector and monitor the psychoemotional state of soldiers.

Besides medicine and security, the technology can be used in teaching and social work. In the future, the scientists plan to conduct a number of additional studies and increase the number of subjects. According to Daria Borovikova, creating such an expanded sample will help to adjust the system parameters and make the diagnostic system more accurate.

The scholars involved in the project besides the employees of the NSTU NETI, include the specialists in psychology from Novosibirsk State Pedagogical University and a phonopaedist researching voice and its training. According to Daria Borovikova, it was thanks to the collective work of engineers, a voice specialist and a psychologist that the entire team managed to achieve such results.

The founder of the scientific development is Vladimir Makukha, Doctor of Technical Sciences, Professor of Radio Engineering and Electronics Faculty. For more than 10 years he has been engaged in the voice-speech characteristics objectification. Vladimir Makukha, the Honorary University Worker, died in July 2019. Now the project is being supervised by Oleg Grishin, Professor of Radio Engineering and Electronics Faculty, NSTU NETI, Doctor of Medical Sciences.

12. EFFECTIVENESS OF BLOOD CLOT MEDICINE WAS DOUBLED WITH THE HELP OF A PULSED MAGNETIC FIELD AT SAMARA UNIVERSITY

https://ssau.ru/english/news

Scientists of the Samara National Research University conducts a series of studies on the effects of a pulsed magnetic field (IMP) with the induction of 1-3 Tesla on drugs.

The pentoxifylline drug is being studied, which reduces blood viscosity, preventing blood clots, and increases the concentration of oxygen in tissues (1).

Earlier, an interdisciplinary group of scientists (2) investigated the influence of a pulsed magnetic field on the biological activity of an antibiotic and established the fact of increasing its antibacterial activity using microorganisms of the genus Escherichia coli. Research was continued on another drug that is an antiplatelet agent - pentoxifylline. Experiments to study anti-aggregation activity were performed in vitro on the blood of healthy donors. The experimental results are reflected in the journals Butlerov Communications (3) and Actual Problems of Biological Physics and Chemistry (4).

"It was found that a pulsed magnetic field almost doubles the antiplatelet activity of pentoxifylline, that is, the blood viscosity decreases by half, which can significantly affect the process of thrombosis," said the design engineer of the “Progressive plastic deformation research laboratory” (NIL-41) Natalia Rodenko.

The safety of irradiated UTI pentoxifylline was tested on mice. The treated medicine was examined for the formation of free radicals by chemiluminescence. No harmful effects from UTI exposure were detected.

The main attention is paid to the study of the mechanism of such a significant change in the biological activity of drugs. Drugs affected by a pulsed magnetic field are inhibitor substances. Acting by the same mechanism, they can change the affinity for the active center of the enzyme upon irradiation.
Scientists have studied the duration of irradiating exposure on drugs. “We wondered how long the effect of irradiating the preparations with a pulsed magnetic field lasts, and we conducted such studies. It was found that the effect of exposure to UTIs lasts from three hours to one day depending on the intensity of the irradiation,” explained the assistant professor of biochemistry and biotechnology and bioengineering Tatyana Vasilieva.

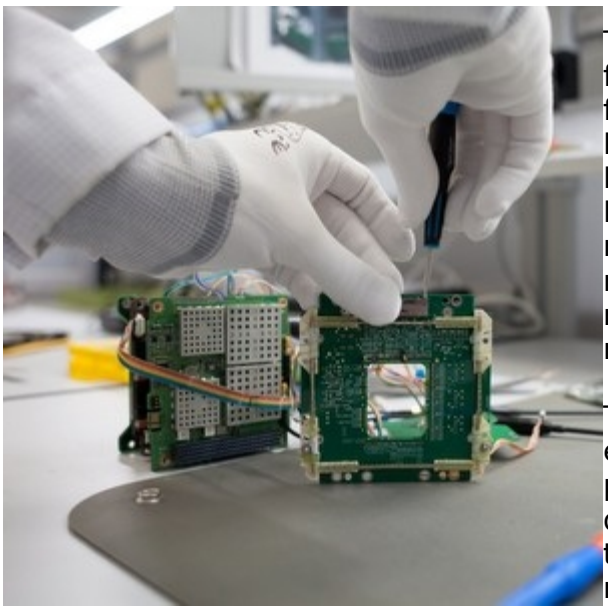
Now scientists are preparing to conduct additional experiments to study the effect of excipients on the biological activity of medicines. It was agreed that experts from the Chemistry Department will help to conduct such experiments.

In parallel with the study of pentoxifylline under the grant, it is planned to continue work on the effects of UTI on antibiotics. The grant was allocated by the Foundation for the Promotion of Innovations - at the end of April Natalia Rodenko became the winner of the project contest for the UMNIK program.

"In the process of work on the grant, it is planned to conduct experiments on the study of substrate-binding constants for enzymes. We will study the antibacterial activity of a pure antibiotic substance without auxiliary substances after exposure to UTI, and study the biological activity and time of effect maintenance when the antibiotic is irradiated using microorganisms of the genus Staphylococcus," informed Natalia Rodenko. According to her, it is also planned to develop a technology for the irradiation of drugs to increase their biological activity. Magnetic-pulse installation (MIU) "Bio" for the irradiation of drugs has already been created on the basis of NIL-41 of Samara University.

13. SCIENTISTS FROM RUSSIA AND BELARUS WILL DEVELOP WAYS TO STUDY THE EARTH'S IONOSPHERE USING GPS AND GLONASS SIGNALS

https://ssau.ru/english/news



The research team, consisting of scientists from Samara University and the Joint Institute for Informatics Problems of the Belarus National Academy of Sciences (OIPI NAS of Belarus) will develop methods for studying the Earth's ionosphere using nanosatellites. As a means of research, scientists suggest using navigation receivers of signals from satellite radio navigation systems located on nanosatellites.

The ionosphere is the upper layer of the earth's atmosphere saturated with charged particles, the concentration of which, depending on the activity of the Sun, affects the propagation of radio waves and has a noticeable effect on the performance of technical systems.

The project is intended at developing methods and tools for processing and converting information from GLONASS and GPS systems, used for building dynamic models of the ionosphere state. Solving this problem is important for predicting possible interruptions in the operation of radio communication systems, as well as correcting errors and improving the accuracy of positioning systems on Earth. In addition, understanding the nature of physical processes in the ionosphere opens up possibilities for creating new promising technologies for transmitting information.

The project's supervisor from the Samara University was the head of the space research interuniversity department, doctor of technical sciences, professor Igor Belokonov, and professor Alexander Krot doctor of technical sciences, the head of the modeling self-organizing systems laboratory from the Institute of Applied Mathematics, Belarus National Academy of Sciences.

"The study of wave processes and identification of local fluctuations in the density of electron concentration will be carried out, which will expand knowledge of ionosphere mechanisms and processes. This is the first joint project of Russia and Belarus scientific communities, which will be implemented at Samara University. Work on this grant will be in demand implementing the project of a consortium of Russian universities aimed at creating a group of nanosatellites for studying the ionosphere, organized by Samara University," said Igor Belokonov.

As previously reported, the consortium of Russian universities aimed at creating a group of nanosatellites for monitoring the ionosphere includes eight universities, the Institute of Physics of the Earth of the Russian Academy of Sciences, and a number of Skolkovo residents. The satellite constellation should include at least four spacecrafts. According to the plan of the consortium participants, nanosatellites will be able to simultaneously measure at different points in the near-Earth space, revealing anomalies in the ionosphere and magnetosphere.

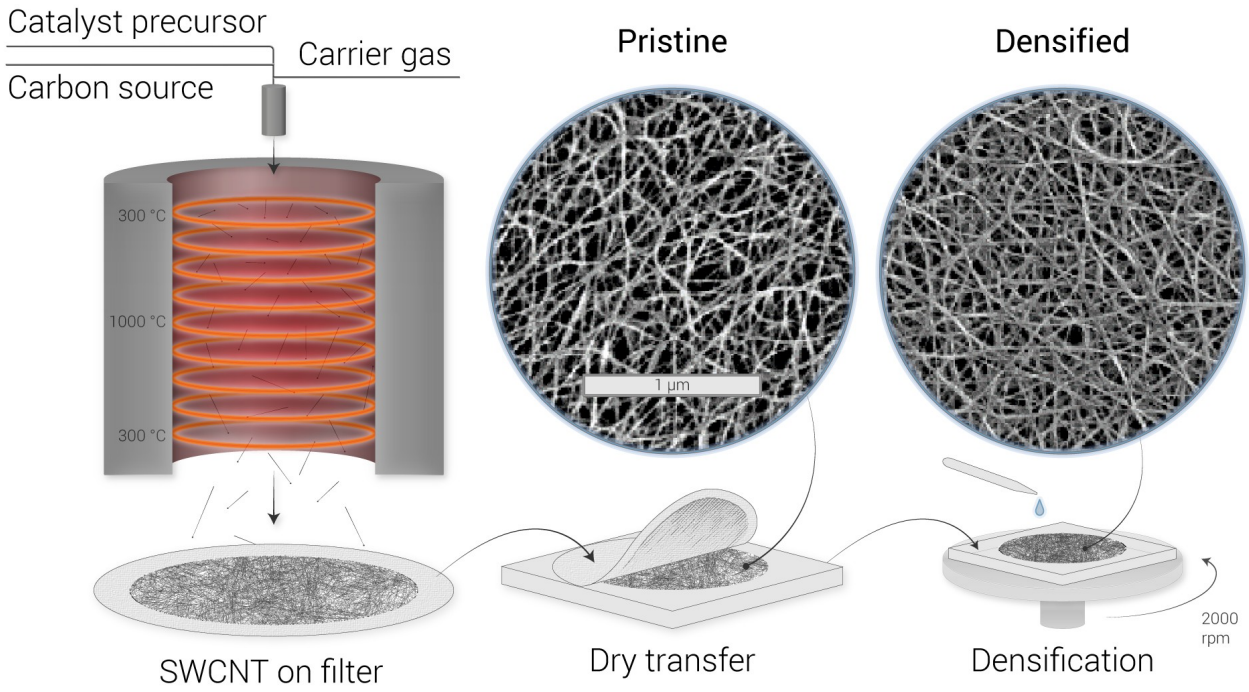
INNOVATIVE PRODUCTS AND SOLUTIONS FROM A LEADING RUSSIAN INSTITUTE- SKOLTECH

1. NO TOUCHING: SKOLTECH RESEARCHERS FIND CONTACTLESS WAY TO MEASURE THICKNESS OF CARBON NANOTUBE FILMS

https://www.skoltech.ru/en/2020/06/no-touching-skoltech-researchers-find-contactless-way-to-measure-thickness-of-carbon-nanotube-films/

Scientists from Skoltech and their colleagues from Russia and Finland have figured out a non-invasive way to measure the thickness of single-walled carbon nanotube films, which may find applications in a wide variety of fields from solar energy to smart textiles. The paper was published in the journal Applied Physics Letters.

A single-walled carbon nanotube (SWCNT) is essentially a sheet of graphite one atom thick that is rolled into a tube. They are an allotrope (a physical form) of carbon, much like fullerenes, graphene, diamond, and graphite. SWCNTs hold a lot of promise in various industrial applications, ranging from solar cells and LEDs to ultrafast lasers, transparent electrodes, and smart textiles.



Preparing SWCNT films for the experiment. Credit: Pavel Odinev / Skoltech

All these applications, however, require rather precise measurements of SWCNT film thickness and optical properties. “Film thickness is quite important for many applications and usually characterised by how much light can be transferred through the film in the visible spectral range: the higher the transparency, the less the thickness of the film. However, precise control over film thickness and optical

constants is critical when one needs to design efficient transparent electrodes. For instance, we need to know the thickness to improve antireflection properties of the surface based on transparent SWCNT window layer for solar cells. To estimate and subsequently utilize the mechanical properties of SWCNT films, we need to predict the geometrical dimensions of the films," says Professor Albert Nasibulin, head of Laboratory of Nanomaterials at Skoltech Center for Photonics and Quantum Materials
Existing methods for optical constant measurements include absorption and electron energy-loss spectroscopies, while geometric parameters can be determined by transmission electron microscopy, scanning electron microscopy or atomic force microscopy. These methods are resource-inefficient and require sample preparation, which might affect the very properties of SWCNT films that one is trying to measure.

A team of researchers led by Albert Nasibulin of Skoltech and Aalto University was able to design a rapid, contactless, and universal technique for accurate estimation of both SWCNT film thickness and their dielectric functions. They figured out a workaround to use spectroscopic ellipsometry (SE), a non-destructive, fast, and very sensitive measurement technique, for SWCNT films.

"*Ellipsometry is an indirect method that we can use to determine film parameters, and standard methods of data processing are not always applicable here. At first glance, a carbon nanotube thin film is a very difficult object for this technique: consisting of many millions of randomly oriented nanometer-sized individual and bundled tubes, it has strong absorption in the entire spectral range, low reflection and anisotropy in its optical properties. Nevertheless, the first author of the paper, Georgy Ermolaev, a student of a joint Skoltech-MIPT Master's program, has found an elegant algorithm to retrieve the thickness and optical constants in a single set of optical measurements," says Yuriy Gladush, one of the coauthors of the paper.*

The researchers manufactured SWCNT films of varying thickness and absorption between 90% and 45% at 550 nm and determined the broadband (250–3300 nm) refractive index and corresponding thickness of the films.

"*It was expected that optical properties would depend on the density of packaging of the carbon nanotubes in the film, but the surprise was in how large this effect is. A single droplet of ethanol can compress or densify the film and change the refractive index from 1.07 to 1.7, opening simple opportunities to adjust the optial properties of the SWCNT films," Albert Nasibulin adds.*

The team believes other scientists can build on their work and, among other things, use their approach beyond the realm of carbon nanotubes for other kinds of these structures. Other organisations involved in this research include the MIPT Center for Photonics and 2D Materials, GrapheneTek and Canatu Ltd.

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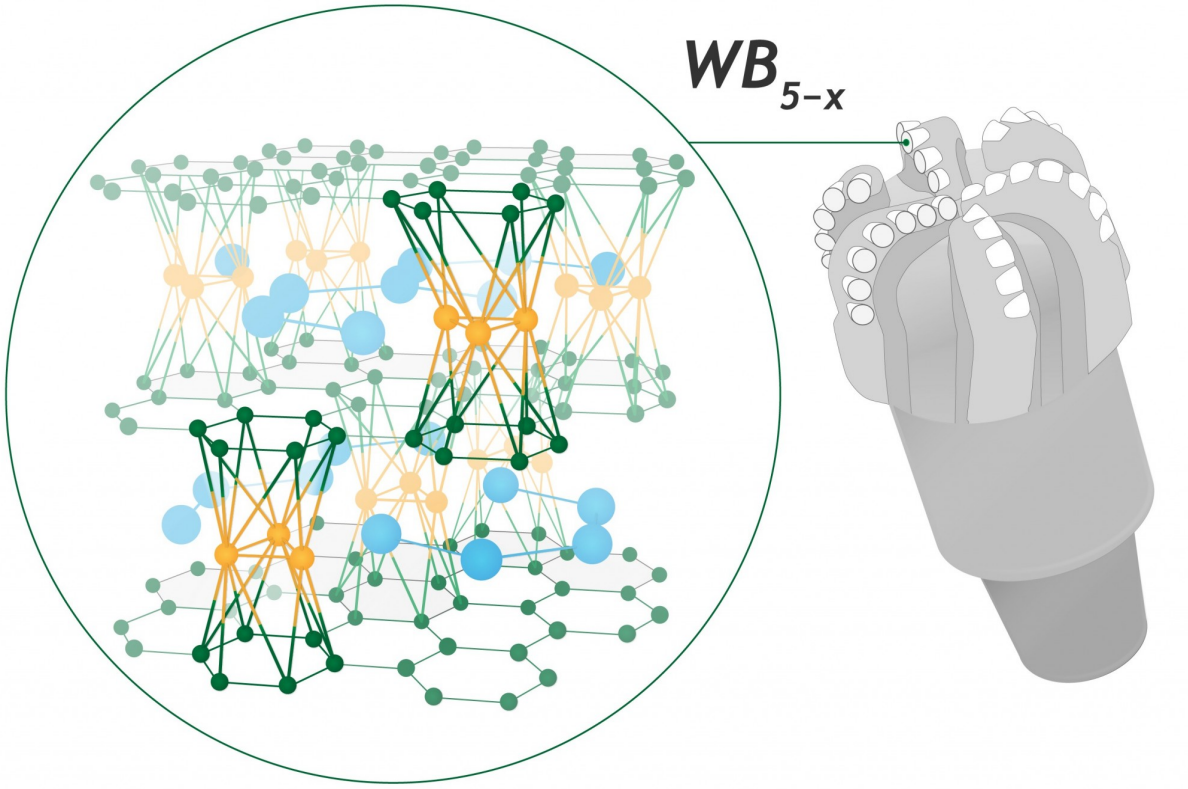
2. SKOLTECH RESEARCHERS SOLVE A 60-YEAR-OLD PUZZLE ABOUT A SUPERHARD MATERIAL

https://www.skoltech.ru/en/2020/07/skoltech-researchers-solve-a-60-year-old-puzzle-about-a-superhard-material/

Skoltech researchers together with their industrial colleagues and academic partners have cracked a 1960s puzzle about the crystal structure of a superhard tungsten boride that can be extremely useful in various industrial applications, including drilling technology. The research, supported by Gazpromneft Science & Technology Center, was published in the journal Advanced Science.

Tungsten borides first captured the imagination of scientists in mid-twentieth century due to their hardness and other fascinating mechanical properties. One long-standing puzzle has been the crystal structure of the highest W-B phases, the so-called “WB4”, which varied wildly between experimental models and theoretical predictions.



Researchers have cracked a 1960s puzzle about the crystal structure of a superhard tungsten boride. Credit: Pavel Odinev / Skoltech

“Experimentally, the crystal structure is determined by X-ray structure analysis. But the large difference in atomic scattering cross sections (heavy tungsten compared to light boron) renders positions of boron atoms in transition metal borides hardly discernable by X-ray diffraction. This can be resolved by neutron diffraction, but any diffraction method can only give the average structure. If the material is disordered, the complete knowledge of its crystal structure (including local arrangement of the atoms) can be obtained only using a combination of experimental techniques (X-ray, neutron diffraction) and computational methods of materials science,” Alexander Kvashnin, Skoltech senior research scientist and first author of the study, explained.

In 2017, Andrei Osiptsov and Artem R. Oganov at Skoltech proposed an idea to search for superhard materials to be used for producing composite cutters installed on bits, which are used for drilling oil and gas wells. The idea was well received by Gazpromneft STC LLC, and the collaboration began between the company, Skoltech, and the Vereshchagin Institute for High Pressure Physics of the RAS. Researchers led by Artem R. Oganov of Skoltech and MIPT predicted the existence of WB5, tungsten pentaboride, which was expected to be harder than the widely used tungsten carbide and having comparable fracture toughness. The compound was successfully synthesized in the lab at Vereshchagin Institute to complete the research loop. In the new paper, Oganov and his colleagues show that the long-debated "WB4" and the newly predicted WB5 are actually the same material.

"*We studied the W-B system in order to predict stable structure of higher tungsten borides as we had already known about this long-standing puzzle. Predicting a new WB5structure was a surprise, especially as it has exciting properties as high Vickers hardness and fracture toughness and remains stable at very high temperatures. Then we thought this material should find application in the industry. Our colleagues from the Vereshchagin Institute successfully synthesized it. The diffraction patterns matched theoretical prediction very well, except a few weak peaks that were present in theory, but not in the experiment. Our predicted WB5 has perfect single crystal structure, but as we showed, experiments produced a closely related disordered WB5-x material," Kvashnin explained.*

The researchers synthesized this new material, measured its properties, and revealed an unexpected connection between the two compounds: the new material has a crystal structure derived from the WB5 structure, with some amount of disorder and nonstoichiometry (this means that proportions of its elemental composition cannot be represented by a ratio of small integer numbers). Thus, the new material was denoted not as WB4 but as WB5−x. Its crystal structure was utlimately predicted by USPEX, an evolutionary algorithm developed by Oganov and his students, and elaborated by a microscopic lattice model.

Since WB5-x is relatively easy to synthesize, its excellent mechanical properties and stability at high temperatures make it a very promising material for many technologies where tungsten carbide-based composites dominated in the last 90 years.

"*This puzzle is solved in full detail. We have a detailed microscopic description of this material and its structure, we know the range of chemical compositions it can adopt, and its properties. Other exciting puzzles are waiting for theorists' attention," said Artem R. Oganov.*

Other organizations involved in this research include A. M. Prokhorov General Physics Institute of RAS and Vereshchagin Institute for High Pressure Physics of RAS.

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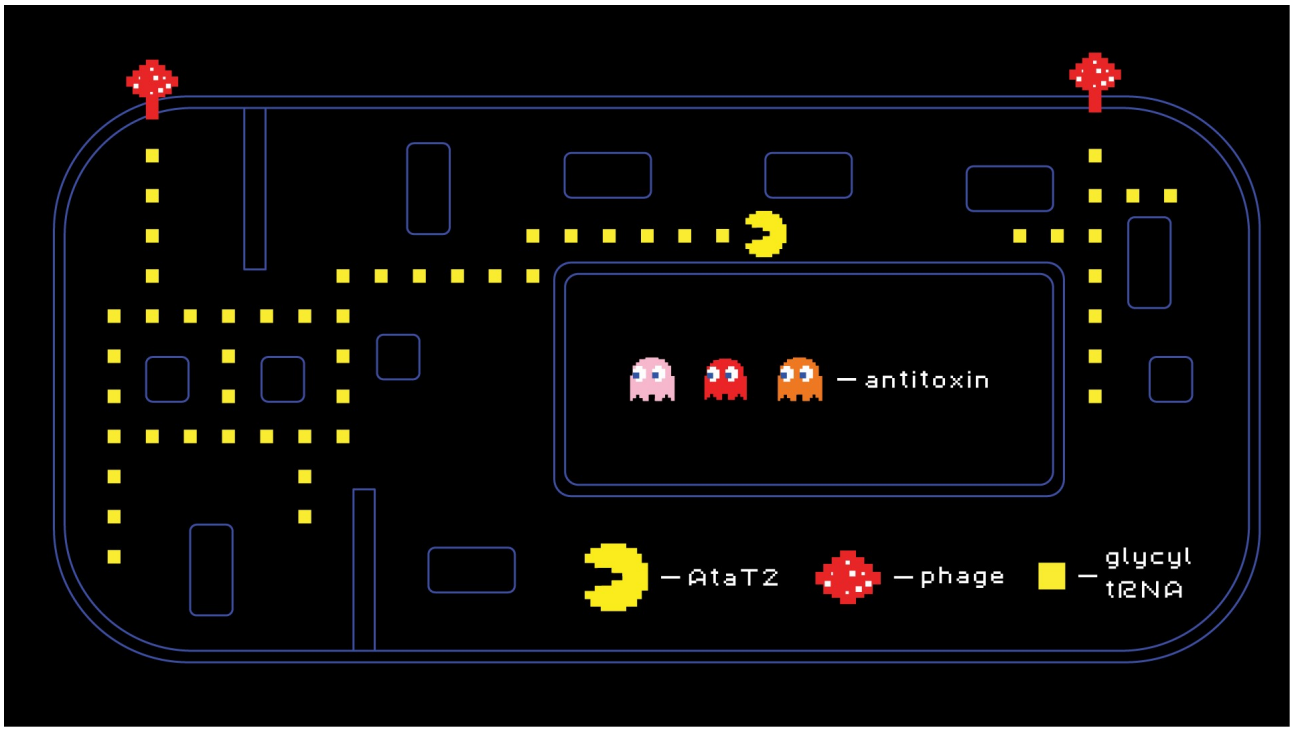
3. VIRUSES BEWARE: SCIENTISTS SHOW HOW BACTERIAL 'ATTACK DOG' TOXIN DISRUPTS PROTEIN SYNTHESIS

https://www.skoltech.ru/en/2020/07/viruses-beware-scientists-show-how-bacterial-attack-dog-toxin-disrupts-protein-synthesis/

A team of Skoltech researchers from the Severinov laboratory and their colleagues have identified the way in which a component of a two-part bacterial self-defense system from the toxin-antitoxin family works, leading to cell dormancy that helps fight off bacterial viruses, antibiotics and other insults. The paper was published in the journal Nucleic Acids Research.



A team of Skoltech researchers and their colleagues have identified the way in which a component of a two-part bacterial self-defense system from the toxin-antitoxin family works. Credit: Pavel Odinev / Skoltech

Toxin-antitoxin systems are a class of multipurpose mechanisms that bacteria can use, among other things, against phage infections. Two adjacent genes encode two proteins, a toxin disrupting various cellular processes and an antitoxin that inhibits the toxin's activity. Much like Fluffy the three-headed dog from the Harry Potter series, the toxin is "dormant" while the music is playing (i.e. while the antitoxin is present), but under stress conditions — say, when a bacteriophage attacks — the antitoxin is no longer produced and the toxin is "unleashed", disrupting protein synthesis needed for viral replication.

"*Toxin-antitoxin systems are very widespread in bacteria, and many people tried to answer what their raison d'être is, why they exist. The answer appears to be elusive, and the story of assigning biological function to these systems is full of drama, retraction of papers and the like. The answer may be the childish "just because": they may be selfish elements concerned with their own propagation more than with the well-being of the cell, which, however, does not make these systems less interesting*

to study or reduce the knowledge about their function to practice," says Konstantin Severinov, Skoltech professor and a coauthor of the paper.
There are various types of toxin-antitoxin systems, which are classified depending on how exactly the antitoxin blocks the toxin. Though thousands of these pairs have been predicted with the help of bioinformatics, only a handful has been thoroughly characterized. Many toxins are ribonucleases that degrade RNA, but some have different activities.

A team of researchers led by Severinov and Svetlana Dubiley of Skoltech Centre for Life Sciences studied AtaT2, a representative of a rare class of toxins called GNAT (for Gcn5-related N-acetyltransferase). They show that this toxin disrupts translation, or the synthesis of proteins by the ribosome, by targeting transfer RNAs for glycine, a common protein-building amino acid.

The scientists modified E. colito express the toxin-antitoxin system genes on demand and then conducted in vivo tests to determine how the toxin works by observing the behavior of intoxicated cells. They also performed in vitro analysis and, by combining the two, found that the toxin interferes with translation by stalling ribosomes at the glycine codons in the protein encoding sequence, so that most of them are unable to complete the process and build a protein.

Interestingly, the antitoxin counterpart of AtaT2 does not have any glycyl residues for the toxin to target, so its synthesis is unaffected by the toxin. The researchers speculate that this might be a built-in feedback loop preventing too much AtaT2 from being produced and helping cells recover from its toxic action.

If the hypothesis about the essentially selfish nature of toxin-antitoxin systems is correct, one can imagine that different systems compete with each other for their hosts, the bacteria they inhabit. If so, the targets of related toxins should diverge with time. The Severinov team hypothesizes that GNAT toxins may thus diversify to target transfer RNAs specific for each of the 20 genetically encoded amino acids.

"*If that is true, a panel of such toxins, whatever their biological function may be, can provide a powerful tool to control each of the elemental steps of protein synthesis inside the cell and may lead to development of powerful new antibiotics," Severinov notes.*

Other organizations involved in this research include the RAS Institute of Gene Biology, Lomonosov Moscow State University, University of Illinois, Rowan University School of Osteopathic Medicine, and Waksman Institute for Microbiology.

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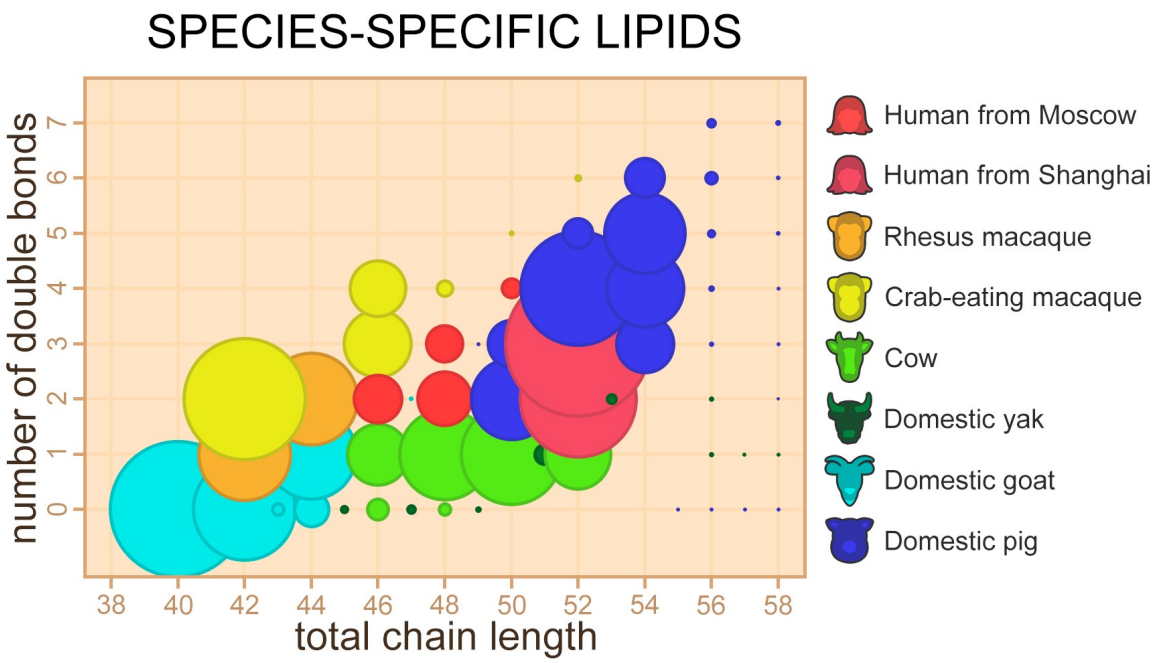
4. MILK LIPIDS FOLLOW THE EVOLUTION OF MAMMALS

https://www.skoltech.ru/en/2020/07/milk-lipids-follow-the-evolution-of-mammals/

Skoltech scientists conducted a study of milk lipids and described the unique features of human breast milk as compared to bovids, pigs, and closely related primates. Their findings could be indicative of co-evolution of milk composition and the specific needs of the developing organism. The study was published in BMC Evolutionary Biology.



Credit: SkoltechMilk is a source of nutrients for growth and development of all mammals. Its composition can adjust to the needs of the baby's organism depending on the habitat, physiology, and reproductive strategy. The main lipids in milk − triglycerides − are composed of three fatty acids and show high diversity depending on the lactation stage, season, and the mother's diet. The baby's body uses fatty acids both as a source of energy and as building blocks for cell membranes, which is particularly important for the brain. Thus, the evolution of milk composition could occur concurrently with the evolution of the brain, and interspecific differences in mammalian milk are of special interest to scientists.

Researchers from Philipp Khaitovich's lab at Skoltech conducted mass spectrometric analysis of milk lipid samples of humans, two species of macaques, cows, pigs, goats and yaks, and made comparisons for their 472 components. The differences in the lipid composition were then compared to the known evolutionary distances between the species, and the majority of samples displayed a good match, except for pig milk. The analysis of triglycerides showed that saturated and monounsaturated fatty acids prevail in the milk of even-toed mammals, while primate milk is rich in unsaturated fatty acids. Pig milk contains a large amount of polyunsaturated fatty acids, which may be indicative of the adaptation to the short lactation period. Human milk, unlike primate milk, also contains a lot of polyunsaturated fatty acids. As both primates and humans have rather long lactation periods, scientists attribute the differences in milk composition to increased needs of the more complex human brain. Polyunsaturated

fatty acids, especially omega-3 and omega-6, mostly come from food and are known to play an important role in the functioning of the nervous system.
"This is the first study that describes lipid composition of milk of seven mammalian species, including humans and primates. Our results show that milk composition differs not only between primates and cows, which was to be expected, but also between humans and monkeys. This means that breast milk is evolving, with its composition reflecting the changing needs of the entire body and the extensively growing brain. As the next step, we want to compare the interspecific differences in the composition of milk and brain," says Aleksandra Mitina, the first author of the paper.

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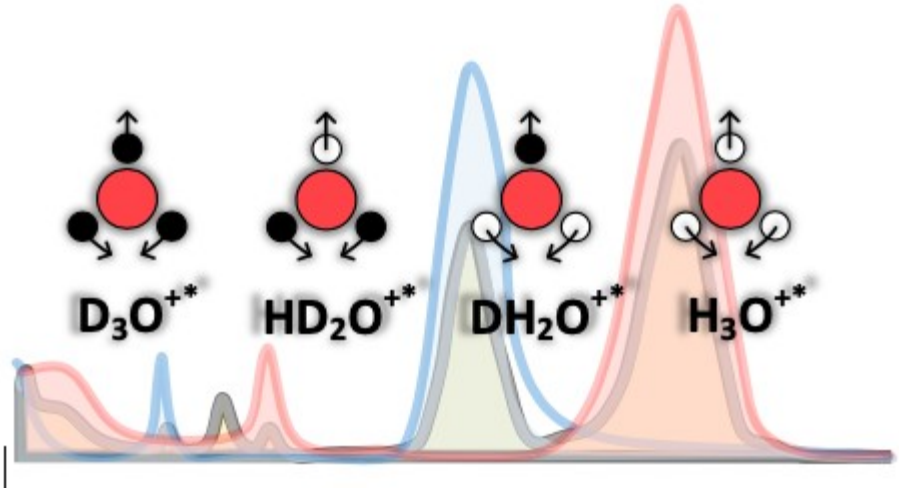
5. LIQUID WATER IS MORE THAN JUST H2O MOLECULES

https://www.skoltech.ru/en/2020/07/liquid-water-is-more-than-just-h2o-molecules/

Skoltech scientists in collaboration with researchers from the University of Stuttgart showed that the concentration of short-lived ions (H3O+ and OH-) in pure liquid water is much higher than that assumed to evaluate the pH, hence significantly changing our understanding of the dynamical structure of water. The results are published in Scientific Reports.



Infrared spectra of light (red), heavy (blue), semiheavy (gray) water, and ionic species that have been identified in the current study. Red, white and black circles depict oxygen, hydrogen and deuterium atoms, respectively. Arrows show the directions of species vibrational deformation Intrinsic ionic species of liquid water play an important

role in the redox processes, catalytic reactions and electrochemical systems. A low-barrier tunneling of hydrogen atom between the H2O molecules, caused by nuclear quantum effects, is expected to generate short-lived excess proton states. However, to date, there has been no information on the concentration of such excess protons states in pure water.

Skoltech scientists in collaboration with German researchers measured the ion-molecular composition of liquid water on the sub-picosecond time scale. The result surprised scientists as they observed that up to several percent of H2O molecules were temporarily ionized.

“We used water isotopologues: ordinary (H2O), heavy (D2O), and semi-heavy (HDO) water, to identify excess-proton states. By gradually substituting the hydrogen atoms (H) with deuterium (D), we changed the relative concentration of excess-proton-related species, such as HD2O+, DH2O+, H3O+ and D3O+, and identified their contributions to the cumulative infrared absorption. We found concentration-dependent spectral features near molecular bending modes of semi-heavy water spectra that no known model was able to explain. We associated these features with excess protons that may be expected to exist on the picosecond time scale,” said one of the co-authors, Prof. Henni Ouerdane from the Skoltech Center for Energy Science and Technology (CEST).

“While previous studies of water structure were based on crystallographic experiments, and did not reflect the dynamics of water, our research brings new insights into the intricate water structure at ultra-short time scale. The finding anticipates new effects of electric field interaction with water, as well as other anomalous properties of water,” concluded the lead author, Dr. Vasily Artemov, Senior Research Scientist at CEST.

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LEADING RUSSIAN TECHNOLOGY GROUPS

RUSNANO Group

Russia has been making rapid advances in the Nano-Tech domain and a few of the leading innovations and solutions have emerged from Russia. RUSNANO Group is the coordinator of innovation activities of the national nanotechnology network of the Russian Federation since 2007, and has developed around 115 portfolio companies (https://en.rusnano.com/portfolio/companies).

Fund for Infrastructure and Educational Programs

The Fund for Infrastructure and Educational Programs was founded during the reorganization of the Russian Corporation of Nanotechnologies. It stimulates nanotechnology infrastructure building to support innovation in the country. The Fund for Infrastructure and Educational Programs primarily focuses its activity in these areas:

- Formation of infrastructure for nanotechnology
- Development of human resources for the nanoindustry
- Market development for nanotechnology products
- Improvement of the legislative framework for innovation
- Standardization and certification of nanoproducts and evaluation of their safety
- Refinements in metrology
- Popularization of nanotechnology and nano-enabled products.

Technology Infrastructure: Nanotechnology Centers

Nanotechnology centers (nanocenters) are an indispensible element of infrastructure for developing Russia's nanoindustry. They incubate start-ups and prepare small innovative companies for market entry. The day-to-day functions of the nanocenters include:

- Engineering development for nanotech products, experimentaldesign and experimental-technological work for commercial customers
- Intellectual property protection
- Management, patent, and marketing support to small innovative companies
- Technology licensing
- Testing and obtaining product certifications.

Nanocenters are organized to attract private capital. They offer opportunities for profitable investment thanks to the division of each center into three independent business units:

- A center for technology transfer
- A property asset, the physical space of the building
- A property asset, the equipment.

Nanocenters are selected through tenders organized by the Fund for Infrastructure and Educational Programs. The following centers are in operation :

- Multifunctional nanotechnology center DUBNA, Moscow Oblast
- Nanotechnology center Zelenogradskiy, Moscow
- Nanotechnology center SIGMA.Novosibirsk, Siberia
- Nanotechnology center SIGMA.Tomsk, Siberia
- Nanotechnology center Ulyanovskiy, Ulyanovsk
- Nanotechnology center TechnoSpark, Troitsk, New Moscow
- Center for Nanotechnologies and Nanomaterials, Saransk
- Nanotechnology Center of Composites, Moscow
- Nanotechnology center T-Nano, Moscow
- Northwestern Nanotechnology Center, St. Petersburg
- Nanotechnology center Idea, Kazan, Republic of Tatarstan
- Nanotechnology center Samarskiy, Samara Region

Technology Infrastructure: Engineering Companies

Engineering companies develop technology and instruments and product prototypes on contract basis, using their own facilities and equipment to devise solutions for specific customers.

Engineering companies differ from manufacturing projects whose goals are to produce and sell products in the mass market. The work of an engineering company is usually unique for each customer and does not go into replication.

Many companies were awarded rights to enter into investment agreements for engineering projects with the Fund for Infrastructure and Educational Programs, namely :

- Institute for Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow Oblast
- Smart Engineering, Moscow
- Noncommercial partnership Center for Innovative Energy Technology, Moscow.

Educational Programs

The educational projects and programs of the Fund are focused on the development of human resources for the nanoindustry.

The development of further training programs for engineers and senior executives of nanotechnology companies, in line with the development of new technologies, is one of the major areas where the Fund interacts with the labour market. The scope of the programs is defined by the companies in accordance with their actual human resources needs. The educational programs have modular structure, and they consist of distance training programs, virtual simulators and training systems that ensure the minimum interruption of the work activities of trainees.

The Fund develops the professional standards for advanced engineering professions in nanoindustry—the regulations that can be used by nanotechnology companies as qualifying standards for professional training of experts. Those professional standards are also used as the basis for independent qualification assessment of engineers and

technical personnel of the companies and graduates. The Fund develops the tests and learning activities for “professional exams”.

The Fund also arranges for the events designed to improve the image of scientific, engineering, technology and business activities among children and young people. Those events include RUSNANO School League designed to promote quality reforming of the natural science education in Russian schools. The Fund holds on regular basis the scientific and practical conferences; competitions; Nanograd vacation summer school; online academic competition “Nanotechnology—Breakthrough to the Future!” for school students, undergraduates, postgraduates and young scientists as pertaining to nanosystems, nanomaterials and nanotechnology; all-Russia national school Week for High Technology and Hi-Tech Business.

Geographical Focus

Investment funds of RUSNANO Management Company invest in both Russian and foreign companies for the purpose of technology transfer to the Russian Federation and/or promoting the development of export potential of Russia’s high-tech sector.

New Investment Funds

Launching and managing new investment funds with participation of RUSNANO

- “Green” energy: Wind Development Investment Fund, First Ecological Fund
- Innovations in Israel: CIR Tech Venture Fund
- Russian-Chinese Growth Fund
- European Venture Capital Fund Rusnano Sistema SICAR
- Chemical Development Fund RUSNANO-SINTEZ
- Far Eastern Fund for Development and Introduction of High Technologies

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