



XXII MENDELEEV CONGRESS  
ON GENERAL AND APPLIED CHEMISTRY

# BOOK OF ABSTRACTS

IN 7 VOLUMES

VOLUME 3

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Federal Territory "Sirius", Russia



**XXII MENDELEEV CONGRESS  
ON GENERAL AND APPLIED CHEMISTRY**

*Dedicated to the 190<sup>th</sup> anniversary  
of D.I. Mendeleev and the 300<sup>th</sup> anniversary  
of the Russian Academy of Sciences*

**BOOK OF ABSTRACTS**

**Volume 3**

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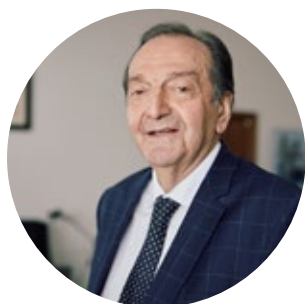
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# CONTENT

## SECTION 7

### **CATALYSIS IN SCIENCE AND INDUSTRY 11**

Keynote lectures	12
Invited lectures	15
Oral lectures	30
Poster session	72

## SECTION 8

### **POLYMERS AND POLYMERIC MATERIALS**

### **(INCLUDING 2ND INTERNATIONAL SYMPOSIUM**

### **"MODERN TRENDS IN DENDRIMER CHEMISTRY**

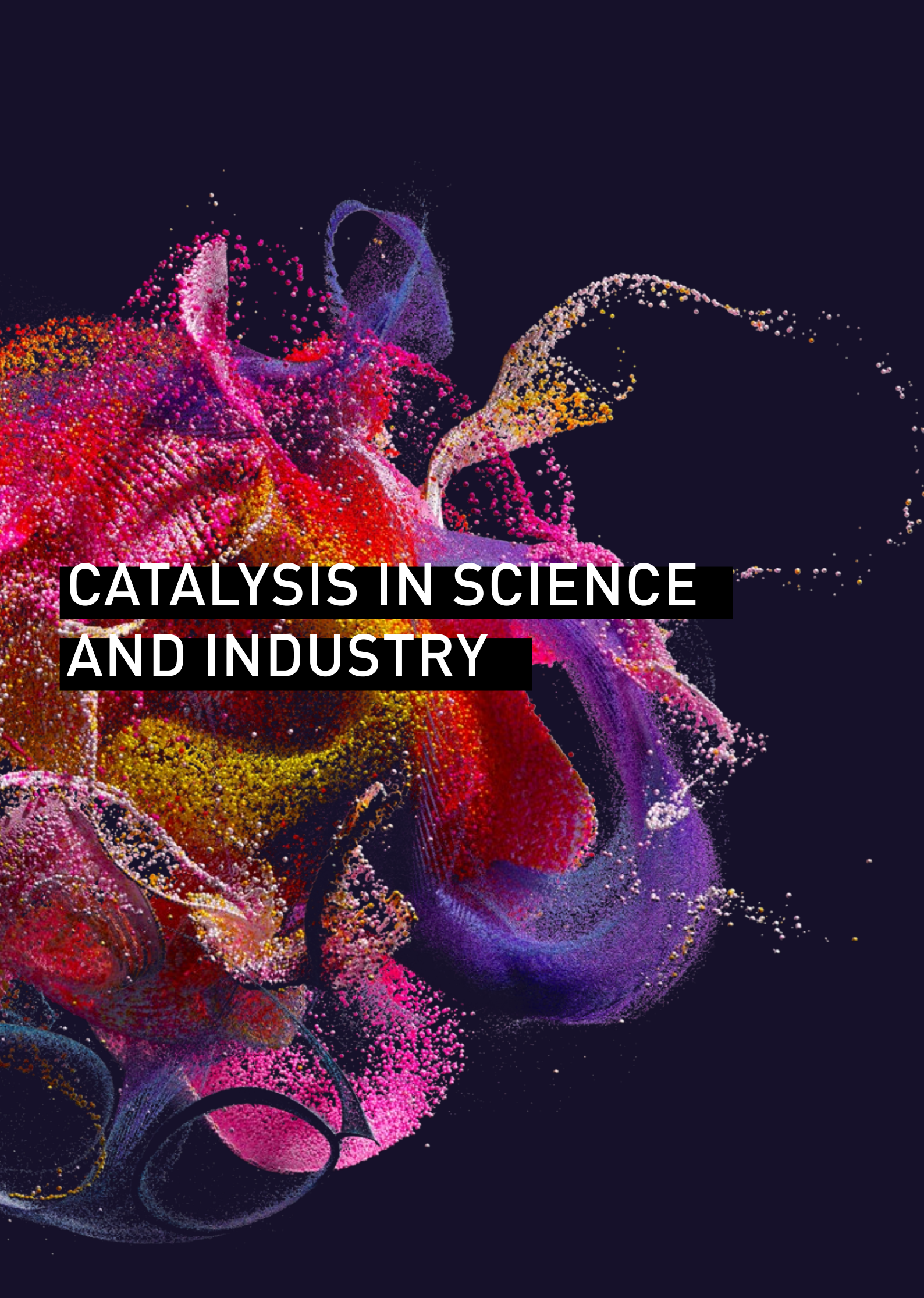
### **AND APPLICATIONS") 125**

Keynote lectures	126
Invited lectures	130
Oral lectures	146
Poster session	170

## SECTION 9

### **CHEMICAL EDUCATION 271**

Keynote lectures	272
Invited lectures	276
Oral lectures	286
Poster session	317



# CATALYSIS IN SCIENCE AND INDUSTRY

# ADSORPTION-INDUCED SEGREGATION AS A TOOL FOR DRIVING CATALYTIC PERFORMANCE OF Pd-BASED BIMETALLIC CATALYSTS

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Bimetallic nanoparticles are of great interest for contemporary research, including the field of heterogeneous catalysis. It is well known that the introduction of a second metal into a system leads to modification of the electronic and structural properties of the active component with respect to the monometallic counterpart, and therefore to improved catalytic properties in a number of industrially important reactions. The surface structure can be purposefully tuned using adsorbate induced segregation by applying specific treatments to a catalyst by heating it in a specially adjusted gas atmosphere at a certain temperature. Hence, the segregation effects could be used as tool for fine-tuning the active sites structure on a catalyst surface.

In the present lecture the nature of the segregation processes for two types of systems: the substitutional solid solutions (Pd-Au, Pd-Ag) and intermetallic compounds (Pd-In) is considered, and the possibility of their use for structure of active sites “fine-tuning” on the surface of catalysts is demonstrated. Finally it was shown using XPS, DRIFTS CO, and catalytic tests that the adsorption-induced segregation effects are efficient surface engineering toolbox to balance the activity and selectivity of the catalyst to a desired optimum in the selective hydrogenation of C≡C ternary bonds into C=C.

*This work was supported by the Ministry of Science and Higher Education of the Russian Federation within the governmental order for SRF SKIF Boreskov Institute of Catalysis (FOUR-2024-0042).*

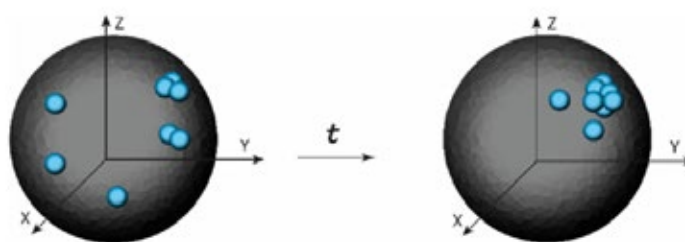


# DYNAMIC BEHAVIOR OF HETEROGENEOUS PALLADIUM-BASED CATALYTIC SYSTEMS

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A series of papers will be presented to study the dynamic behavior of metallic nano- and subnanoscale particles on the surface of heterogeneous catalyst under reaction conditions using palladium as an example. The modern understanding of the course of catalytic organic reactions based on metal complexes and nanoscale particles is based on multithreaded and conjugated processes of transformation of one form of metal into another initiated by chemical reaction reactants. Therefore, even when using a single catalyst precursor, such as a soluble salt, hundreds of new compounds with this metal capable of exhibiting high catalytic activity are formed in the system. If such methods of analysis as mass spectrometry or NMR spectroscopy are suitable for the study of homogeneous systems, the study of the dynamic behavior of heterogeneous systems requires the use of electron microscopy methods. For this purpose, it is necessary to develop a new methodology for the study of catalytic systems within the concept of dynamic catalysis, as well as to systematize and classify surface dynamic phenomena that differ in their manifestation from the behavior of homogeneous catalytic systems.



**Figure 1.** Example of dynamic behavior of nanoparticles on a support surface

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# NEW APPLICATIONS OF KINETIC DATA IN MECHANISTIC STUDIES IN CATALYSIS

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Kinetic studies are extremely effective tools for establishing the fine details of the mechanisms of catalytic reactions. Unfortunately, the kinetic methods applications in the studies of catalytic processes are quite limited. First of all, it is resulted from high labor intensity of kinetic data acquisition; also, the determination of reaction rates, which are the most frequently assessed kinetic parameter, needs for a correct processing of such data using differentiation procedures. In the report, using the examples of cross-coupling reactions of aryl halides and related processes, the approaches are discussed for the mechanistic studies of the reactions by analyzing of the kinetic patterns using integral kinetic data only without the need for their differentiation. In particular, the examples of the use of primary kinetic data on the concentrations of the reactants to study the patterns of the differential selectivity of the catalyst, determined in different conjugation nodes of complex catalytic processes under so-called natural and artificial multirouteness. The results obtained made it possible to discriminate between alternative hypotheses for the mechanisms of complex chemical reactions. In particular, for Pd-catalyzed cross-coupling reactions, using these approaches under the real catalytic conditions unique data were obtained about the pathways of the transformations of catalytically active species, as well as about the roles of substrates and additional components of the catalytic systems in these transformations. The report also presents the examples of the integral kinetic data application to develop descriptive and predictive models of the complex catalytic processes using machine learning algorithms.

*This work was supported by the Russian Science Foundation, grant 24-23-00382.*



# PHOTOCATALYSTS BASED ON FUNCTIONALIZED 1,10-PHENANTHROLINE RUTHENIUM(II) COMPLEXES

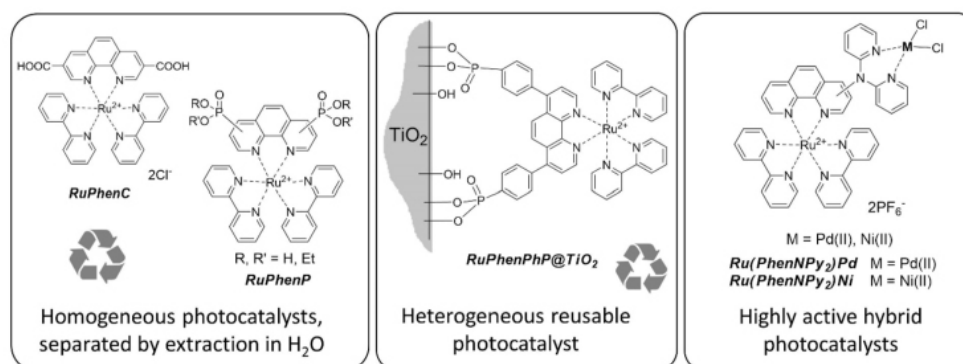
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Polypyridine ruthenium(II) complexes possess a unique combination of electrochemical and photophysical properties, due to which they are widely used as photocatalysts and components of photovoltaic cells.<sup>1,2</sup> The significant cost of ruthenium compounds limits their application. This problem can be overcome by increasing the activity of catalysts, allowing to reduce catalyst loading, as well as by developing methods for their separation from the reaction mixture for further reuse.

Synthesis of new homogeneous and heterogeneous photocatalysts based on ruthenium(II) complexes with substituted 1,10-phenanthrolines (Fig. 1) will be discussed in the report, as well as the advantages and limitations of their use in various photocatalyzed reactions.



**Figure 1.** Photocatalysts studied in this work.

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*The work was financially supported by Russian Science Foundation, grants 22-73-00031 and 24-43-00069.*

# PERSPECTIVE BIOMIMETIC PROCESSES FOR SELECTIVE FUNCTIONALIZATION OF ORGANIC COMPOUNDS

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Designing highly efficient and environmentally benign approaches to deliberately selective oxidative functionalization of organic compounds at the abundant C–H and C=C groups is a hot topic at the interface of the state-of-the-art synthetic chemistry and catalysis. The urgency of this area is largely dictated by the growing need for powerful and versatile general approaches to site-predictable modification of bioactive natural products and drug-like molecules at C(sp<sup>3</sup>)–H bonds. In particular, *late-stage functionalization*, aimed at selective transformations of complex molecules without the necessity for installation of directing or protecting groups, is now considered as a key strategy of medicinal chemistry, enabling rapid access to a range of derivatives and metabolites without *de novo* synthesis of individual counterparts, and facilitating total syntheses.<sup>1</sup>

Transition metal based catalysts offer unsurpassed opportunities for such processes, nowadays enabling treatment of “nonfunctional” aliphatic C–H groups as a useful synthetic handle. To a large extent, this is achieved via adopting principles of *biomimetic control of chemical selectivity*<sup>2</sup> for C–H functionalization of complex molecules. Recent years have witnessed noticeable growth in the number of works dedicated to synthetically-focused biomimetic catalytic approaches, aimed at modeling the catalytic properties of natural metalloenzymes (such as Cytochrome P450, methane monooxygenase, and others) with synthetic transition metal based catalysts. This contribution highlights recent advancements in designing biomimetic catalyst systems for direct oxidative modifications of organic molecules and understanding the molecular mechanisms of their catalytic action.

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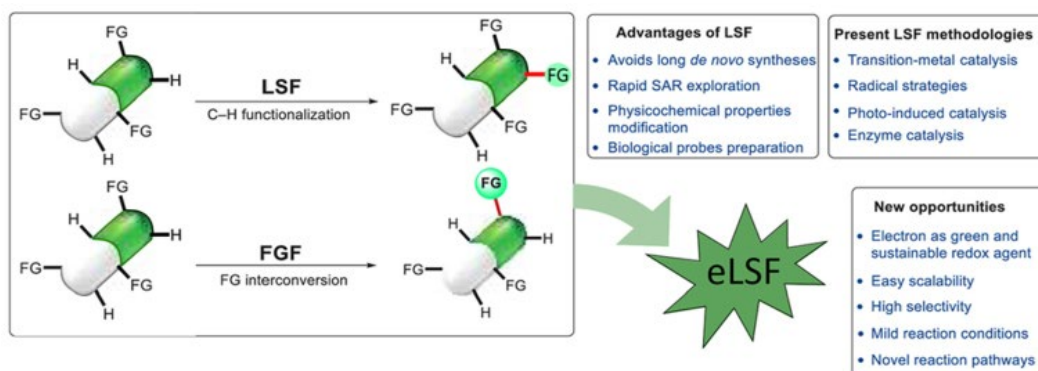
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# ELECTROCHEMICAL C-H FUNCTIONALIZATION. OPPORTUNITIES IN LATE STAGE SYNTHESIS (e-LSF)

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Organic electrosynthesis is of particular importance in the field of new drugs and biologically active molecules preparation, primarily through direct selective functionalization of C-H bonds. Direct selective modification of structurally complex molecules at late stage functionalization (LSF) has great potential for drug discovery, materials science, plant protection, etc. This approach avoids complete *de novo* synthesis of the target molecule, allows rapid generation of large libraries of compounds, and therefore promises rapid investigation of structure–activity relationships. The most synthetically useful LSF strategy is often the direct selective introduction of fluorophores or small groups, including CH<sub>3</sub>, OH, P, F, CF<sub>3</sub>, into a biologically relevant molecule. The development of organic synthesis methods that comply with the concept of sustainable development and meet such principles of “green” chemistry as atom-saving, low-waste, and energy efficiency remains an urgent task, and electrochemical synthesis has a number of advantages in solving these problems. Development of an effective strategy for targeted synthesis based on direct activation and functionalization of C-H bonds with the formation of new C-P, C-N, C-C bonds under mild electrocatalytic conditions (including eLSF), by identifying key intermediates and their properties, reaction mechanisms by modern methods, including electrochemical and ESR, is the subject of this report.



*The work was supported by the Russian Science Foundation grant No. 22-13-00017.*

# NOVEL CATALYTIC METHODS FOR THE SELECTIVE C-H FUNCTIONALIZATION OF THE FURAN NUCLEUS

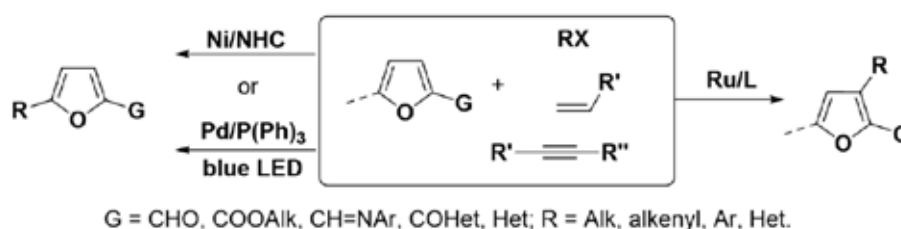
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Furfural (FF) and 5-hydroxymethylfurfural (HMF) derivatives are used as renewable raw materials in the chemical industry.<sup>1</sup> C-H functionalization of the furan nucleus is considered an efficient way to convert furan platform molecules into value-added products. However, known methods for C-H functionalization of the furan nucleus are mainly based on reactions involving the more active C5-H bond, while activation of the less reactive C3-H and C4-H bonds is difficult.<sup>2</sup>

The methods developed by the authors for the selective C3-H and C5-H alkylation, alkenylation, and (hetero)arylation of the furan core of FF and HMF derivatives under ruthenium, nickel, and palladium catalysis are discussed.



Particular attention is paid to solving the selectivity problem of C3-H and C5-H bond functionalization through the choice of metal, ligands, directing and protecting groups, and activators of the catalytic system.<sup>3,4</sup>

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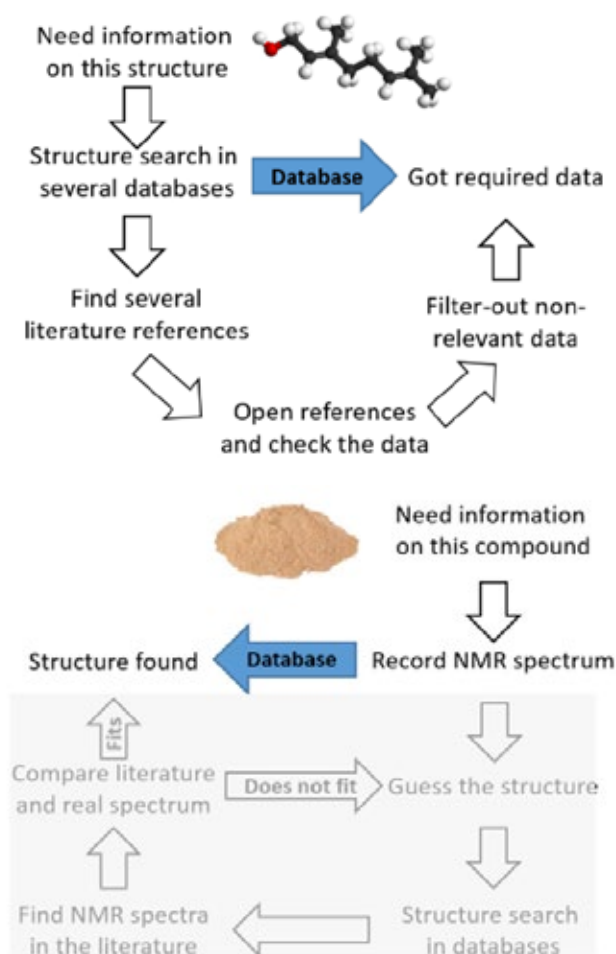
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# CHEMICAL INFORMATION SEARCH AND NEW APPROACHES TO REENGINEERING

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The search for chemical information requires special approaches and specific databases. This study discusses options for searching experimental properties from the structure of a molecule, as well as for solving the inverse problem - searching the structure of a substance from experimental spectra.





# GOLD-CATALYZED DIFFUNCTIONALIZATION OF ALKYNES

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Today, gold catalysis is recognized as powerful synthetic tool<sup>1</sup>. Do to the high affinity of cationic Au(I) and Au(III) species to double and triple carbon-carbon bonds, gold complexes can serve as potent activators of nucleophilic additions to unsaturated compounds. Gold catalysis is especially widely used for the difunctionalization of alkynes, which serve as convenient molecular building blocks for the rapid assembly of valuable organic products.

The presented report combine the following results obtained in the author's research group, namely:

- gold-catalyzed interaction of electron-deficient and electron-rich alkynes with OH- and NH-nucleophiles allows the selective preparation of various hydroxylation and hydroamination products [*Green Chem.*, 2022, 3314; *Adv. Synth. Catal.*, 2023, 2428; *Org. Lett.*, 2023, 8756];
- in the presence of gold complexes, ynamides and cyanamides are involved in formal (2+2+2) and (4+2) cycloaddition reactions, leading to polyamino-substituted azaheterocycles [*Adv. Synth. Catal.*, 2020, 2672; *Org. Biomol. Chem.*, 2021, 4577; *J. Org. Chem.*, 2021, 7218; *J. Org. Chem.*, 2021, 17804];
- oxidation of gold-activated alkynes under the action of oxygen and nitrene transfer reagents led to a variety of O- and N-containing products [*Eur. J. Org. Chem.*, 2019, 1856; *J. Org. Chem.*, 2020, 745; *Org. Lett.*, 2019, 4116; *J. Org. Chem.*, 2021, 1748; *Adv. Synth. Catal.*, 2019, 2926; *Adv. Synth. Catal.*, 2022, 3697; *J. Org. Chem.*, 2021, 12964; *Org. Chem. Front.*, 2022, 5133].

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# NEW HORIZONS FOR THE APPLICATION OF NMR AND MRI IN CHEMISTRY, BIOLOGY AND MEDICINE

**Burueva D.B.,<sup>a</sup> Kononenko E.S.,<sup>a</sup> Skovpin I.V.,<sup>a</sup> Salnikov O.G.,<sup>a</sup> Chukanov N.V.,<sup>a</sup>  
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NMR-based techniques are efficient tools for the studies of physico-chemical and biological processes of various nature. Because their sensitivity is limited, much attention is paid to the development and application of spin hyperpolarization techniques, to enhance NMR signals by a factor of 10,000 or more<sup>1</sup>. One promising approach is based on the use of parahydrogen in catalytic hydrogenation and related processes, which makes it possible to hyperpolarize a number of natural metabolites and drugs. An injection of such compounds into a living organism allows one to monitor their transformations in vivo for the development of novel highly sensitive methods for biomedical diagnostics of a wide range of pathologies. The use of homogeneous and heterogeneous hydrogenation processes with parahydrogen makes it possible, in particular, to hyperpolarize metabolites of the Krebs cycle and a number of nitrogen-containing drugs. In addition, the use of hyperpolarized gases for functional diagnostics of the lungs is highly promising. Based on hydrogenation with parahydrogen, an original approach was implemented to produce hyperpolarized propane, butane and diethyl ether, which were used in MRI experiments on animal lungs<sup>2</sup>.

The use of parahydrogen in reactions involving H<sub>2</sub> is also applicable to significantly increase sensitivity in the studies of operating reactors and the mechanisms of catalytic processes. To make such studies informative, it is additionally required to significantly increase the resolution in the NMR spectra of highly inhomogeneous objects. To this end, a number of promising approaches are proposed for making NMR signals much narrower, based on optimizing the structure of the catalytic layer, using the properties of multiquantum spin coherences, and performing NMR experiments at zero magnetic field.

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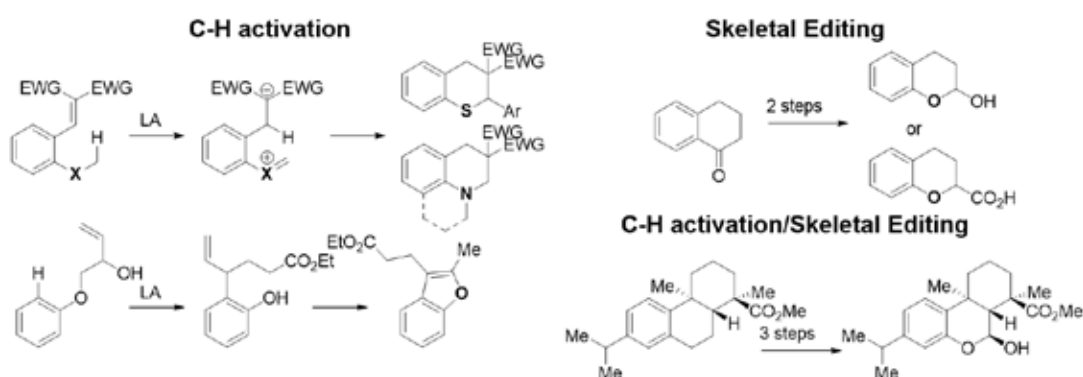
# C-H ACTIVATION AND SKELETAL EDITING FOR SYNTHESIS OF POLYCYCLIC STRUCTURES

Ikonnikova V.A.,<sup>a</sup> Smirnov A.Yu.,<sup>a</sup> Baranov M.S.,<sup>a</sup> Korlyukov A.A.,<sup>b</sup> Mikhaylov A.A.<sup>a</sup>

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Reaction proceeding with atomic precision are of the most valuable in the recent organic chemistry.<sup>1</sup> Answers to this challenge are: for peripheral editing – reactions of C-H activation – the direct substitution of hydrogen atom at unactivated hydrocarbon fragment, and for skeletal editing – reactions of «atom swap» and atom transposition. In this report there would be covered our recent development in the areas of C-H activation and skeletal editing, which focus on synthesis of biologically relevant polycyclic molecules, such as julolidines, tetrahydroquinolines, thiochromans, benzofurans and chromans.<sup>2-5</sup>



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# POROUS AROMATIC POLYMERS AS SUPPORTS FOR THE CATALYSTS OF HYDROGENATION AND CROSS-COUPLING

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The study of approaches to the stabilization of catalytically active forms of metals is a promising area of research. Functionalized polymeric supports can serve as an effective tool for stabilizing particles of active phase performing various organic transformations. Depending on the characteristics of the catalytically active metal, as well as the type of selected polymeric support, the catalytic properties of such systems can be varied. The overall efficiency of the catalyst depends both on the state of the active component itself and on the interaction between the catalytically active forms of the metal and the support, which determines the catalyst morphology.

This work is devoted to the possibilities of using porous aromatic polymers as supports for catalysts of hydrogenation and cross-coupling. The factors influencing the distribution of the metal-catalyst (Pd and Ru) in the polymeric environment are investigated. It is shown that the key parameter is the relative hydrophilicity/hydrophobicity of the aromatic polymer, due mainly to the oxygen content in combination with the nature of the metal precursor and the solvent selected for the synthesis of the catalytic system. In the resulting polymer-containing catalyst, several forms of the metal-catalyst are simultaneously present (molecular dispersion of salt or oxide, clusters and nanoparticles). At the same time, the aromatic nature of polymers contributes to the stabilization of small metal-containing clusters, which, however, do not reveal high activity in hydrogenation and cross-coupling reactions, but can serve as precursors of catalytically active forms and a reservoir of metal-catalysts.

It should be noted that the issue of the stability of polymer-containing catalytic systems as a whole is complex and depends on the mutual combination of the relative hydrophobicity of both the support itself and the reagents involved in the catalytic process and the solvent.

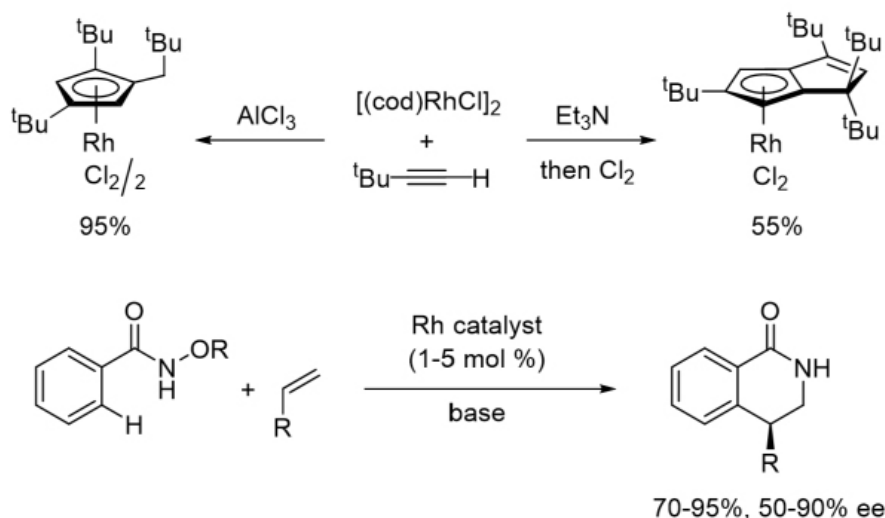
*The work was supported by the Russian Science Foundation, project 23-29-00604.*

# CYCLOPENTADIENYL RHODIUM COMPLEXES AS CATALYSTS FOR SELECTIVE C-H ACTIVATION REACTIONS

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Rhodium complexes with bulky cyclopentadienyl ligands can be obtained in just couple of steps by unusual cyclization of several molecules of *tert*-butyl-acetylene.<sup>1-3</sup> These complexes catalyze activation of C-H bonds in aryl hydroxamic acids and their reaction with alkenes giving valuable dihydroisoquinolones in excellent yields with high regio- and stereoselectivity. Critical analysis revealed that noble metals, such as rhodium, typically contribute less than 10% to the total cost of fine organic synthesis and their replacement by cheap 3d metals can in fact make catalytic reactions more expensive.<sup>4</sup>



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# PLASMON-ASSISTED ACTIVATION OF ORGANIC REACTIONS ALTERNATIVE APPROACH FOR CATALYSIS

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The development of catalytic technologies has led to the emergence of conceptually new approaches to initiating classical organic transformations. These reactions could be carried out on the surface of semiconductors<sup>1</sup> and via plasmon-initiation.<sup>2</sup>

Among plasmon-driven transformations, a special role belongs to reactions of homolytic cleavage of C-Het bonds, which make it possible to generate radical intermediates from appropriate precursors effectively. Thus, plasmon initiation has been successfully applied to generate aryl radicals from iodonium salts<sup>3</sup> and the stable nitroxide formation as the result of alkoxyamines homolysis.<sup>4</sup>

Not least important in plasmon chemistry is the establishment of the mechanisms of activation processes of organic molecules under the excited plasmons. In this context, reactions of homolytic cleavage of alkoxyamines represent a unique tool for kinetic studies of the plasmon-initiated reactions.<sup>5</sup>

The presented report will be devoted to the fundamental and applied aspects of plasmon-driven organic reactions.

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# THIRD GENERATION OF SILICONE PRODUCTION. DIRECT SYNTHESIS OF ORGANOALKOXYSILANES.

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The development of the direct synthesis of organochlorosilanes (DSCI) has revolutionized the world of silicones. It allowed to avoid energy-consuming and low-productivity organomagnesium synthesis and enabled production of tens of thousands of tons of organosilicon monomers in a single reactor, marking the turnover from the first- to the second-generation production of these polymers. As a result, silicones have moved from being specialty materials to being used in virtually all areas of human activity.<sup>1</sup>

An obvious disadvantage of DSCI is the environmental risks associated with the use of large quantities of chlorine-containing compounds. Another disadvantage is economic. Separation of a mixture of organochlorosilanes is a highly energy-intensive process due to the small difference in their boiling points. Organoalkoxysilanes can be an alternative chlorine-free raw material for the production of silicones. However, today the method of their synthesis involves the use of the same organochlorosilanes.

The development of direct synthesis of organoalkoxysilanes can solve all the problems described above. In addition to eliminating chlorine from the process of silicone synthesis, the use of organoalkoxysilanes is also beneficial and economical due to the greater difference in boiling point. This report analyzes the main problems, possible ways to solve them, as well as recent advances in the field of direct synthesis of organoalkoxysilanes. The first example of the preparation of methylmethoxysilanes by direct reaction of silicon with dimethyl ether in gram quantities is presented.

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# NEW APPROACHES TO ACTIVATION OF C=C AND C-H BONDS

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The development of new approaches to the activation of multiple C-C, sp<sup>3</sup>- and sp<sup>2</sup>-C-H bonds, catalyzed by complexes of s- and f-elements will be reported. Efficient and selective catalysts have been developed for intermolecular reactions of hydrosilylation/dearomatization of nitrogen-containing pyridine type heterocycles, stereoselective migration of the C=C double bond in  $\alpha$ -olefins and allylbenzenes, hydrophosphination, hydroamination of olefins and acetylenes, as well as dehydrocoupling of hydrosilanes with arenes, amines and phosphines.

New coordinatively unsaturated Ca(II) and Yb(II) hydrides turned out to be efficient catalysts for the addition of hydrosilanes to nitrogen-containing pyridine-type heterocycles at room temperature. Dearomatization of pyridines and quinolines easily proceeds with exceptional regioselectivity and gives the 1,2-addition product. The chemoselectivity of the reaction strongly depends on the steric properties of the heterocyclic substrate. Reactions of PhSiH<sub>3</sub> with pyridines and isoquinoline lead to double addition products, whereas only single addition was observed for quinoline and its derivatives. However, when the reaction temperature is increased to 90°C, the same complex catalyzes the reverse reaction: the release of the original silane and the restoration of the aromaticity of the pyridine system.

Heterobimetallic ate-complexes {[*p*-*t*BuC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>CH]<sub>3</sub>M<sup>1</sup>}M<sup>2</sup> (M<sup>1</sup> = Ca, Sr, Ba, Yb; M<sup>2</sup> = Li, Na, K) proved to be efficient catalysts for the migration of the terminal double bond of allylbenzenes and  $\alpha$ -olefins, allowing the reaction to be carried out at room temperature with high rates and quantitative conversions, achieving high E-stereoselectivity (90-98%). A synergistic effect of the two metal ions was discovered, causing coordinated activation of each of the substrates on different metal centers.

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# CATALYSIS AS PART OF NEW STRATEGIES FOR THE DEVELOPMENT OF ACETYLENE CHEMISTRY

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The article presents a brief overview of work on the chemistry of acetylene with a laconic consideration of the results obtained over the last decade (2015-2024). The chemistry of acetylene and its derivatives is developing dynamically and effectively. New fundamental reactions are being discovered that fundamentally complement existing knowledge about the reactivity of a triple carbon-carbon bond, reflecting development trends in this area.

B.A. Trofimov School proposes an effective strategy for the development of previously unknown acetylene reactions occurring in highly basic conditions. These reactions include for the first time ethinylation of the C=N bond (aza-Favorsky reaction), an unexpected dimerization-cyclization reaction of acetylene ketones, leading under mild conditions to oxaspiro[2.4]heptanones and other practically important compounds.

V.P. Ananikov School proposed an original strategy for using calcium carbide as a source of acetylene generated *in situ* during the reaction of  $\text{CaC}_2$  with water. This is a rational solution to the problem of using acetylene gas associated with its fire and explosion safety.

Progress in the chemistry of acetylene was reflected in a series of works by I.V., Alabugin, in which the well-known rules of D. Baldwin on the cyclization of unsaturated compounds, which for many years were and remain one of the most effective tools for organic synthesis, were critically revised, supplemented and clarified. For synthesis of compound a certain structure.

I.P. Beletskaya's works on improvements and modifications of one of the most famous Sonogashira's reaction are well known. One of these novelties is the use of a phase transfer catalyst to activate the  $\text{Ph}_3\text{P}$ -TMEDA catalytic system.

*The bibliography includes 30 publications in highly rated journals (2015-2024).*

# ELECTROCHEMICAL SYNTHESIS OF HOMOGENEOUS CATALYSTS FOR SELECTIVE ETHYLENE DIMERIZATION AND TRIMERIZATION

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The catalytic systems based on nickel and chromium are the most important industrial catalysts for homogeneous catalytic dimerization and trimerization of ethylene.<sup>1</sup> The search for new environmentally friendly and resource-saving methods for production of such catalysts is one of the priority areas in the development of modern synthetic chemistry and catalysis. We have previously shown that a combination of classical chemical synthesis and electrochemical methods can be effectively used to develop new methods for the preparation of various types of organometallic compounds and transition metal catalysts.<sup>2</sup>

This lecture will discuss the developed industrially acceptable electrochemical methods for the preparation of organonickel complexes of type [NiBr(Aryl)(L)], where Aryl – *ortho*-substituted aromatic group, L – 2,2'-bipyridine (bpy) or substituted 1,10 -phenanthroline (phen), as well as organochromium compounds (chromium(III) 2-ethylhexanoate), which are effective pre-catalysts for the production of 1-butene and 1-hexene by selective catalytic dimerization and trimerization of ethylene.<sup>3,4</sup>

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# HYDROSILYLATION – A KEY CATALYTIC APPROACH TO Si-C-BOND FORMATION

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Hydrosilylation is the most successful and large-scale example of the application of homogeneous Pt-catalysis in industry. In addition, hydrosilylation is the main method for the preparation of organosilicon compounds and one of the most important atom-efficient approaches to the functionalization of unsaturated compounds.

Industrial catalysts for hydrosilylation are Pt-complexes – Speier’s and Karstedt’s catalysts, used since the mid-twentieth century. However, intensive research into this reaction and the development of new catalysts are still ongoing. On the one hand, this is due to the high cost of platinum and its irreversible “scattering,” contamination of products with colloidal platinum, etc. On the other hand, this is due to low activity towards sterically hindered compounds, low selectivity for hydrosilylation of functionalized alkenes/alkynes, etc.

In modern chemistry, several main approaches can be distinguished aimed at solving the above-mentioned economic, environmental, chemical and technological problems:<sup>1</sup> (1) development of organo-catalyzed hydrosilylation; development of new homogeneous [M] catalysts based on (2) cheap and available 3d metals (3) platinum series metals; and the transition to regenerated and recyclable heterogeneous and heterophasic catalytic systems. Findings of our research group in these areas will be discussed.<sup>2-5</sup>

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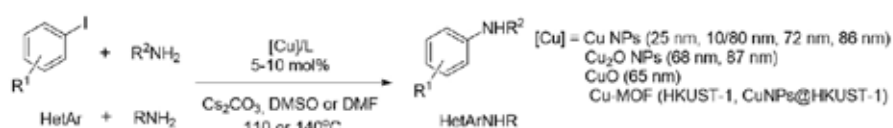
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# COPPER NANOPARTICLES IN THE CATALYSIS OF CARBON-NITROGEN BOND FORMATION

**Averin A.D., Fomenko V.I., Murashkina A.V., Kuliukhina D.S., Borisova A.S., Malysheva A.S., Beletskaya I.P.**

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A detailed study of homogeneous Cu(I)-catalyzed arylation and heteroarylation of various monoamines, diamines, polyoxadiazines and polyamines helped to outline main regularities of this process.<sup>1</sup> In this work we have thoroughly studied the use of copper and copper oxides nanoparticles, as well as copper-containing metal-organic frameworks (Cu-MOFs), as catalysts for the formation of the C-N bond.<sup>2</sup> The amination of aryl and heteroaryl iodides and bromides (benzene, naphthalene, pyridine, quinoline) with aliphatic monoamines and NH-heterocycles have been studied. The reactions employed free copper nanoparticles of various average sizes (25 nm, 72 nm, 86 nm, bifractional nanoparticles 10/80 nm), copper (I) and (II) oxides (65, 68, 87 nm) which were not deposited on any substrate. A comparison was made with the catalysis by Cu-MOFs. It has been found that the best results of (hetero)arylation are obtained in the presence of the ligands like 2-isobutyrylcyclohexanone, *rac*-BINOL and, in some cases, *L*-proline. A systematic study of the induction period of the reaction, leaching of copper into solution, analysis of changes in the catalyst using TEM and SEM electron microscopy was carried out, and the possibility of recycling nanocatalysts up to 8 times, and Cu-MOCF up to 10 times without a noticeable decrease in the products yields was demonstrated.



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# DESIGN OF NEW SINGLE COMPONENT Ni- AND Pd-CATALYSTS FOR ADDITION POLYMERIZATION OF CYCLOOLEFINS

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Topchiy M.A.<sup>1</sup>, Asachenko A.F.<sup>1</sup>, Bermeshev M.V.<sup>1</sup>**

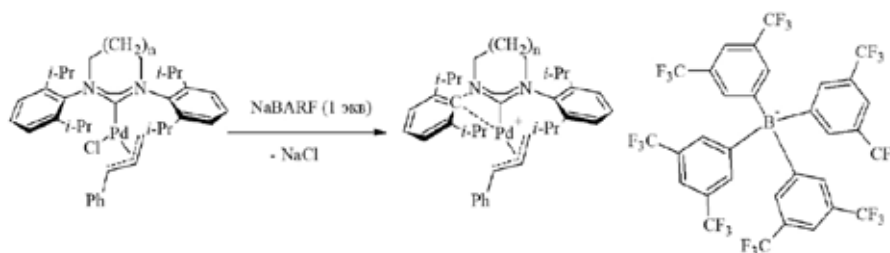
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The development of new polymers and the simplification of approaches to obtaining existing polymers is a highly demanded task in the synthesis of modern polymer materials. Strained cyclic monomers containing a double bond in the cycle seem to be particularly promising for this purpose. Two mechanisms of polymerization of these monomers (addition and metathesis) are the most widespread. Metathesis polymerization has been studied in detail, and efficient catalysts have been developed for it, while addition polymerization is currently a poorly understood process requiring the development of versatile catalysts.

In the presentation, the results on the development of single-component Ni- and Pd-catalysts for addition polymerization of cycloolefins will be discussed, as well as systematic studies on the optimization of the structure of such complexes for polymerization catalysis [1, 2]. The main steps of the mechanism of addition polymerization in the presence of these complexes will be also considered.



**Figure 1.** Synthesis of single-component Pd-complexes.

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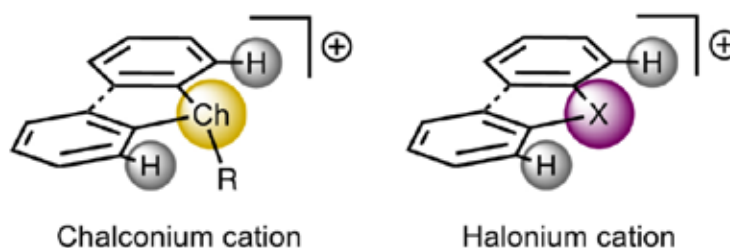
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# ELECTROPHILIC CATALYSIS WITH ORGANIC LEWIS ACIDS

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One of the directions in the development of the field of electrophilic organocatalysis is the preparation of analogues of metal complex catalysts featuring a nonmetal element with a kinetically labile coordination vacancy as the central atom. The report will discuss the latest experimental data on the kinetics of reactions in the presence of cationic organochalcogen and organohalogen compounds (Figure 1), xenon derivatives, as well as the results of quantum chemical calculations that reveal the essence of the observed catalytic effects.<sup>1-6</sup>



**Figure 1.** Structures of chalconium and halonium cations utilized for the catalysis.

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# SYNTHESIS OF N-ALKYL-5-METHYL-2-PYRROLIDONES OVER NICKEL PHOSPHIDE CATALYSTS

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An attractive approach for the preparation of N-alkyl-5-methyl-2-pyrrolidones is the heterogeneous catalytic reductive amination of levulinic acid esters with primary amines in the presence of hydrogen. Since this process involves imine formation and intramolecular amidation steps, phosphide catalysts containing both metal and acid sites are of interest for use in this reaction. The work studied the effect of the preparation method, the nature of the support ( $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$ ) and the precursor of Ni and P ( $\text{Ni}(\text{CH}_3\text{COO})_2$  and  $(\text{NH}_4)_2\text{HPO}_4$  or  $\text{Ni}(\text{OH})_2$  and  $\text{H}_3\text{PO}_3$ ) on the catalytic properties of supported  $\text{Ni}_2\text{P}$  catalysts in the reductive amination reaction of ethyl levulinate (EL) with n-hexylamine to N-hexyl-5-methyl-2-pyrrolidinone (HMP).

The catalysts were characterized by elemental analysis, low-temperature nitrogen adsorption,  $\text{NH}_3$ -TPD, X-ray diffraction, and TEM; a study of their catalytic properties in a flow reactor was carried out by varying temperature, pressure, and the nature of the solvent and amine.

It was found that the  $\text{Ni}_2\text{P}/\text{SiO}_2$  catalyst prepared using  $(\text{NH}_4)_2\text{HPO}_4$  and reduced at 600 °C provides a HMP yield of  $\geq 98\%$ , while the selectivity for the formation of pyrrolidones is influenced by the nature of the primary amine, solvent and ratio of reagents. Thus, a decrease in selectivity is observed in the reaction with aniline derivatives when using alcohol solvents (isopropanol and methanol) instead of toluene. The  $\text{NiP}/\text{Al}_2\text{O}_3$  catalysts showed lower HMP selectivity due to the high rate of hydrogenation of ethyl levulinate to gamma-valerolactone. Taking into account the observed dependences of the main and by-products on the nature of the catalyst and reaction conditions, a scheme for the conversion of EL on nickel-phosphide catalysts is proposed, taking into account the role of acid and metal centers.

*The work was carried out with financial support from the Ministry of Science and Higher Education of the Russian Federation within the framework of a state assignment from the Institute of Catalysis of the Siberian Branch of the Russian Academy of Sciences, using the equipment of the Center for Collective Use "National Center for Catalyst Research".*

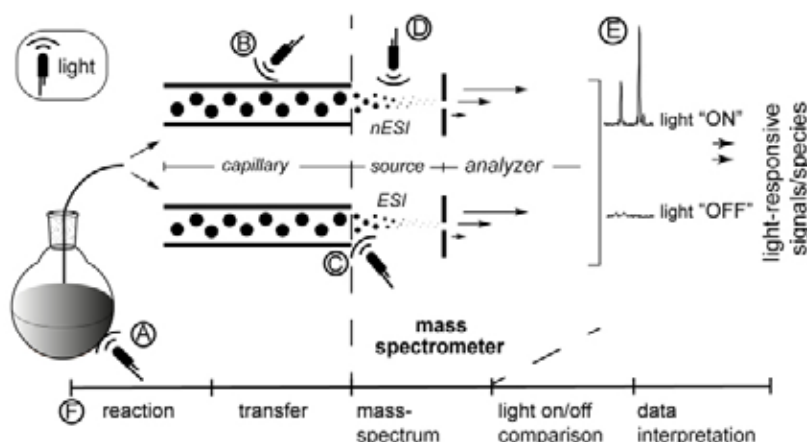


# INVESTIGATION OF PHOTOCATALYTIC TRANSFORMATIONS USING MASS SPECTROMETRY IN OPERANDO MODE

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The demand for using a mass spectrometric approach to analyze photocatalytic reaction mixtures today is due to the increasing complexity of these systems and the limitations of other structural methods of analysis.<sup>1</sup>



**Figure 1.** A - Photochemical reaction with irradiation in the flask or syringe; B - Irradiation of the reaction mixture in the capillary; C - irradiation of the reaction mixture on the tip of the capillary and plume at the needle tip (inside ESI-MS hardware); D - irradiation of the nESI tip (inside ESI-MS hardware); E - registering mass spectra in two regimes, light on/off; F – schematic diagram of the stages involved.

Intermediates, by-products and major products of the reaction can be recorded by mass spectrometry in *operando* mode. The proposed approach is based on continuous feeding of the reaction mixture inside the ionization source of the mass spectrometer and irradiation of the reaction vessel, transparent capillary or nebulizer needle inside the ionization source with light (Figure 1).<sup>2-3</sup>

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# STRUCTURE-DRIVEN TUNING OF O AND CO ADSORPTION ON Au-Cu NANOPARTICLES: A DENSITY FUNCTIONAL THEORY STUDY

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Nanoparticles are fascinating nanoobjects that are actively studied and widely employed in various fields, such as heterogeneous catalysis and advanced electrode materials. Their local atomic structure and composition can significantly impact their properties. We employed the state-of-the-art first-principles calculations to investigate the effects of AuCu nanoparticle structure and composition on the electronic properties, charge distribution, and CO and O adsorption energies. Two types of nanoparticles were examined in this study; specifically core-shell nanoparticles (Cu@Au, Au@Cu) and bimetallic alloy particles (Au-Cu), all with an average diameter of 2 nm (321 atoms) and exhibiting fcc, icosahedral, and amorphous structures. The research comprehensively investigated the electronic and adsorption properties of the proposed nanoparticles with regard to their ability to adsorb CO and O, revealing the potential for finely tuning of their properties by modifying their atomic structure and composition. Adjusting the core-to-shell ratio allows one to precisely tune the O and CO adsorption energies on the nanoparticle surface, particularly in fcc nanoparticles. This results in a narrower range of adsorption energies, specifically for CO adsorption, which cannot be achieved in bimetallic alloys. Our study shows the significance of this approach for fine-tuning adsorption energies on a nanoparticle surface.

# METAL-FREE ELECTROCATALYSTS FOR PRODUCTION OF MOLECULAR HYDROGEN AND SYNTHESIS GAS: KINETICS, MECHANISM AND STRUCTURAL DESIGN OF CATALYSTS

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One of the ways to solve the problem of rapid utilization of excess CO<sub>2</sub> is to use it as a building block for the synthesis of various organic compounds using the Fischer-Tropsch reaction (processes based on synthesis gas (CO and H<sub>2</sub>)). The development of efficient electrocatalytic systems capable of coupled hydrogen production and controlled selective reduction of carbon dioxide to CO to produce “green” synthesis gas from saturated aqueous solutions of CO<sub>2</sub> in water, at low potentials and rates, is a key challenge for future electrochemical conversion systems. CO<sub>2</sub> processing technologies.

The report will present data on the creation based on “molecular platforms”, based on heterocyclic organic compounds - acridine, pyridine, 2,2'-bipyridine and 2,2':6',2''-terpyridines, phenanrolines, benzimidazoles, Ganz esters and others, capable, depending on the process conditions, of generating hydrogen, as well as the coupled process of hydrogen formation and controlled selective multielectron reduction of carbon dioxide to CO, to obtain a mixture of CO and H<sub>2</sub> (the initial components in the Fischer-Tropsch process). The combination of two or more pyridine-based catalytic centers in one molecule leads to an increase in the efficiency and selectivity of the process (synergetic effect). In addition, the use of monoalkylated derivatives of 2,2'-bipyridine and 2,2':6',2''-terpyridines allows the implementation of electrocatalytic reactions for the selective production of CO and H<sub>2</sub> at “separate” centers: at an unsubstituted center - the formation of CO, at a substituted center - the formation molecular hydrogen.

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# SYNTHESIS AND CATALYTIC ACTIVITY OF CARBONATE-STABILIZED RHODIUM NANOPARTICLES

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Rhodium nanoparticles have pronounced catalytic properties, therefore they are used in the hydrogenation of organic compounds, such as benzene and cyclohexane, arenes, quinoline and its derivatives, hydroformylation of olefins, reduction of NO by carbon oxide, introduction of carbenoids into amines, asymmetric arylation, oxidation of CO, ring opening of cyclohexane and many others<sup>1</sup>.

We set a goal to synthesize rhodium nanoparticles by a method consistent with the principles of green chemistry. Such a method is the reduction of  $\text{Rh}^{3+}$  ions in the presence of oxalate ions  $\text{C}_2\text{O}_4^{2-}$  under the action of UV radiation. UV radiation is used to initiate the ion reduction reaction in the synthesis processes of nanoparticles of many metals<sup>2</sup>. The synthesized rhodium nanoparticles should have high catalytic activity. As an example, a model reaction of reduction of 4-nitrophenol to 4-aminophenol was investigated.

The action of UV irradiation on a deaerated aqueous solution of rhodium ions ( $0.5\text{--}3 \times 10^{-4} \text{ mol L}^{-1}$ ) containing oxalate ions ( $1.5\text{--}9 \times 10^{-4} \text{ mol L}^{-1}$ ) was found to initiate the reduction of metal ions and the formation of nanoparticles.

According to TEM data, the particles are predominantly spherical in shape. The average diameter is  $3.4 \pm 0.8 \text{ nm}$ . According to DLS data, the average size is  $4.1 \pm 1.2 \text{ nm}$ . The diffraction pattern indicates the presence of rhodium in metallic form.

The nanoparticles were found to have high catalytic activity in the reduction reaction of 4-nitrophenol to 4-aminophenol using  $\text{NaBH}_4$  as a reducing agent. Thus,  $\tau_{1/2}$  for this reaction ( $C_0$  [4-nitrophenol] =  $1 \times 10^{-4} \text{ mol L}^{-1}$ ,  $C$  [ $\text{NaBH}_4$ ] =  $1 \times 10^{-2} \text{ mol L}^{-1}$ ,  $C$  [Rh] =  $5 \times 10^{-6} \text{ mol L}^{-1}$ ) is 330 seconds.

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# METALLOCENE/ISOBUTYLALUMINUM ARYLOXIDE CATALYTIC SYSTEMS FOR SYNTHESIS OF ETHYLENE-PROPYLENE COPOLYMERS

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Ethylene-propylene copolymers are widely used in various industries such as automotive, rubber, cable, construction materials, and impact-resistant plastics. The synthesis of these copolymers is facilitated by modern and efficient catalysts such as metallocene and post-metallocene complexes [1]. To activate organometallic catalysts in polymerization processes, methylalumoxane (MAO) is commonly used as an activator. However, MAO is expensive, unstable during long-term storage, and used in large molar excesses with respect to the organometallic complex ( $Al/M=10^3-10^4$ ). Therefore, an important task is to develop new effective activators and create catalytic systems with their participation.

New catalytic systems based on metallocenes and aryloxides of isobutylaluminum of different structures have been developed for copolymerization of ethylene(E) with propylene (P). The influence of the structure of metallocenes and aryloxides of isobutylaluminum on the activity of catalytic systems, composition, and molecular weight characteristics of copolymers, which, in turn, determine the physical and mechanical properties of polymer samples, has been shown. By varying the components of the system it is possible to regulate the activity of the catalytic system (from 70 to 4600 kg of copolymer/mol  $M \cdot h \cdot atm$ ), the content of comonomers in copolymers (P from 0 to 39 wt.%), molecular weights ( $M_w=60-500$  kDa), tensile strength (2-20 MPa), and elongation at break (100-1000%) of copolymers. The obtained results suggest the potential use of presented catalytic systems for producing ethylene/propylene and ethylene/propylene/5-ethylidene-2-norbornene copolymers with a wide range of properties.

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# Ag-Cu CATALYSTS SUPPORTED ON MIXED OXIDES FOR OXIDATIVE EXHAUST GAS PURIFICATION

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Nowadays, solving environmental problems is among the most important challenges facing chemical science. Research programs to reduce the level of harmful substances from emissions of industrial enterprises, transport, heat- and power plants and, as a result, prevent their negative impact on human health and the environment are topical.

Promising materials comprise transition metal oxides and their mixtures used as supports or modifiers for noble-metal-based catalysts. The combination of properties and a large number of active sites of such materials make it possible to predict their high catalytic performance both in the oxidation of CO and volatile organic compounds (VOCs) and in soot combustion, even in the absence of noble metals and/or their low content.

This work is aimed at the design of  $\text{CeO}_2\text{-ZrO}_2\text{-MnO}_x$  ( $\text{SnO}_2$ ) and bimetallic Ag-Cu (Ag and Cu content of no more than 2 wt.%) materials on the basis thereof, which makes it possible to obtain accessible (less expensive) catalysts for CO oxidation and soot combustion, while maintaining their high efficiency and stability. The work will show the influence of the preparation method (citrate, solvothermal and template approaches) and the catalyst composition on its structure, texture and catalytic activity. The work discusses the role of modifying additives  $\text{MnO}_x$  and  $\text{SnO}_2$  to  $\text{CeO}_2\text{-ZrO}_2$  from the point of view of the defect structure and interphase boundaries [1,2]. The question is raised about the features of the formation of bimetallic Ag-Cu particles on the surface of mixed oxides depending on the ratio of metals and, as a consequence, the peculiarities of the silver-copper interaction and the surface of the supports as well as the changes in the state of the active surface under the influence of redox treatments.

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# A NEW CLASS OF CATALYSTS FOR PETROCHEMICALS AND ORGANIC SYNTHESIS BASED ON GRANULATED HIERARCHICAL ZEOLITES

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In the laboratory of catalyst preparation at the IPC UfRC RAS, new materials have been developed - granulated zeolites with hierarchical (micro-meso-macro) porous structures. In these new catalytic systems, the concentration and accessibility of active centers are higher than in traditional zeolite-containing catalysts obtained by granulation with a binding material, due to the higher concentration of zeolite, presence of nano-sized crystals, and hierarchical porous structure. Additionally, these catalysts are 1.3-1.5 times stronger.

The new materials have been tested as catalysts for various petrochemical and organic synthesis processes. At LLC "Gazprom neftekhim Salavat", a domestic catalyst based on granulated hierarchical FAU (Yh) zeolite has been implemented for the production of ethylbenzene through the transalkylation reaction of diethylbenzene and benzene.

A new generation of catalysts for diesel fuel dehydroisomerization is being developed based on SAPO-11 zeolite granules with a hierarchical pore system, yielding over 95% winter diesel fuel output. Methods for the oligomerization of C5 and C8-12 olefins, cycloolefins (cycloheptene, cyclooctene, norbornene), vinylarenes on hierarchical Yh zeolite have been developed, showing high oligomer yields (up to 99%) and more stable operation compared to microporous zeolites.

In the presence of hierarchical Yh and ZSM-5h zeolites, efficient syntheses (up to 95% yields) of several practically significant N-heterocyclic compounds (alkylpyridines, alkylquinolines, alkyl-tetrahydroquinolylamines, alkylbenzimidazoles, benzodiazepines) have been achieved, which are either impossible or have low yields on microporous zeolites.

New catalytic systems for selective heterogeneous catalytic processes to obtain methylarenes, isophorone, and 3,5-xyleneol through acetone condensation are being developed based on metal-modified granulated hierarchical Yh and ZSM-5h zeolites.\*

*\* The work was carried out with the financial support of the Russian Science Foundation, grant No. 23-13-00213.*

# NEW APPROACHES TO THE FORMATION OF METALLOCARBON CATALYZERS FOR HYDROGENATION OF CO

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Catalysts of carbon oxides processing are the basis of realized technologies for obtaining valuable petrochemical products. Depending on the nature and method of the catalytic system synthesis of various products is possible: methane, liquid hydrocarbons, alcohols, etc. Therefore, the search for new approaches to the catalyst formation is an urgent task, since the results can expand the ways of influencing the properties of the synthesized active systems.

One of the promising methods for the formation of catalytic systems is the synthesis of material in a solution of metal precursor salts in subcritical water - hydrothermal synthesis. In the process of catalyst production the formation of carbon-containing matrix occurs under hydrothermal carbonization conditions and parallel immobilization of metal ions on the carrier surface due to interaction with active groups of polymers takes place. Various carbon-containing polymers of natural origin - cellulose, lignin, and synthetic polymers - polyvinyl alcohol - can be used as raw materials for obtaining catalytic systems.

It was established by a complex of physicochemical methods that in the process of hydrothermal synthesis the formation of ultradisperse composite material with metal oxide nanoparticles distributed in the carbon matrix with the size of 6-30 nm, depending on both the nature of the metal and the nature of the polymer. It was found that a carbon matrix with oxygen-containing functional groups and polyspore fragments in the carbon skeleton is formed based on the polymer molecule. The effective capture of metal ions from solution was confirmed by the results of XPS and AES-ICP.

Application of the hydrothermal synthesis method to the formation of CO hydrogenation catalysts (20 atm, CO/H<sub>2</sub>=1/1, 1000 h<sup>-1</sup>) allowed to obtain systems exhibiting high activity (X<sub>co</sub>,% reached 100%), with C<sub>5</sub>+ selectivity from 20 to 90% and with the content of iso-paraffins ~49-50 wt.% and olefins ~20-30 wt.% in C<sub>5</sub>+ hydrocarbons.

*This work was carried out within the State Program of TIPS RAS*

# HIGH-PERFORMANCE CATALYTIC HYDROGEN SENSORS FABRICATED ON ANODIC ALUMINA SUBSTRATES

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Hydrogen is now an important part of the global economy. Green hydrogen fuel already makes up a significant share of the energy sector. It is predicted that hydrogen will become the basis of the global economy and ensure sustainable development of humanity in the future.

However, hydrogen is characterized by a high fire and explosion hazard. Catalytic sensors are one of the most widely used in industry for detecting the concentration of hydrogen. Their main disadvantage is the high power consumption required to heat the sensor to operating temperatures (300 – 500 °C).

The aim of this work is to create highly efficient catalytic hydrogen sensors with examination of the functional characteristics of the obtained devices in various operating modes.

The sensitive element of the sensors is a platinum microheater (500 nm thick), formed by photolithography and magnetron sputtering on the surface of porous anodic aluminum oxide (AAO) (30 μm thick). Catalyst particles were obtained in AAO channels by incipient wetness impregnation with solutions of Pd and Pt complexes in a molar ratio of 3:1 followed by annealing.

The sensitivity of the developed sensor is 76 mV/vol. % hydrogen. Relative air humidity in the range of 6 to 90% does not affect the value of the sensor response. The short response time of the sensors ( $t_{90} = 0.4$  s) allows the use of a pulsed power supply mode, which reduces the power consumption of the sensor to 3.2 mW.

The characteristics of catalytic hydrogen sensors achieved during the work indicate their high competitiveness in the market and the prospects for their industrial application.

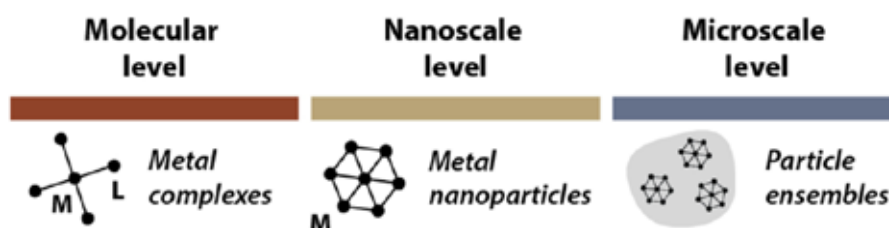
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# MULTILEVEL CATALYTIC SYSTEMS: FROM MOLECULAR COMPLEXES TO PARTICLE ENSEMBLES

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Carbon-carbon and carbon-element bond formation reactions catalyzed by transition metal compounds are widely used in the synthesis of various organic compounds. The evolution of views on the regularities of the functioning of catalytic systems used to carry out these transformations has led to a shift from the description of the mechanisms of action of catalysts within the framework of the consideration of transformations in the coordination sphere of a single active center to the consideration of the whole variety of metal-containing particles at different levels of organization of the catalytic system, their interconversions and their contribution to the overall efficiency of the process.



In the framework of the present work, the efficiency of using a multilevel approach for the study of catalytic systems and the optimization of chemical transformations involving transition metal-based particles and complexes is demonstrated using the example of Heck<sup>1</sup> and C-S cross-coupling<sup>2-3</sup> reactions catalyzed by palladium, copper or nickel compounds. Special attention is given to the application of liquid phase electron microscopy for direct visualization of the catalytically active phase in *in situ* mode.<sup>4</sup>

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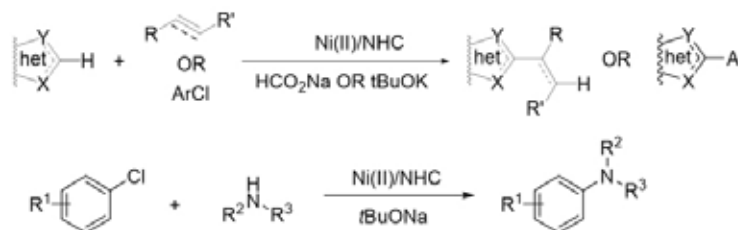
# APPLICATION OF Ni(II) COMPLEXES WITH N-HETEROCYCLIC CARBENES IN CATALYSIS OF C-H ACTIVATION AND C-N CROSS-COUPLING REACTIONS

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Catalytic systems based on nickel complexes with N-heterocyclic carbenes (Ni/NHC) are widely used in organic synthesis. To achieve high efficiency of such systems in most cases it is necessary to use Ni(0)/NHC complexes. However, often Ni(0) compounds are extremely unstable in air, which greatly complicates the work.

Herein we discuss the recent achievements of our research group on the use of air-stable Ni(II)/NHC precatalysts in the catalysis of C-H arylation, alkylation and alkenylation reactions of heteroaromatic compounds,<sup>1,2</sup> as well as in C-N cross-coupling reactions<sup>3</sup>:



To achieve high activity of catalytic systems based on Ni(II)/NHC complexes, we have used the following approaches: 1) addition of HCO<sub>2</sub>Na, tBuONa or tBuOK to the reaction for *in situ* generation of catalytically active forms of Ni(0)/NHC; 2) synthesis of Ni(II)/NHC precatalysts with two cyclopentadienyl-anion co-ligands acting as internal reducing agents of Ni(II) to Ni(0)

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# SYNERGISTIC CATALYSTS FOR ELECTROCATALYTIC REDUCTION OF CARBON DIOXIDE AND HYDROGEN EVOLUTION REACTION

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We discuss the targeted design of efficient catalysts for carbon dioxide reduction (CO<sub>2</sub>RR) and the hydrogen evolution reaction (HER). The focus will be on innovative approaches that enhance the electrocatalytic efficiency and selectivity of these vital environmental reactions.

The work introduces three main strategies in developing effective electrocatalysts for CO<sub>2</sub>RR. Firstly, the incorporation of specific functional groups into catalyst structures will be highlighted. These functional groups are strategically chosen to enhance the adsorption and activation of CO<sub>2</sub> molecules, thereby facilitating their reduction. Secondly, the creation of specialized surfaces from solutions during the electrochemical reduction process will be discussed. This approach involves engineering the catalyst surfaces at the molecular level to optimize their interaction with CO<sub>2</sub> molecules. The modifications aim to increase the number of active sites and improve the electron transfer characteristics, which are crucial for the efficiency of CO<sub>2</sub> reduction. Thirdly, we demonstrate catalytic systems that, due to their unique geometric configurations, provide selective CO<sub>2</sub> reduction. The design of these catalysts focuses on shaping the spatial arrangement of atoms to create selective pathways for CO<sub>2</sub> conversion, thereby minimizing unwanted reactions and improving overall catalytic performance.

Additionally, the synergistic effects of combining catalysts for CO<sub>2</sub>RR and HER will be explored. By designing catalysts that can effectively perform both reactions, we aim to develop integrated systems that can simultaneously reduce CO<sub>2</sub> and produce hydrogen, a valuable clean energy carrier. This dual functionality not only enhances the practicality of such systems in sustainable energy applications but also increases the overall energy efficiency of the process.

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# VISIBLE-LIGHT PHOTOCATALYSIS WITH METALLA-N-HETEROCYCLIC CARBENE COMPLEXES

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Synthetic approaches of fine organic synthesis based on reactions occurring under the influence of visible light in the presence of photocatalyst allow to obtain organic compounds from available raw materials and to carry out syntheses of complex molecules with high selectivity and in environmentally safe conditions. The development of these approaches can be achieved through the development of novel highly efficient photocatalysts.

In the last two decades, complexes of transition elements with diaminocarbene ligands have occupied a key position in coordination chemistry and catalysis.<sup>1</sup> One type of highly donative diaminocarbene ligands are metalla-*N*-heterocyclic carbenes (MNHC), whose structure is imidazole-2-ylidene, in which instead of a carbon atom in the main chain there is a transition metal atom. The project on the chemistry of diaminocarbenes shows that Pd<sup>II</sup> and Pt<sup>II</sup> complexes with MNHC ligands can be prepared under mild conditions using a one-reactor protocol involving a metal-promoted combination of aromatic isocyanide with  $\alpha$ -aminoazaheterocycles.<sup>2,3</sup> Pt<sup>II</sup>-MNMHC showed high catalytic activity in the hydrosilylation reaction of alkynes upon irradiation with blue or green light.<sup>3</sup>

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# NEW PHOTOCATALYSTS FOR CO<sub>2</sub> REDUCTION UNDER VISIBLE LIGHT

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The involvement of carbon dioxide in chemical transformations is an urgent task not only from the point of view of using CO<sub>2</sub> as a source of carbon, but also to reduce its concentration in the atmosphere. The reduction of CO<sub>2</sub> under mild conditions occurs under the action of additional physical influences, such as light radiation. Thus, exposure to visible or UV irradiation removes thermodynamic restrictions on the reduction transformations of CO<sub>2</sub>. The main factor limiting the practical use of photocatalytic reduction of CO<sub>2</sub> is the lack of effective heterogeneous photocatalysts operating under the influence of visible light, which makes up about 43% of the solar spectrum.<sup>1</sup>

Titanium dioxide is most often used as a semiconductor photocatalyst for CO<sub>2</sub> reduction, the main disadvantage of which is the lack of sensitivity to visible light for pristine TiO<sub>2</sub>. The main strategies leading to sensibilization of TiO<sub>2</sub> to visible light and increase in photocatalytic activity due to interfacial heterojunctions are the creation of composites in which TiO<sub>2</sub> is in contact with narrower bandgap semiconductor materials, as well as the deposition of metallic and nonmetallic cocatalysts on the surface of titanium dioxide.

The report will review new composite photocatalysts for CO<sub>2</sub> reduction under the influence of visible light based on titanium dioxide, such as WB5/TiO<sub>2</sub>, TiZrNbHfTaC<sub>5</sub>/TiO<sub>2</sub>, Ti<sub>3</sub>C<sub>2</sub>/TiO<sub>2</sub> and TiO<sub>2</sub>/Mo<sub>2</sub>C, and compare these materials with traditional g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> heterostructures.

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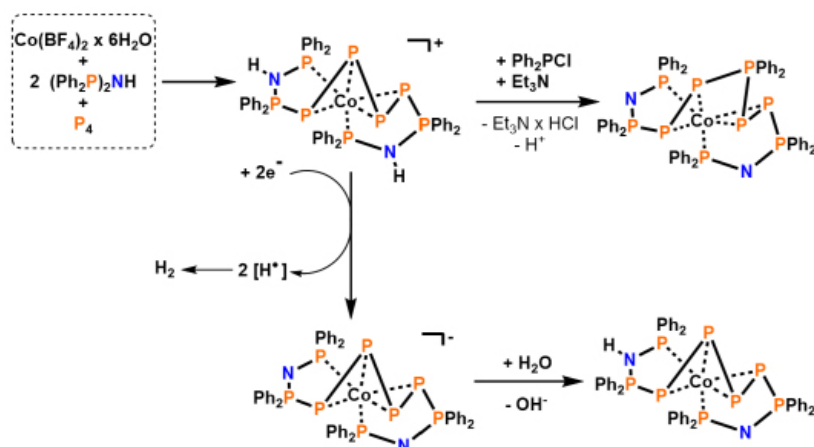
*The work was carried out with the financial support of the Russian Science Foundation, project 24-13-00416.*

# WHITE IS THE NEW BLACK. COORDINATION COMPOUNDS DERIVED FROM WHITE PHOSPHORUS ACTIVATION AS ELECTROCATALYSTS OF WATER SPLITTING TO H<sub>2</sub>

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Transition-metal-mediated white phosphorus (P<sub>4</sub>) activation and transformation have attracted increasing attention as an ecological alternative to organophosphorus compounds. However, the properties of the complexes obtained this way are little studied.



We report a facile approach for P<sub>4</sub> activation and transformation using cobalt complexes bearing PNP ligands.<sup>3</sup> The use of *N,N*-bis(diphenylphosphino)amine as a ligand allows one to transform P<sub>4</sub> tetrahedron into a *zig-zag* chain with the formation of complex [Co(Ph<sub>2</sub>PNHP(Ph<sub>2</sub>)PPPPP(Ph<sub>2</sub>)NHPPH<sub>2</sub>)]BF<sub>4</sub>. This complex reacts with Ph<sub>2</sub>PCl with the functionalization of the polyphosphorus chain and exhibits catalytic activity in hydrogen evolution reaction under the conditions of homogeneous electrocatalysis.

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# CYCLIZATION OF DIHALOARENES IN THE PRESENCE OF NICKEL COMPLEXES WITH DIAZABUTADIENE LIGANDS

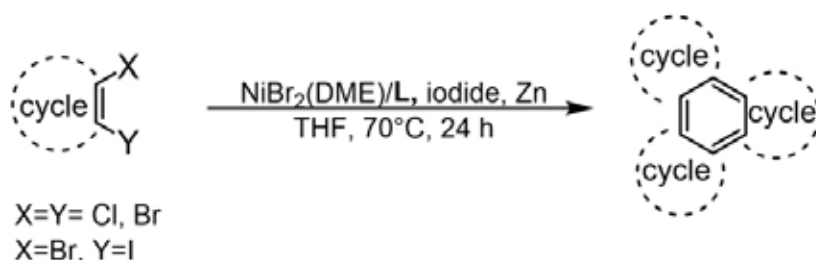
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Due to their unique properties, triphenylenes are important compounds for the development of new materials as well as for a number of applications in analytical, medical and supramolecular chemistry. There are several synthetic strategies for triphenylene derivatives, but most of them are multistage approaches. In this regard, the investigation of alternative one-step and preparative procedures for synthesis of triphenylenes would be a relevant task.

1,2-Dihaloarenes seem to be the most convenient substrates for one-step synthesis of symmetric triphenylenes. Though the scientific literature describes scarce examples of synthesis of triphenylenes from 1,2-dihaloarenes as a result of the reductive cyclization in the presence of nickel catalysts,<sup>1</sup> there are no systematic studies of this method, especially the respective preparative procedures.

In this work, nickel complexes with nitrogen-containing ligands (including diazabutadiene and 2,2'-bipyridyl ligands) were shown to be efficient catalysts of the reductive cyclization of various 1,2-dihaloarenes to form the corresponding triphenylenes. First, optimal conditions of the triphenylene synthesis from 1,2-dibromobenzene and, alternatively, 1,2-dichlorobenzene were found. Further on, the developed catalytic system was studied for the reductive cyclization of 1,2-dihaloarenes bearing various substituents. As a result, various substituted triphenylenes (and, in some cases, tetraphenylenes) were obtained with moderate to high yields followed by unambiguous characterization of the isolated products.



**Figure 1.** Tricyclization of 1,2-dihaloarenes under nickel catalysis

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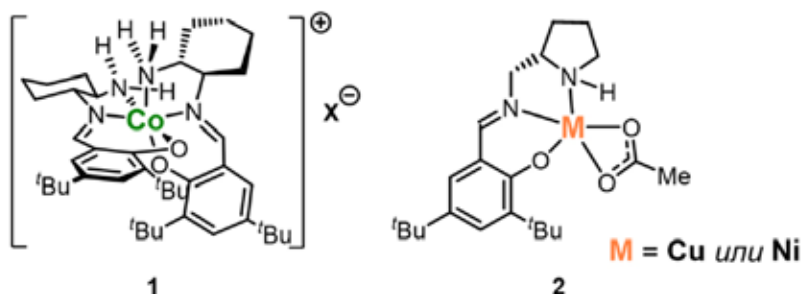
# META-TEMPLATED APPROACH FOR THE DESIGN OF CHIRAL HOMOGENEOUS CATALYSTS

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The rapid development of asymmetric catalysis is driven by the creation of new, efficient, and multifunctional catalytic systems. One area of focus is the use of metal-templated approach to create enantioselective catalysts.<sup>1</sup>

Our laboratory is actively working in this area and has developed new classes of homogeneous catalysts based on octahedral cationic Co(III) complexes,<sup>2-4</sup> and chiral Cu(II) and Ni(II) complexes based on *NNO* ligands.<sup>5</sup> The resulting catalysts demonstrated high activity and stereoselectivity in such asymmetric reactions as the alkylation of O'Donnell's substrate under phase-transfer conditions<sup>2,3</sup> and the Henry reaction.<sup>5</sup> The desired enantioenriched amino acid derivatives and nitro alcohols were produced with enantiomeric excess values of up to 96%.<sup>2-5</sup>



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# SIMPLE PLATINUM ACIDO COMPLEXES IN CATALYSIS OF C-C COUPLING REACTIONS

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Metal-catalyzed cross-coupling reactions have now become a versatile tool in fine organic synthesis as they allow easy assembly of complex chemical structures from simpler building blocks<sup>1-2</sup>. The key intermediates of these reactions are usually metal complexes bearing two organic ligands in a mutual cis-position, the subsequent reductive elimination (RE) of which yields C-C coupling products. In the classic C-C coupling<sup>1</sup>, bis-organic metal derivatives are mostly generated by oxidative addition (OA) of C-electrophile to a metal complex followed by transmetalation of the resulting organometallic intermediate with an organometallic nucleophile. Using Pt, we have shown that such intermediates can be easily generated with no need of pre-formed organometallic nucleophiles, but by play on the electrophilic or nucleophilic properties of Pt in its various oxidation states.

Electrophilic Pt<sup>IV</sup> iodo complexes are able to activate C≡C bond by its iodoplatination forming bis-vinyl Pt<sup>IV</sup> derivatives, which decompose via reductive elimination (RE) to give C(sp<sup>2</sup>)-C(sp<sup>2</sup>) coupling products, *E,E*-1,4-diiodo-1,3-dienes<sup>3</sup>. Using nucleophilic properties of Pt<sup>II</sup> made it possible to realize<sup>4</sup> the sequential OA of two C-electrophiles – MeI and vinyl iodide – to form the methylvinyl derivative of Pt<sup>IV</sup>. Finally, the combination of nucleophilic properties of Pt<sup>II</sup> in the OA and electrophilic properties of the resulting Pt<sup>IV</sup> in the activation of C≡C bond allowed us<sup>5</sup> to generate the MePt<sup>IV</sup>(CH=CHI) species in a sequence of steps: OA of MeI to Pt<sup>II</sup> and further acetylene iodoplatination by MePt<sup>IV</sup>.

The mechanisms of C-C coupling reactions based on combining experimental and dft-computational approaches will be discussed in detail.

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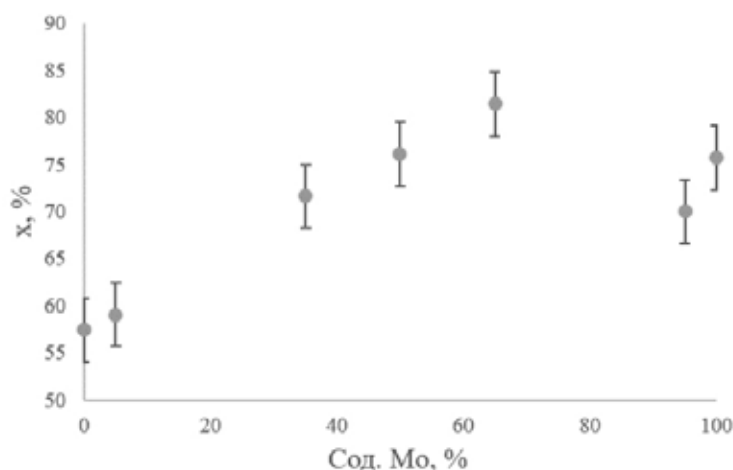
# PHOTOCATALYTIC PROPERTIES OF MIXED MOLYBDENUM AND TUNGSTEN TRIOXIDES WITH DISCOLORATION OF METHYLENE BLUE AS AN EXAMPLE

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Molybdenum and tungsten trioxides are promising candidates for photocatalytic application in wastewater purification from organic dyes. Their mixed trioxides  $\text{MoO}_3\text{-WO}_3$  show synergetic effects on different properties<sup>1</sup> but the influence of  $[\text{Mo}]/[\text{W}]$  molar ratio on photocatalytic properties remains little-studied.

In this work,  $\text{MoO}_3\text{-WO}_3$  oxides in a wide range of  $[\text{Mo}]/[\text{W}]$  molar ratios were obtained by precipitation from ammonium paratungstate and heptamolybdate followed by precipitate peptization. Figure 1 shows the results of a photocatalytic experiment for the model methylene blue decomposition reaction with a UV exposure time of 30 minutes.



**Figure 1.** Dependence of photocatalytic activity on molybdenum content in the sample.

According to the results of XRD and Raman spectroscopy, phase composition corresponds to orthorhombic  $\text{MoO}_3$  [05-0508] and monoclinic  $\text{WO}_3$  [43-1035] for samples with molar ratios  $[\text{Mo}]/[\text{W}]$  95/5, 5/95; at close  $[\text{Mo}]/[\text{W}]$  ratios – compositions  $\text{W}_x\text{Mo}_{1-x}\text{O}_3$  (ex. [32-1391]). Average diameters of particles are in the range of 0.5-1.7 microns, depending on their composition. The highest catalytic activity was demonstrated by a sample with a  $[\text{Mo}]/[\text{W}]$  molar ratio of 65/35: after 180 minutes of reaction, the decomposition of methylene blue is 95.57%.

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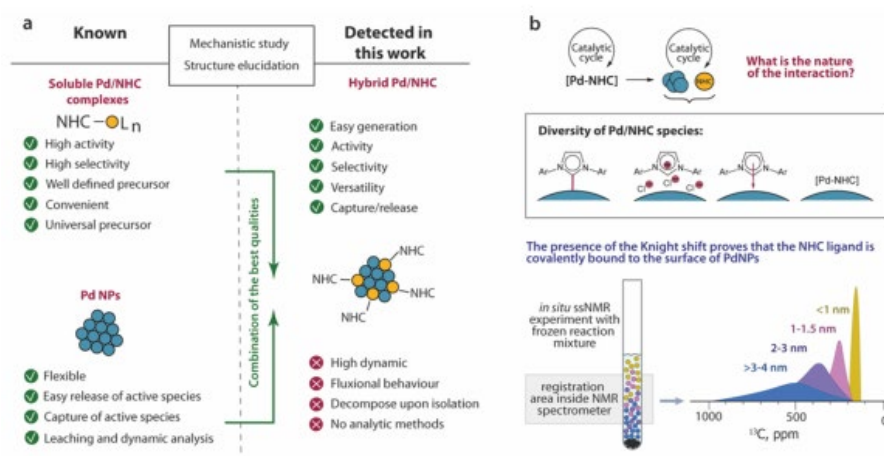
## CONCEPTION OF HYBRID PD/NHC SYSTEMS

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The formation of transient hybrid nanoscale metal species from homogeneous molecular precatalysts has been demonstrated by *in situ* NMR studies in catalytic reactions involving transition metals with *N*-heterocyclic carbene ligands (M/NHC). These hybrid structures provide benefits of both molecular complexes and nano-particles, enhancing activity, selectivity, flexibility, and regulation of active species. However, they are challenging to identify experimentally due to unsuitability of standard methods for homogeneous or heterogeneous catalysis. Using a sophisticated solid-state NMR technique, we provide evidence for the formation of NHC-ligated catalytically active Pd nanoparticles (PdNPs) from Pd/NHC complexes during catalysis. The coordination of NHCs *via* C(NHC)-Pd bonding to the metal surface was first confirmed by observing the Knight shift in the <sup>13</sup>C NMR spectrum of the frozen reaction mixture. Computational modeling revealed that as little as few NHC ligands are sufficient for complete ligation of the surface of the formed PdNPs. Catalytic experiments combined with *in situ* NMR studies confirmed the significant effect of surface covalently bound NHC ligands on the PdNPs catalytic properties formed by decomposition of Pd/NHC complexes. This observation shows the crucial influence of NHC ligands on the activity and stability of nanoparticulate catalytic systems.



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# BIMETALLIC CATALYSTS – NEW IDEAS FOR NEW PROCESSES

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It is impossible to imagine the modern chemical industry without catalytic technologies. More than 80% of all industrial processes occur under conditions of heterogeneous catalysis. The development of new types of heterogeneous catalysts is a key point in the creation of new technologies. We have proposed the concept of producing bimetallic catalysts by selectively modifying supported metal nanoparticles - the active phase or oxide support - with non-noble metal oxides. This approach made it possible to synthesize a highly efficient Pt/CeO<sub>2</sub>-ZrO<sub>2</sub> system for the hydrogenation of carbonyl compounds,  $\alpha$ ,  $\beta$ -unsaturated aldehydes to the corresponding alcohols and nitro compounds of various structures to primary amines at room temperature and atmospheric pressure, which is due to the ability of the system to activate hydrogen already at negative temperatures.<sup>1,2</sup> Selective modification of supported nanoparticles of iron and copper oxides with gold in ultra-low concentrations (<0.1% wt.) provides high activity of catalysts in the oxidation of glycerol to glyceric acid under mild conditions.<sup>3</sup> Modification of supported Pd nanoparticles with Cr<sub>2</sub>O<sub>3</sub> nanoparticles allows the creation of a new type catalysts with an “inverse” structure and new active centers that provide selective hydrogenation of the triple C-C bond to a double bond under normal conditions.<sup>4</sup> Modification of synthetic copper phyllosilicate – a nature mineral – with cerium oxide made it possible to obtain an active catalyst for the unique “one-pot” process of hydroamination of 5-HMF with nitro compounds to obtain a number of hard-to-find N-furfurylamines.<sup>5</sup>

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# SYNTHETIC OPAL IN THE SYNTHESIS OF CO OXIDATION CATALYSTS

**Eurov D.A.,<sup>a</sup> Kurdyukov D.A.,<sup>a</sup> Shilina M.I.,<sup>b</sup> Udalova O.V.,<sup>c</sup>  
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Macroporous materials based on densely packed sub-micron-sized spherical SiO<sub>2</sub> particles, so-called synthetic opals, are applicable in catalysis. For example, the effectiveness of opals decorated with Co and Ce oxides in CO oxidation significantly exceeded that of similar samples based on micro- and mesoporous silicas [1,2]. In the present work, optimal conditions for the use of opal matrices in the synthesis of CO oxidation catalysts based on Co and Ce oxides have been found. Opals were prepared by sedimentation of SiO<sub>2</sub> particles from an aqueous suspension followed by drying and annealing at 800 °C as described in [1,2]. Co and Ce oxides were introduced by capillary impregnation; their loading and order of introduction were varied.

Catalytic oxidation of carbon monoxide was carried out in three modes: in an inert atmosphere, in excess of H<sub>2</sub> (PROX), and in the presence of hydrocarbons and nitrogen oxides under conditions of prompt thermal aging when heated to 1000 °C, simulating the operation of automotive three-way catalysts. In all test modes, the best results were achieved for bimetallic systems obtained by consecutive deposition of cerium oxide and then cobalt oxide on the opal matrix in a ratio of 1:3. According to SEM, TEM, XPS, and IR-spectroscopy, under these conditions, a uniform distribution of highly dispersed oxides on the surface of the silica matrix is achieved. The synergistic effect of Co and Ce oxides is manifested in increased activity, selectivity, and stability of the obtained catalysts.

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# SUPPORTED Pt-MeO<sub>x</sub>/CNT CATALYSTS FOR THE DBT OXIDATION IN HYDROCARBON FUELS

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Oxidative desulfurization (ODS) is a non-hydrogen technology for the removal of dibenzothiophene (DBT) and its alkyl-substituted derivatives from hydrocarbon fractions [1]. The use of molecular oxygen as an available oxidizer under mild conditions determines the advantages of the technology in the production of low-sulfur diesel fuel (with a sulfur content of less than 10 ppm) at low-capacity refineries [2]. For the practical application of the ODS technology, it is necessary to solve a number of problems, primarily related to the synthesis of highly active and selective catalysts.

Carbon nanomaterials (CNT), including those with deposited Pt nanoparticles, are of interest for the oxidation of sulfur compounds at low temperatures and atmospheric pressure [3]. The aim of this work was to develop effective CNT-based catalysts for the oxidative desulfurization of hydrocarbon fractions.

The presentation describes the influence of various methods of synthesis and activation of CNTs, their modification by oxides of transition (CuO, MoO<sub>x</sub>, etc.) and noble (Pt, Pd) metals on their effectiveness in the ODS process. The composition, morphology and structure of catalysts were studied using a complex of physicochemical methods (CHNS-analysis, DTA-TG-MS, TEM, TPR, etc.). The selection of optimal conditions for the ODS process was carried out. The mechanisms of oxidation of typical sulfur compounds of hydrocarbon fuels (thiophene, benzothiophene, DBT and alkyl-substituted derivatives) were studied.

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# NANOSTRUCTURED TITANIUM DIOXIDE IN POLYMER MATRIX AS AN EFFECTIVE PHOTOCATALYST FOR WASTE WATER TREATMENT

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The photocatalytic activity of nanostructured poly(titanium oxide) (PTO NPs), including doped Au or Ag NPs, in polymer matrix of different nature - organic-inorganic copolymers based on poly(hydroxyethyl methacrylate) and chitosan - has been investigated. A comparison of the PTO NPs properties and powdered  $\text{TiO}_2$  with micron-sized particles of anatase polymorphic modification was carried out. Polymer composites were prepared as films using  $\text{Ti}(\text{OPr})_4$  and precursors of Au and Ag NPs. During the synthesis process, anatase-type PTO NPs, whose size can be controlled from 6 to 900 nm, Au NPs (6 - 12 nm) and Ag NPs (9 - 20 nm) uniformly distributed in the organic polymer matrix were formed. The samples' structure was confirmed by SAXS, XRD and SIMS methods. Photocatalytic properties of nanocomposites were confirmed:

1) in the decomposition of organic water pollutants - azo-dyes (methylene orange, congo red, methylene blue), phenol and para-nitrophenol under UV and visible light irradiation. It was found that nanostructured PTO and PTO doped with Au or Ag NPs were 50% and 90-100% more effective than powdered  $\text{TiO}_2$ , respectively, under UV-irradiation. Moreover, doping of PTO with Au or Ag NPs leads to an increase in water purification by ~200 times under visible light irradiation.

2) in the decomposition of pollutants on the materials' surface - on the example of stearic acid as a model system.

3) in the neutralization of pathologically dangerous bacteria. The samples inactivate Gram-positive microorganism *S. aureus* for 1 hour by 100%, and Gram-negative microorganism *E. coli* – by 54.1%.

The developed materials are promising for use in elements of water treatment systems and self-cleaning coatings under irradiation with light in a wide range of wavelengths.

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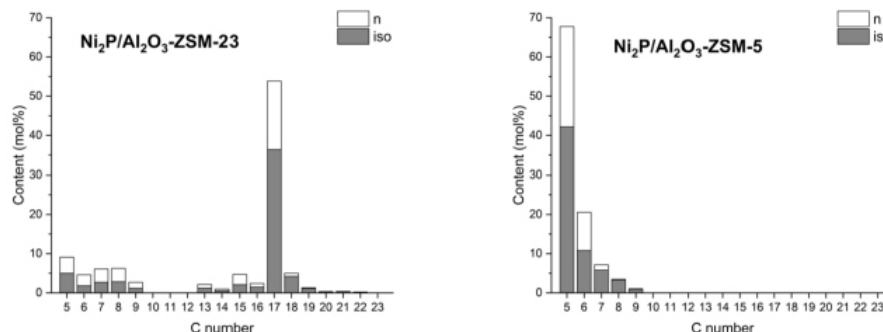
# RAPESEED OIL HYDROCONVERSION OVER NICKEL PHOSPHIDE CATALYSTS SUPPORTED ON ALUMINA-ZEOLITE COMPOSITES

**Shamanaev I.V., Vlasova E.N., Pakharukova V.P., Gerasimov E.Yu., Yakovlev I.V., Fedorov A.Yu., Bukhtiyarova G.A.**

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One-step hydrodeoxygenation – hydroisomerization – hydrocracking (hydroconversion – HC) is an attractive way to produce high quality fuels from triglyceride-based feedstocks such as nonedible vegetable oils. Nickel phosphide has high efficiency in hydrodeoxygenation and does not require addition of sulfur-containing compounds like conventional hydrotreating NiMoS/Al<sub>2</sub>O<sub>3</sub> catalysts.<sup>1</sup> In this work we prepared Ni<sub>2</sub>P catalysts on composite Al<sub>2</sub>O<sub>3</sub>-zeolite supports, studied their physicochemical properties (by chemical analysis, N<sub>2</sub> adsorption, XRD, TEM, XPS, <sup>27</sup>Al and <sup>31</sup>P MAS NMR) and catalytic properties in HC of rapeseed oil (290–350 °C, 2.0 MPa, LHSV=5.3 h<sup>-1</sup>). As zeolite component we used ZSM-23, ZSM-22, and ZSM-5. The content of zeolite was 30%, the content of Ni was 5–6%.

Both XRD and TEM analysis confirmed formation of Ni<sub>2</sub>P. Particle size distributions in all catalysts were similar with mean size of 6–8 nm. The quality of the products was shown to depend both on the zeolite nature as well as on reaction conditions (Figure 1). By tuning the properties of the catalyst, it is possible to obtain products such as biogasoline, bio-jet, and green diesel.



**Figure 1.** Rapeseed oil hydroconversion products distribution. 340 °C, 2.0 MPa, 5.3 h<sup>-1</sup>.

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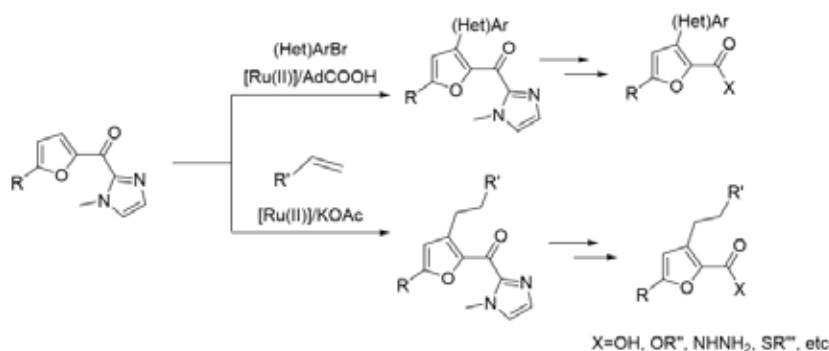
# A NEW APPROACH TO THE SYNTHESIS OF C-3-FUNCTIONALIZED DERIVATIVES OF 2-FURANCARBOXYLIC ACIDS BASED ON RUTHENIUM-CATALYZED REACTIONS OF C-H FUNCTIONALIZATION

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Derivatives of furancarboxylic acids obtained from plant biomass carbohydrates are of interest as a renewable source of chemical feedstock for the production of polymers, bioactive substances, and other valuable chemical products<sup>1-3</sup>. However, the methods of functionalization of such compounds currently include either the use of functional groups or reactions, including transition metal catalysis, at the more active position 5, while selective functionalization of position 3 of the furan core is a more difficult task<sup>4</sup>.

Here a new methods for selective C(3)-H functionalization of furan core of 2-furoyl-N-methylimidazoles under ruthenium catalysis will be presented. In this case, the imidazole fragment acts as a directing group, and the resulting C-3 functionalized products can be easily converted to the corresponding furan carboxylic acid derivatives.



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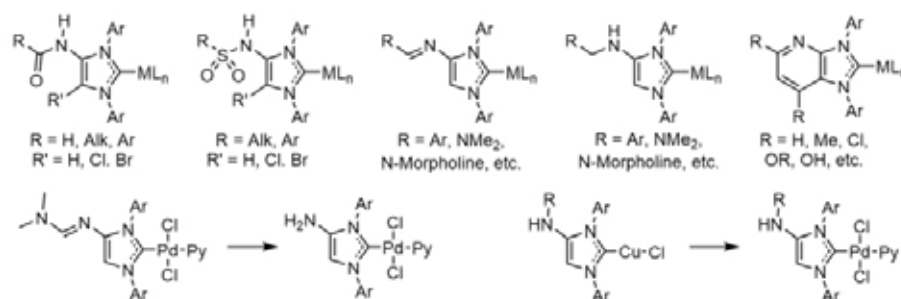
# 4-AMINOIMIDAZOLIUM SALTS AS PRECURSORS OF FUNCTIONALIZED M/NHC

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The design of the N-heterocyclic carbene (NHC) molecule remains a pressing problem in modern organic synthesis due to the wide application of M/NHC complexes as homogeneous catalysts.<sup>1</sup> In particular, 4-(NHR)imidazole derivatives have proven to be of interest.<sup>2</sup>

The synthetic potential of previously unknown 4-(NH<sub>2</sub>)imidazolium salts, for which a convenient method of synthesis has been developed by our team, is considered in this work.<sup>3</sup> The regularities of their interaction with electrophilic reagents and further transformations are shown. The optimal conditions for the metalation of the obtained proligands on the carbene atom C2 have been demonstrated, taking into account the minimization of the undesirable formation of "abnormal" C5 complexes, revealed in a number of cases of palladation of NH-acid derivatives.



In addition to obtaining various functionally substituted M/NHC complexes (M = Pd, Ni, Cu, Au, etc.), the possibilities of their post-modification and transmetalation are considered, and the high catalytic activity of some representatives in Suzuki-Miyaura, Buchwald-Hartwig, etc. cross-coupling reactions is shown.

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# CATALYSTS BASED ON Cu/Ce-MODIFIED ZEOLITES FOR OXIDATION OF CARBON MONOXIDE

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The peculiarities of the crystal structure of zeolites make it possible to specifically create catalysts on their surface with new types of active centers that are not typical for traditional oxide systems. We recently showed that in catalysts based on cobalt modified zeolite ZSM-5, cobalt  $[\text{Co}_x\text{O}_y]^{n+}$  ( $n = 1, 2$ ) oxocations containing Co(III) play the key role in adsorption and catalysis<sup>1</sup>. The introduction of cerium into such systems leads to an increase in catalytic activity<sup>2,3</sup>. This work examines the activity and synergy in the action of bimetallic systems based on Cu/Ce zeolites in the reaction of CO oxidation in the absence (TOX) and presence (PROX) of hydrogen. A series of catalysts with different ratios of copper and cerium were synthesized using ZSM-5 zeolites with different ratios of Si/Al = 40, 28 and 15 and Beta (Si/Al = 19). According to TEM, XRD, XPS, diffuse reflectance UV-vis spectroscopy, DRIFT spectroscopy of adsorbed CO and H<sub>2</sub>-TPR, the effect of metal synergism in the oxidation of CO on copper/cerium catalysts is due to the participation of two types of active centers, the contribution of which is determined by the ratio of metals and the aluminum content in zeolite framework. At Cu/Ce  $\geq 1$ , the key role is played by Cu<sup>+</sup> ions associated with CeO<sub>2</sub> particles on the surface, and at Cu/Ce < 1 and low Si/Al values, the largest contribution to catalysis is made by mixed copper-cerium oxocations in zeolite channels<sup>4,5</sup>. The Cu/Ce-ZSM-5 catalyst with Cu/Ce=0.5 allows reducing the residual CO concentration in hydrogen to 10 ppm.

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# ISOMERIZATION OF $\alpha$ -PINENE OXIDE ON ALUMINUM SILICATE NANOTUBES IN GREEN SOLVENTS

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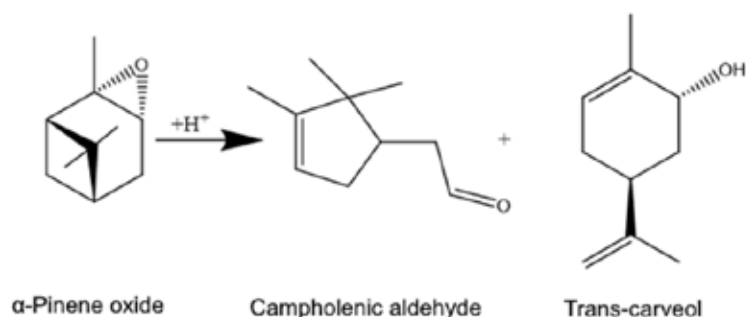
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The main products of  $\alpha$ -pinene oxide isomerization are campholenic aldehyde and Trans-carveol, used in the perfume industry<sup>1</sup>. Aluminosilicate nanotubes are promising catalysts for such reactions<sup>2</sup>. In this work, the catalytic properties of halloysite (HNT, Sigma-Aldrich) and synthetic kaolin nanotubes (KNT) were studied for the first time. KNT was obtained by sequential intercalation of kaolin (Uzbekistan) with dimethyl sulfoxide (DMSO), methanol and cetyltrimethylammonium chloride. After functionalization of nanotubes with piranha solution ( $\text{H}_2\text{SO}_4\text{-H}_2\text{O}_2$ ), the concentration of acid sites on their surface reached 59.0  $\mu\text{mol/g}$ .



It was established that on the studied catalysts (HNT-Pir, KNT-Pir) the reaction proceeds efficiently in a number of “green” solvents with the highest selectivity to *trans*-carveol (56.8%) in DMSO, and to campholenic aldehyde (50.4%) in ethyl lactate upon complete conversion of the reagent.

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# MECHANISM OF INTENSIFICATION OF GAS-CHEMICAL REACTIONS IN A REACTOR WITH A MEMBRANE CATALYST

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The intensification of the gas-chemical catalytic reaction of dry reforming of methane (DRM) was established by us on porous membrane catalysts (MC) and is based on a new type of activated mass transfer for catalysis – thermal slip. This phenomenon is observed in the pores of the Knudsen range and is induced by the tangential temperature gradient in the open pore channels of the catalytic layer MC. As it was established<sup>1</sup>, intensification in the DRM process is expressed in an increase in the methane cracking reaction rate constant by about an order of magnitude (20-40 times) compared to a similar constant on a traditional catalyst (crushed or powdered) of identical composition under the same conditions (same process temperature, same composition of the reagent mixture) of this process. Taking into account the peculiarities of mass transfer in the pores of the MC under conditions of thermal slip, the kinetic scheme of the DRM was substantiated and its mathematical description was obtained.

Using this mathematical description, the rate constants of forward and reverse reactions were determined at all intermediate stages of the DRM, both on membrane and traditional catalysts. We also used a mathematical description in the analysis of the operating modes of a reactor with a membrane catalyst. It was found that intensification is observed in all modes of the membrane reactor, but with different values of the rate constants of direct and reverse reactions at the intermediate stages of the DRM. It turned out that the manifestation of thermal slip is not limited only to the intensification of heterogeneous stages, but also manifests itself in a change in the state of equilibrium. For example, in the contactor mode, all heterogeneous stages of DRM took place as irreversible reactions. At first glance, this unexpected result was explained not by the "selectivity of the transfer of one of the products of the reversible reaction across the membrane", as it happened in the experiments of Academician V.M. Gryaznov, but by two features of UKM on membrane catalysts. First, all the heterogeneous stages of tDRM-process occur with an increase in the volume of reaction products. And, secondly, due to the rarefied state of gases in the pore channels of the catalytic layer of the membrane catalyst.

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# STRUCTURED CATALYSTS FOR FUEL PROCESSORS AND ELECTROCHEMICAL GENERATORS: FROM R&D TO PILOT-SCALE PRODUCTION

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The report summarizes the results of long-term works carried out at the Boreskov Institute of Catalysis on the development of structured catalysts and their synthesis methods, and discusses examples of reactor designs, based on these catalysts, for producing synthesis gas from various hydrocarbon feedstock: natural gas, liquefied petroleum gas (propane-butane mixtures), alcohols, ethers, liquid hydrocarbons for fuel cell feeding applications [1-3]. Approaches are discussed regarding the use of platform solutions for unifying the basic stages of the catalyst manufacturing process in order to improve its technological effectiveness (manufacturability) and reduce costs at organizing pilot scale production.

The data are summarized on the performance of variously composed catalysts based on noble metals (Rh, Ru, Pd, Pt), transition elements (mainly Ni, Co, Cu), bimetallic systems in combination with varying the support from individual or mixed oxides of Zr, Ce, Gd, La, Y, Pr, Al, as well as those doped with alkali and alkaline earth metals. The experience of their use in electrochemical generators based on fuel cells is discussed.

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# IMMOBILIZED IONIC LIQUIDS WITH METAL-CONTAINING ANIONS IN CATALYSIS

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Ionic liquids (ILs) are widely used as solvents and extractants, and, in the presence of an active center in the cation or anion, as catalytic compositions. These properties are also preserved when ILs are applied in the form of thin layers onto supports of various natures, and the resulting solid materials have all the advantages of heterogeneous catalysts<sup>1</sup>.

This work presents the results of many years research conducted by the authors using a wide range of physicochemical methods on the composition, structure and catalytic properties of immobilized ILs with metal-containing anions, such as halide complexes of iron and copper, as well as tungsten and molybdenum polyoxometalates. Imidazolium derivatives with different alkyl substituents, including those containing acid centers, were used as organic cations. The resulting solid catalysts were used in various organic reactions involving halocarbons, sulfur- and nitrogen-containing compounds<sup>2-4</sup>. One of the important areas of these materials application is the peroxide oxidation of heteroatomic components of hydrocarbon feedstocks<sup>5,6</sup>.

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# APPLICATION OF SHAPE SELECTIVITY CONCEPT FOR PREDICTION OF CATALYTIC AND ENANTIO SELECTIVITY OF POROUS MATERIALS

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Based on the Shape Selectivity concept, an algorithm is proposed to predict the selective effect of porous materials, for example zeolites, carbon tubes containing regular nanoscale pores on chemical and electrode processes. The algorithm is based on the theoretical determination of the adsorption energies of molecular "probes" on clusters of tested porous materials.

The use as molecular probes of cyclic transition states of multichannel reactions, for example, the Prince reaction, makes it possible to identify, according to the calculation of adsorption energy differences ( $E_{ads}$ ), the range of diameters at which zeolites and nanotubes should exhibit the greatest selective catalytic activity with respect to a given channel<sup>1-3</sup>. The nature of the dependence of the calculated values  $E_{ads}$  of the transition state on the diameter of the cavity coincides well with the experimental dependence of the change in the activation energy on the same materials.

Considering enantiomeric analytes as molecular "probes" using the same algorithm makes it possible to determine chiral modifiers in the composition of composite enantioselective sensors with the highest enantioselectivity for a given analyte. The application of the algorithm was tested not only on the example of homochiral zeolites and nanotubes, but also on cyclodextrins, substances of molecular structure also having cavities of a certain size. In all cases, there is a correlation between the calculated difference  $E_{ads}$  of the enantiomers of the analyte on the chiral modifier and the experimental value of the enantioselectivity of the sensor containing the same chiral modification<sup>4-5</sup>.

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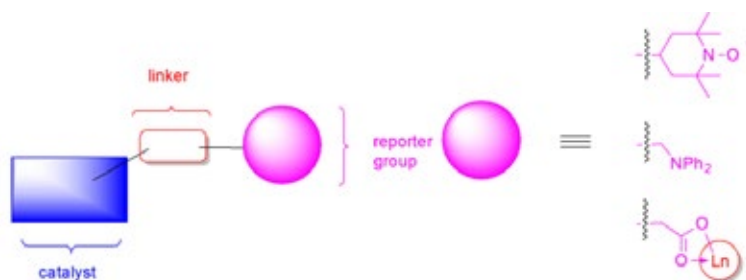


# BISPIDINE ORGANOCATALYSTS WITH LUMINESCENT AND RADICAL LABELS

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Our laboratory works on the creation of catalysts based on catalytically active bispidines conjugated with additional "reporter" fragments. Changes in the response of the system during the reaction process can be monitored due to changes in the response of the reporter group. As the latter, the following are used: (a) chelating fragments for coordination with luminescent lanthanide ions; (b) free-radical TEMPO-type fragments; (c) luminescent organic fragments of the triarylamine type.



The report discusses the most recent achievements of our laboratory in the field of synthesis of bispidines labeled with free radicals<sup>1,2</sup> and luminescent groups<sup>3</sup>, and the possibilities of their application to the study of the mechanism of the Michael reaction<sup>4</sup>.

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# INFLUENCE OF PROMOTER ADDITIVES Pt, Pd, Ru AND Ni ON THE CATALYTIC PROPERTIES OF BIFUNCTIONAL COBALT CATALYSTS FOR THE SYNTHESIS OF HYDROCARBONS FROM CO AND H<sub>2</sub>

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XTL (X-to-liquid) technology for the production of fuels and other products with high added value from synthesis gas by catalytic Fischer-Tropsch synthesis combined with hydroprocessing of the resulting hydrocarbons in one reaction apparatus is commercially promising. Synthetic oil produced on a bifunctional cobalt catalyst developed at the Nanotechnologies and New Materials Research Institute contains a large amount of alkenes (> 40%), which negatively affect the performance properties of motor fuels. It is possible to reduce the proportion of unsaturated hydrocarbons by adding additional hydrogenating components to the catalyst, for example, Pt, Pd, Ru and Ni. In this case, the method (impregnation, ion exchange) and sequence (into an acidic or cobalt-containing catalyst, onto a finished catalyst, etc.) of introducing promoting additives is important. Thus, the purpose of the work is to study the effect of the method of introducing Pt, Pd, Ru and Ni promoting additives on the catalytic properties of a bifunctional cobalt-based catalyst for the combined process of Fischer-Tropsch synthesis and hydrocarbon hydroprocessing.

It has been shown that the content of unsaturated hydrocarbons in the synthesis products when introducing a hydrogenating component by impregnation of zeolite increases in the series: Pd<Pt<Ru<Ni, and the content of branched hydrocarbons decreases in the series: Pt>Pd>Ru>Ni. In the synthesis products obtained on catalysts containing Pt and Pd, the proportion of unsaturated hydrocarbons is practically the same, and the content of branched hydrocarbons is 30% higher on a catalyst promoted by Pt.

It has been established that the most effective way to introduce the hydrogenating additive Pt into the catalyst is to apply Pt to the zeolite using the ion exchange method. The catalyst obtained by this method is characterized by the highest iso/n index at the studied temperatures of 240 °C and 250 °C - 1.55 and 1.86, respectively.

*The work was carried out within the framework of the Russian Science Foundation grant 23-73-10108.*

# DEVELOPING PALLADIUM CATALYSTS FOR REDUCTIVE DEBENZYLATION OF HEXAAZAISOWURTZITANE DERIVATIVES

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Recently, the chemistry of hexaazaisowurtzitane derivatives has received a new boost in development, including not only powerful explosives but also promising biologically active compounds. For example, thiovercine, developed at the IPCET SB RAS, is a promising non-narcotic analgesic that has passed the preclinical stage. The two-stage reductive debenzylation of the hexabenzyl derivative with hydrogen on palladium catalysts in the presence of acylating agents is the key step in the known schemes for the industrial synthesis of hexaazaisowurtzitane derivatives. The process is complicated by the high requirements for the size of the palladium particles on the support. This is associated with a low TOF value. Accordingly, catalyst deactivation occurs mainly by increasing the size of the Pd particles from 3-5nm in the original catalyst to 20-30nm or more in the spent catalyst.

A number of catalysts based on activated carbons and carbon materials and ceramic supports, including those coated with carbon<sup>1</sup>, were developed. Methods of stabilising Pd particles have been proposed. These involve the use of carbon materials obtained by pyrolysis of nitrogen and oxygen containing polymers in a matrix of activated carbons and on the surface of ceramics. It has been shown that the most active catalysts are those prepared on supports based on nitrogen-containing precursors. In this case, the amount of Pd can be reduced to 3%. The catalysts prepared have a low Pd loss during reductive debenzylation and are suitable not only for the classical process using acetic anhydride, but also for the use of other acylating agents, such as Boc- anhydride<sup>2,3</sup>. This leads to an extension of the synthetic possibilities of the method and makes it possible to obtain hexaazaisowurtzitane derivatives substituted in positions 2, 6, 8 and 12.

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# SYNTHESIS OF IMINE DERIVATIVES OF CAMPHOR USING Zn-CONTAINING IONIC LIQUIDS

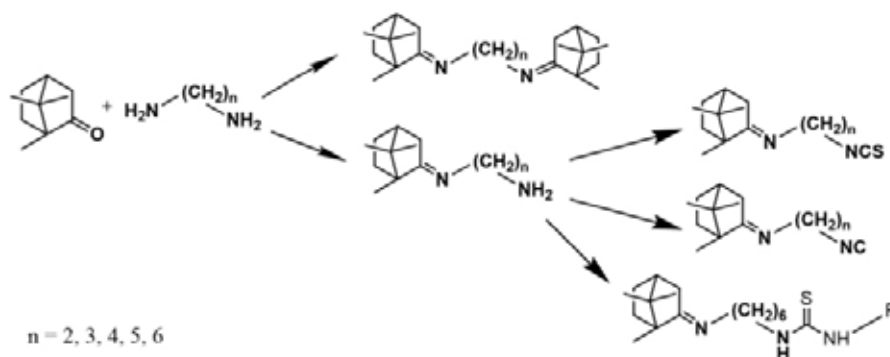
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Currently, there is increased interest in two areas of application of ionic liquids: in the processing of biomass and lignocellulosic waste to obtain valuable chemical products, as well as the development of heterogeneous catalytic systems involving ionic liquids or catalysts in which the ionic liquid is a structural element.

The condensation reaction of camphor with aliphatic diamines does not occur without the use of catalysts. Traditionally used catalysts (p-toluenesulfonic acid,  $\text{BF}_3 \cdot \text{Et}_2\text{O}$ ,  $\text{ZnCl}_2$ ) do not allow the achievement of high yields of products, even when carrying out the reaction under harsh conditions (e.g. boiling the reaction mass without a solvent). In this work, we propose the use of Zn-containing ionic liquids as catalysts for this reaction.

The catalytic activity of zinc neodecanoate and zinc 2-ethylhexanoate in the condensation reaction of camphor with diamines was studied. Zinc carboxylates that we used showed higher efficiency compared to the standard catalyst for this process -  $\text{BF}_3 \cdot \text{Et}_2\text{O}$ , and also allow the process to be carried out under mild conditions. Methods for the synthesis of symmetrical diimines and monosubstituted imines containing an amino group in the presence of Zn-containing ionic liquids with yields of more than 90% have been developed. The resulting monosubstituted imines were modified at the amino group to produce isothiocyanates, isonitriles and 1,3-disubstituted thioureas.



*This work was carried out within the framework of the state assignment for scientific research of the interregional scientific and educational center of the South of Russia with the financial support of the Ministry of Science and Higher Education of the Russian Federation (FZUS-2024-0001)*

# BIFUNCTIONAL CATALYSTS BASED ON TRANSITION METAL CHLORIDES AND IONIC LIQUIDS IN SILANE PRODUCTION

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In Russia, the need for polycrystalline silicon (poly-Si) in the micro- and nanoelectronic industry against the background of the foreign supplies cessation necessitates the development and expansion of domestic production of high-purity poly-Si precursors (monosilane, dichlorosilane, trichlorosilane, etc.). As a consequence, there is a problem of disposal of a large amount of a highly toxic by-product of its production – silicon tetrachloride (STC). Thus, research in the field of improving the traditional poly-Si production in order to increase industrial and environmental safety, as well as to reduce its production cost through the development and use of highly selective catalytic systems is relevant today. In this work, bifunctional catalysts based on a porous polymer support (copolymer of divinylbenzene and 4-vinylbenzyl chloride) functionalized with imidazolium ionic liquids, which exhibit high catalytic activity in the process of trichlorosilane disproportionation (TCS)<sup>1</sup>, and metal chlorides (rhenium, nickel and cobalt), which have shown good results in the STC hydrogen reduction reaction<sup>2</sup>, are proposed. The catalytic activity was evaluated by holding a mixture of TCS and helium in a thermostatically controlled reactor filled with the catalyst with subsequent hydrogen supply for the STC hydrogenation reaction. The gas mixture from the reactor was analyzed by gas chromatography-mass spectrometry. The bifunctional catalyst exhibits its activity both in the TCS disproportionation reaction (monosilane yield is 2.73% with the maximum theoretical 5.9%) and in the STC reduction reaction (STC conversion is 23%).

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*This work was financially supported by the Ministry of Science and Higher Education of the Russian Federation project number FSWR 2022-008.*

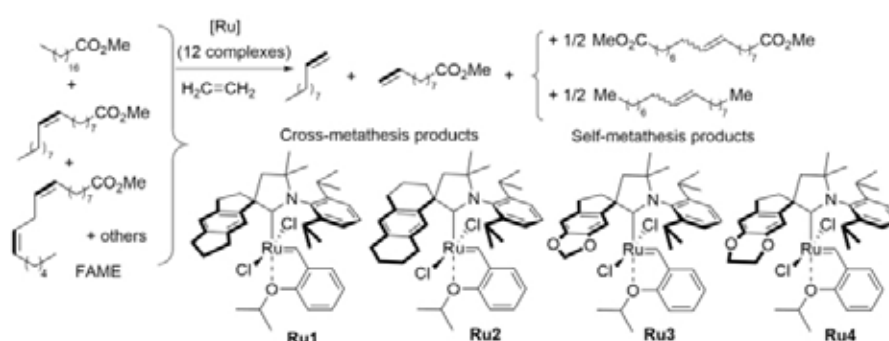
# OLEFIN METATHESIS: DEVELOPMENT OF ORIGINAL ETHENOLYSIS CATALYSTS FOR THE PROCESSING OF RENEWABLE PLANT RAW MATERIALS

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Cross-metathesis of renewable fatty acid esters (FAME) derived from vegetable oil with ethylene (ethenolysis) using selective catalysts (Fig. 1) is a commercially promising way to produce methyl ester of decenoic acid and 'bio'decene-1, environmentally and economically more favourable compared to traditional methods of synthesis of these compounds used in the production of group IV motor oils and surfactant compounds.



**Figure 1.** Etenolysis of FAME

In the course of our research, a new one-pot approach to high-performance catalysts for ethenolysis has been developed, allowing scaling of catalyst synthesis and their use in the production of decene-1 and decenoic acid methyl ester from FAME. A series of new ruthenium-carbene complexes Ru1-Ru12 were synthesised. The Ru2 complex proved to be the most productive catalyst for the cross-metathesis of FAME with ethylene, demonstrating a TON of 215800 and a selectivity of 98% at a loading of 2 ppm.

*This work was supported by the Russian Science Foundation, grant 24-43-20016.*



# HYDROCARBONS PROCESSING ON COFENI-M (M= Pd, Cu) MULTICOMPONENT SYSTEMS FOR THE PRODUCTION OF CARBON NANOMATERIALS

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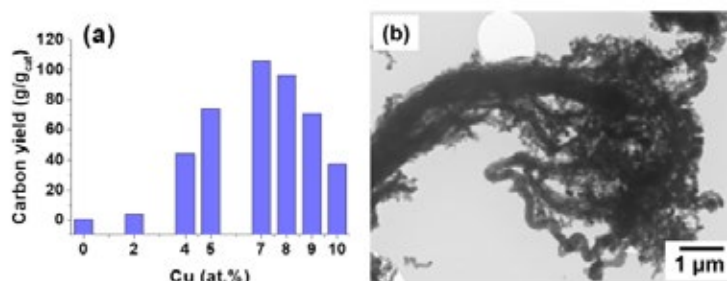
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Decomposition of associated petroleum gas (APG) is one of the main challenges for the oil and gas industry. Catalytic pyrolysis of APG, consisting mainly of light hydrocarbons  $C_1$ - $C_6$ , is a promising approach. As a result, hydrogen and carbon nanomaterial in the form of nanofibers (CNF) can be produced<sup>1</sup>. In turn, CNF are of particular attention in the field of materials science because of their unique physical and chemical properties.

Multi-component alloy systems (MCA) containing from 4 different metals are attracting more and more interest of scientists due to the striking synergetic effect. It is manifested when MCA are used in various catalytic processes<sup>2</sup>.

In this work it is shown that using CoFeNi-M alloy systems (M=Pd, Cu) it is possible to obtain more than 50 g of CNF per 1 g of catalyst (Fig. 1) in the catalytic pyrolysis reaction.



**Figure 1.** (a) - Dependence of carbon yield (g/g<sub>cat</sub>) on Cu concentration in the sample. Experimental conditions:  $C_2$ - $C_4$ /H<sub>2</sub>/Ar, 30 min. (b) - TEM data of CNF sample.

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# SYNTHESIS OF HETEROGENEOUS MANGANESE-OXIDE CATALYSTS USING PHYSICAL INFLUENCES AND THEIR APPLICATION IN THE OXIDATION OF HYDROCARBONS

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Manganese has been used as an active component in the development of heterogeneous catalysts for the oxidation of isopentane, since, compared to other metals, such as cobalt, it provides a soft oxidation of hydrocarbons.

The main principles of the process of liquid-phase oxidation of isopentane with an oxygen-nitrogen mixture in the presence of a heterogeneous manganese oxide catalyst under periodic conditions have been established. With an increase in the duration of oxidation, as well as the concentration of Mn in the catalyst, the conversion of isopentane in the reaction mass increases, accompanied by the accumulation of isopentane hydroperoxide (HPIP) and other oxygen-containing products in the reaction mass. With an increase in the process temperature in the range of 90-120°C, the conversion of isopentane increases, the content of oxygen-containing products in the reaction mass increases from 0.2 to 69.9%, but the selectivity for alcohols decreases.

To increase the efficiency of manganese-oxide heterogeneous catalysts, ultrasonic (US) and supercritical fluids were used at the stage of catalyst synthesis.

Conditions for the preparation of a manganese-oxide catalyst in an ultrasonic field were selected, providing an isopentane conversion of 69.75%, a selectivity for oxygen-containing products of 85.74%, compared to a catalyst sample obtained without ultrasonication, an isopentane conversion of 22.50%, a selectivity for oxygen-containing products 62.21%. This indicates the prospects of using ultrasonics in the production of heterogeneous manganese oxide catalysts for the oxidation of hydrocarbons.

Samples of manganese-oxide catalysts obtained by impregnating gamma aluminum oxide with an excess of aqueous solutions of manganese salts with different manganese contents under supercritical conditions were synthesized and characterized.

It has been shown that maximum activity is observed for catalysts obtained with a manganese content of 2.5% at  $T = 350^{\circ}\text{C}$ , while the selectivity for alcohols increases with increasing manganese concentration.

# INVESTIGATING THE RELATIONSHIP BETWEEN THE ACTIVITY OF METAL-FREE OXYGEN REDUCTION REACTION CATALYSTS AND THE STRUCTURE OF NITROGEN-CONTAINING DEFECTS CREATED THROUGH TARGETED ION BEAM IRRADIATION.

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The oxygen reduction reaction (ORR) is a key process for a number of promising electrochemical energy storage devices, such as fuel cells and metal-air batteries. The performance of these devices is limited by the slow kinetics of ORR at the cathode, which requires the use of catalysts. Commercially available catalysts contain significant amounts of platinum. Although platinum catalysts have the highest activity towards ORR, they are expensive and have low stability. Therefore, reducing the platinum content or eliminating it from the catalyst composition is one of the main directions in the development of electrochemical energy storage technologies using ORR as the electrode reaction.

In this work, a new method for obtaining metal-free ORR catalysts by irradiating the surface of multi-walled carbon nanotubes (MWCNTs) with an ion beam is presented. Pyridinic and pyrrolic nitrogen defects are created in the walls of MWCNTs by this method. The method involves irradiation of MWCNTs with nitrogen ion beams. This leads to the incorporation of nitrogen atoms into the nanotube structure. The structural and chemical changes caused by ion beam treatment have been studied in detail.

It is known that the structure and properties of carbon materials, as well as their nitrogen doping, significantly influence the properties of the resulting catalysts. In this study, the dependence of the activity of the obtained metal-free catalysts on the structure of the nitrogen-containing defects was determined.

*This work was financially supported by the Russian Science Foundation (grant No. 22-13-00035)*

# IDENTIFICATION OF MOLECULAR STRUCTURE OF PHOSPHONIUM SALTS FROM MICROCRYSTALLINE FILMS WITH DEEP LEARNING

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Determining the molecular structure is a fundamental task in chemistry. Classical analytical chemistry methods such as NMR spectroscopy, mass spectrometry, IR spectroscopy and X-ray diffraction analysis are typically used. The recognition of molecular structure from visual appearance is an underestimated and understudied area of research. Advances in microscopy techniques and the application of machine learning methods allow the development of new approaches to this challenging task. The new methodology opens up perspectives for the development of new substances and materials<sup>1-3</sup>. At the same time, the use of micromorphology and microstructure data to predict the properties of new materials is one of the most challenging modern problems in chemistry<sup>4-5</sup>.

In the present work, a neural network model capable of recognition the molecular structure and predicting the properties of quaternary phosphonium salt homologous from scanning electron microscope images of microcrystalline films has been developed and successfully applied. In addition, deep learning was used to transfer the method on optical microscopy images. To demonstrate the versatility of the approach, the model was also tested on binary co-crystallized mixtures of phosphonium salts, which allowed the identification of domains which represent morphologies different from those of individual compounds.

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# INFLUENCE OF PROCESS PARAMETERS ON THE CONVERSION OF CO<sub>2</sub> INTO CYCLIC CARBONATES

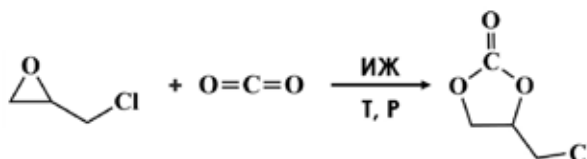
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Due to the continued dependence on fossil fuels, there is currently a problem of capturing CO<sub>2</sub> and converting it into valuable products. One of the approaches is the chemical fixation of CO<sub>2</sub> into cyclic carbonates (CCs), which are used as solvents in various products such as lithium-ion batteries, cleaning and degreasing agents, industrial lubricants and fuel additives. Synthesis of CCs by cycloaddition of CO<sub>2</sub> and epoxides is an atom-economical and safer alternative to the toxic phosgene route. The preparation of CCs using ionic liquids (ILs) as catalysts is evaluated as a promising approach for CO<sub>2</sub> conversion.

In the present work, the influence of various factors on the course of carboxylation reactions of oxides of unsaturated compounds was studied on the example of the model reaction with epichlorohydrin in a wide range of technological conditions of the process with ILs as catalysts.



*The effects of pressure, temperature, catalyst loading, ultrasound and microwave radiation on the conversion and selectivity of the reaction were studied.*

*The work was financially supported by the Russian Science Foundation, project No. 22-79-10302.*

# GRANULAR HIERARCHICAL ZEOLITES YH IN THE SYNTHESIS OF 3,5-XYLENOL BY ACETONE AROMATIZATION

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3,5-Xylenol is a crucial raw material for the production of hydraulic and lubricant fire-resistant liquids, as well as an intermediate in the manufacturing of highly effective disinfectants, insecticides, pharmaceuticals, antioxidants, and dyes. Currently, the most promising method in terms of technology and environmental safety is the production of isophorone through aldol condensation of acetone on heterogeneous catalysts.

There have been no examples found of using zeolite catalysts in the process of obtaining 3,5-xylenol by aromatization of isophorone. Therefore, the goal of this work is to investigate the catalytic properties of new catalysts based on modified metal oxide granulated zeolite with a hierarchical (micro-meso-macro) porous structure Na-Yh in the mentioned reaction.

It has been established that among the zeolite catalysts Na-Yh, HNa-Yh, H-Yh, MgO/Na-Yh, La<sub>2</sub>O<sub>3</sub>/Na-Yh, TiO<sub>2</sub>/Na-Yh, the most active and selective in the synthesis of 3,5-xylenol is the zeolite La<sub>2</sub>O<sub>3</sub>/Na-Yh (the selectivity of the target compound formation is 69% at 94% isophorone conversion). Similar results to zeolite La<sub>2</sub>O<sub>3</sub>/Na-Yh were achieved with the MgO/Na-Yh sample (selectivity for 3,5-xylenol 63%, isophorone conversion 87%).

The high activity and selectivity of zeolites La<sub>2</sub>O<sub>3</sub>/Na-Yh, MgO/Na-Yh are due to the presence of fundamental centers, Lewis acid centers, and a low concentration of weak Brønsted acid centers. Zeolites with strong Lewis and Brønsted acid centers on their surface contribute to the transformation of isophorone into trimethylbenzenes (mesitylene, pseudo-cumene, and hemimellitol), and further into *o,m,p*-xylols.

*The work was carried out with the financial support of the Russian Science Foundation, grant No. 23-13-00213.*



# DEVELOPMENT OF ALUMOSILICATE CATALYSTS FOR SELECTIVE SYNTHESIS OF HIGH-VALUE PRODUCTS FROM VEGETABLE RAW MATERIALS

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Creating valuable chemical compounds from plant raw materials is a key task for the industry. One promising raw material component is  $\alpha$ -pinene, which can be utilized in the production of various products ranging from resins to pharmaceutical intermediates and high-density fuels. Isomerization of  $\alpha$ -pinene yields valuable compounds such as camphene and limonene. Montmorillonites hold potential as catalysts for this process. However, natural montmorillonites have several drawbacks, including variability in composition, structure, and surface properties, which hinder control over their catalytic activity. To address these issues, layered silicates with montmorillonites-like structure and a wide range of isomorphic substitutions of magnesium atoms with aluminum in octahedral layers ( $\text{Na}_{2x}(\text{Al}_2(1-x)\text{Mg}_{2x})\text{Si}_4\text{O}_{10}(\text{OH})_2 \cdot n\text{H}_2\text{O}$ , where  $0 < x < 1$ ) have been synthesized. The presence of isomorphic substitutions and control over synthesis conditions will allow obtaining samples with different chemical compositions, various porosity-textural characteristics, and surface properties, thus establishing the influence of these characteristics on the catalytic activity of montmorillonites in  $\alpha$ -pinene isomerization.

All samples without acid activation exhibit activity, yielding camphene as the main product with a selectivity of around 50%, which is comparable to the results obtained with commercial montmorillonite K-10. Moreover, only those samples that, besides weak and medium acid centers, have some amount of strong acid centers demonstrate high conversion percentages. A correlation between the composition of the samples and changes in their overall acidity was also established.

*Thus, targeted synthesis of layered aluminosilicates with specified characteristics opens up broad possibilities for developing new catalysts with improved properties.*

# STRAINED DOUBLE C=C BOND: NEW OPPORTUNITIES IN SYNTHESIS AND CATALYSIS

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Strained carbocyclic compounds are the most important objects in organic chemistry of hydrocarbons and their derivatives. The use of catalytic methods and approaches makes it possible to obtain unique compounds with specified properties on the basis of these compounds using a very limited number of technological stages. An important feature of such reactions is implementation of the possibility of using additional strain energy contained in the carbocyclic structure to solve selectivity issues at various levels – regio-, stereo-, enantio-. Promising representatives of such compounds are norbornadiene (NBD) and derivatives of the norbornene (NB) series. Catalytic processes with their participation open up opportunities for synthesis of a wide range of hard-to-reach polycyclic hydrocarbons. The effective use and combination of different synthetic techniques allows us to develop a unique strategy for obtaining saturated and unsaturated carbocyclic structures.

Problems of selectivity in multi-route reactions involving NB derivatives acquire a paramount role. Using reactions of dimerization and allylation of NBD and NB and their codimerization with unsaturated compounds as an example, the possibility of regulating the rate and selectivity of the processes at various levels is shown. The formation pathways of Ni- and Pd catalysts have been studied, key intermediates have been identified by spectral and isotopic methods, kinetic patterns have been established, and consistent mechanisms have been proposed. New technologically advanced heterogeneous catalysts have been developed. The efficiency of using homogeneous and heterogeneous catalysts was compared, and common features in the reaction mechanisms were identified. Quantum chemical modeling of nickel- and palladium-catalyzed processes involving NBD was performed. Theoretical approaches have made it possible to carry out the molecular design of catalytic systems, predict the most likely reaction routes, and optimize the conditions for their occurrence.

*The work was carried out with the support of the RSF as part of a scientific project №23-73-00123.*

# [M]-/ORGANO-CATALYZED AEROBIC Si-H- AND C-H- FUNCTIONALIZATION AS THE GREEN WAY FOR THE PREPARATION OF FUNCTIONALIZED ORGANOSILICON COMPOUNDS

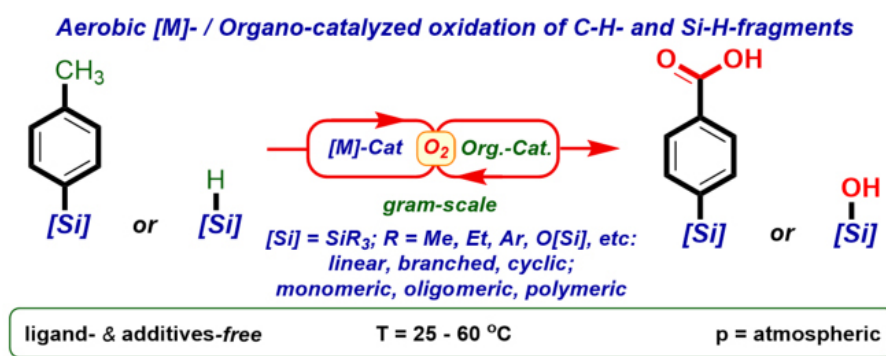
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Synthesis of organosilicon products with a “polar” functional group within organic substituents is one of the most fundamentally and practically important challenges in today’s chemistry of silicones. Incorporation of a “polar” function into organosilicon compounds opens unique opportunities for their subsequent modification and preparation of new copolymers, MOFs, HOFs and other hybrid materials. The aerobic oxidation of hydride or p-tolyl-siloxanes was suggested. This approach is based on “green”, commercially available, simple, and inexpensive reagents and employs mild reaction conditions: TM / organic catalyst – catalytic system, O<sub>2</sub> as the oxidant, process temperature from 30 to 60 °C, atmospheric pressure.<sup>1-3</sup>



All the organosilicon products were obtained and isolated in gram amounts (up to 5 g). The synthesized products can serve as building blocks for MOFs, HOFs, COFs, and siloxane polymers.<sup>4</sup>

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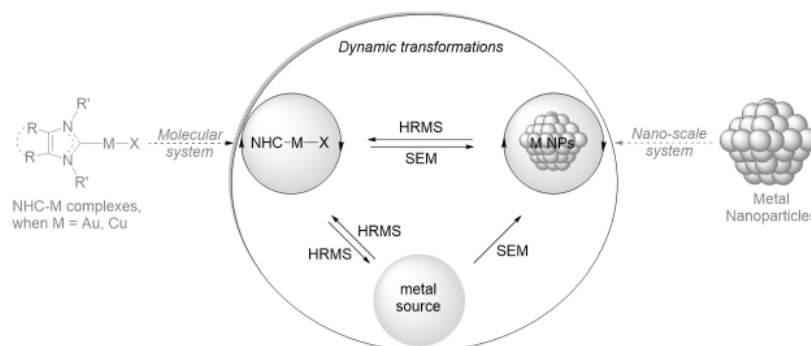
# GOLD AND COPPER COMPLEXES: COMPARISON OF TRANSFORMATIONS AND CATALYTIC ACTIVITY

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With their distinctive chemical and catalytic properties, gold and copper compounds have been the subject of extensive research in recent decades.<sup>1,2</sup> Either well-defined complexes or metal particles with a well/poorly defined structure, each demonstrating unique catalytic behavior uses in this area of catalytic research.



**Figure 1.** Dynamic behavior of the metal complexes and nanoparticles in the M-NHC systems (when M = Au, Cu).

In this study, the chemical and physical properties of gold and copper complexes were investigated.<sup>3,4</sup> Due to electrospray ionization high resolution mass spectrometry (ESI-HRMS) and the dynamic transformations occurring within the investigated gold and copper system were established. Furthermore, the mutual transformations of metal complexes into micro- and nanoscale particles (metal species) as well as the formation of gold complexes from Au NPs were studied by ESI-HRMS and electron microscopy. To compare the action of the metal complexes several more characteristic catalytic reactions (such as A<sup>3</sup>-coupling, hydration of alkynes, Chan-Lam coupling, *etc*) were examined.

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# SYNTHESIS AND STUDY OF PHOTOCATALYTIC ACTIVITY OF BISMUTH FERITE ( $\text{BiFeO}_3$ ) SUBSTITUTED BY BARIUM (BA)

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Photocatalytic decomposition of organic pollutants is one of the most promising methods for purifying water resources. Semiconductor materials such as  $\text{TiO}_2$ ,  $\text{ZnO}$ ,  $\text{Fe}_2\text{O}_3$ ,  $\text{CdS}$ ,  $\text{ZnS}$  act as photocatalysts<sup>1</sup>. Most photocatalysts have a large bandgap, which is a major problem due to the low photocatalytic activity in the visible light region.

Against their background, multiferroics with a small band gap appear to be the most attractive in the field of photocatalysis. The most studied multiferroic is  $\text{BiFeO}_3$ , with a rhombohedrally distorted perovskite structure and a band gap of about 2.2 eV<sup>2</sup>.

Recent studies have reported Ba-doped  $\text{BiFeO}_3$  nanostructures<sup>3</sup>. Substitution of Ba can reduce the band gap and increase the specific surface area, which will benefit the photocatalytic activity of  $\text{BiFeO}_3$ .

In this study, Ba-doped  $\text{BiFeO}_3$  nanoparticles were synthesized by combustion of a mixture of nitrate-organic precursors. The effect of Ba content on morphology, structure and photocatalytic activity was investigated.

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# NEW HIGH-ENTROPY OXIDE CATALYSTS WITH PEROVSKITE STRUCTURE FOR ETHANOL REFORMING

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Hydrogen's high-energy content, clean combustion and renewable production potential make it an attractive alternative fuel for energy storage and transportation. Ethanol reforming is one of the methods used in hydrogen production<sup>1</sup>.

High-entropy oxides (HEOs) are systems containing numerous cations in the equimolar ratio are particularly interesting to research. High entropy perovskite catalysts have shown potential for ethanol reforming due to their high degree of disorder and entropy.  $\text{La}(\text{Cr}_{0.2}\text{Mn}_{0.2}\text{Fe}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2})\text{O}_3$  and  $\text{La}(\text{Ti}_{0.2}\text{Mn}_{0.2}\text{Fe}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2})\text{O}_3$  were synthesized via Pechini and citrate methods. Catalysts with 5 wt.% Ni were prepared by the incipient wetness impregnation. After calcination at 700 °C XRD shown the single-phase nature of all the samples with perovskite structure. TEM pictures showed the homogeneous distribution of cations of the HEOs before and after Ni deposition. Ethanol steam and dry reforming was carried out in a continuous flow fixed-bed quartz reactor under atmospheric pressure in the temperature range of 600- 800 C°. The main products were H<sub>2</sub>, CO, CH<sub>4</sub> and CO<sub>2</sub>. Both the yield of hydrogen and the conversion of reagents increase with temperature. The highest ethanol conversion for both reactions was achieved for the  $\text{La}(\text{Cr}_{0.2}\text{Mn}_{0.2}\text{Fe}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2})\text{O}_3$  and is ~96% already at 600 °C. After the catalytic test, it is observed that the samples surface contains low carbon filaments. After 16 hours of reaction, the catalyst was stable with high conversion of ethanol and hydrogen yield.

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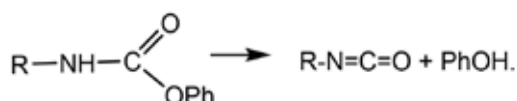


# CARBOXYLIC ACIDS AS CATALYSTS FOR THE REACTIONS OF PRIMARY AMINES WITH DIFENCARBONATE

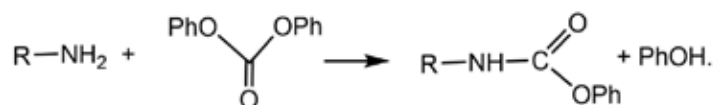
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Isocyanates are monomers for the production of polyurethanes and polyureas, which are widely used in a wide variety of industries. Based on them, structural parts, coatings, adhesives, sealants, varnishes, electrical, heat and sound insulation materials, and explosion-proof products are obtained. The classical technology for the production of isocyanates is based on the interaction of highly toxic phosgene with primary amines. During the reaction, a lot of hydrogen chloride is released, which must be disposed of. Therefore, phosgene-free methods for producing isocyanates are relevant. Among these methods, the production of isocyanates by thermal decomposition of phenyl esters of carbamic acids attracts the most attention:



Phenyl esters of carbamic acids are prepared by reacting primary amines with diphenyl carbonate:



The released phenol can be used to produce diphenyl carbonate, making this approach virtually waste-free.

We have studied the interaction of 4,4'-methylenedianiline with diphenyl carbonate, leading to the diphenylcarbamate 4,41-diphenimethane diisocyanate.

Non-catalytic interaction proceeds slowly. Therefore, it cannot be used as the basis for industrial processes. The influence of various catalysts on the considered process was studied. It has been shown that effective catalysts for this process are carboxylic acids, among which acetic acid showed high activity (yield more than 95% at 80°C). It also has the advantage of easy removal from bis-carbamate.

The mechanism of the catalytic effect of carboxylic acids on the interaction of primary amines with organic carbonates is discussed, suggesting that carboxylic acids act as both acids and Brønsted-Lowry bases in this transformation.

# MECHANISM OF PROPANE DEHYDROGENATION ON CATALYSTS BASED ON VANADIUM OXIDE

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Dehydrogenation of propane on a monolayer vanadium-titanium catalyst<sup>1</sup> was studied in situ using FT-IR spectroscopy and X-ray photoelectron spectroscopy. It has found that complete reduction of  $V^{5+}$  to  $V^{4+}$  and  $V^{3+}$  occurs in propane at 420°C. At the same time, the atomic ratio  $[V]/[Ti]$  decreases significantly, which indicates the formation of amorphous 3D vanadium oxide clusters. This process is reversible, and the complete oxidation of vanadium to the  $V^{5+}$  state is accompanied by the restoration of the  $[V]/[Ti]$  atomic ratio in oxygen even at 350°C. During the oxidative dehydrogenation of propane, partial reduction of  $V^{5+}$  to  $V^{4+}$  was found without a significant change in the atomic ratio  $[V]/[Ti]$ . This means that propane adsorption initiates the reduction of  $V^{5+}$  to  $V^{3+}$ , accompanied by a weakening of the vanadium-titanium interaction. According to FT-IR spectroscopy, propane is adsorbed mainly as isopropoxide, which is then converted to propylene. In the presence of oxygen in the gas phase, rapid oxidation of  $V^{3+}$  occurs with restoration of the structure of the monolayer  $V_2O_5/TiO_2$  catalyst.

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# MITIGATION OF CARBON DIOXIDE HYDROGENATION CONDITIONS BY NEW CATALYTIC SYSTEMS

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The reduction reaction of CO<sub>2</sub> with hydrogen, water or other proton sources using a thermochemical, electrochemical or photochemical process allows the production of fuels such as methane (CH<sub>4</sub>), methanol (CH<sub>3</sub>OH) and carbon monoxide (CO). Due to the thermal stability of the CO<sub>2</sub> molecule, achieving high conversions during hydrogenation to valuable products is a difficult task<sup>1</sup>.

In this work, catalytic systems based on metal nanoparticles obtained by induction flow levitation were developed and modes for different types of metals and physico-chemical characterization of the obtained nanoparticles were tested. The evaluation of the catalytic activity of pure metals, metals deposited on inert substrates and inversion catalytic systems of the “core-shell” type resistant to oxidation and mechanical degradation has been carried out.

The obtained catalytic systems for hydrogenation of carbon dioxide made it possible to reduce the reaction pressure to 30 atm while maintaining a high CO<sub>2</sub> conversion rate of 57%. According to the data obtained, it was determined that pressure does not have a significant effect on the course of the catalytic reaction, compared with temperature. The core-shell nanoparticle-based catalyst has demonstrated the best performance.

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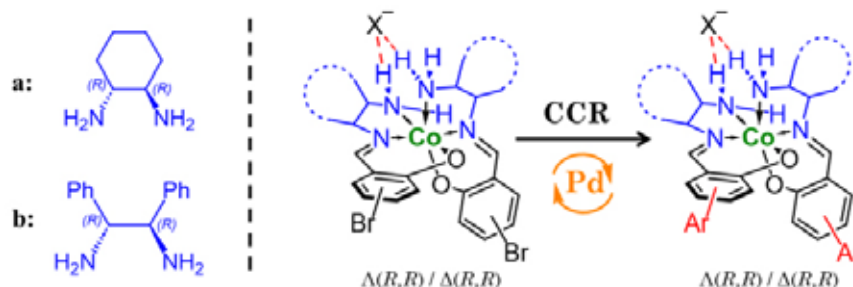
# SYNTHESIS AND MODIFICATION OF ASYMMETRIC CATALYSTS BASED ON CHIRAL Co(III) COMPLEXES OF $\Lambda$ - AND $\Delta$ -CONFIGURATIONS

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Metal-templated organocatalysis is a promising and less explored field in asymmetric synthesis. Such an original approach to the preparation of enantiomerically enriched compounds involves the use of coordinatively saturated chiral transition metal complexes as catalysts. Specifically, positively charged chiral-at-metal Co(III) complexes with two chiral tridentate ligands are an effective hydrogen bonding phase-transfer catalysts<sup>1</sup>.

In this work, the effect of ligand structure on the formation of diastereomeric Co(III) complexes with  $\Lambda$ - and  $\Delta$ -configuration at the metal ion has been studied for the first time and the direct modification of chiral catalysts using the Suzuki-Miyaura cross-coupling reaction (CCR) has been demonstrated<sup>2</sup>. The role of Co(III) complexes' stereochemistry on their enantioselectivity has been shown using the benchmark asymmetric epoxidation and asymmetric Michael addition reactions<sup>3</sup>.



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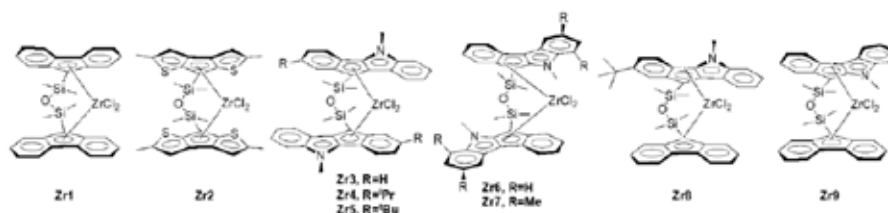
# DESIGN OF NEW ANSA-HETEROCENES WITH A LONG SIOSI BRIDGE AS A CATALYSTS FOR SELECTIVE DIMERISATION OF OCT-1-ENE

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Methylenealkanes  $RC(=CH_2)CH_2CH_2R$  are valuable raw materials for the synthesis of branched functionalized organic compounds with a wide variety of uses. Selective coordination dimerization of  $\alpha$ -olefins is a simple and inexpensive way to methylenealkanes, however, currently known dimerization catalysts possess low productivity, TON  $\sim 10^3$ .



**Scheme 1.** Promising (**Zr1-Zr9**) heterocenes for selective dimerisation.

Novel  $-SiMe_2OSiMe_2-$  bridged **Zr1-Zr9** *ansa*-zirconocenes derivatives of 9*H*-fluorene, cyclopenta[1,2-*b*:4,3-*b'*] dithiophene, 5,10-dihydroindeno[1,2-*b*]indole and 5,6-dihydroindeno[2,1-*b*]indole have been synthesised. The complexes were characterised by NMR spectroscopy and X-ray diffraction analysis [1] and studied in the dimerisation of oct-1-ene using the activators MMAO-12 and TIBA/[PhNMe<sub>2</sub>H][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>] at [oct-1-ene]/[Zr] molar ratio of  $3 \cdot 10^4$  in the absence and in the presence of H<sub>2</sub>. In the absence of H<sub>2</sub>, **Zr6** and **Zr7** complexes showed high activity and dimerisation selectivity up to 94%, when [PhNMe<sub>2</sub>H][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>] was used as an activator. In H<sub>2</sub> atmosphere, when the **Zr9** complex was activated with TIBA/[PhNMe<sub>2</sub>H][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>], the dimerisation selectivity reached more than 99% and no dimer hydrogenation was observed.

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# ELECTROCATALYTIC HYDROGEN EVOLUTION REACTION IN THE PRESENCE OF HYDRO-DERIVATIVE SALTS OF ORTHO-BIPYRIDINE

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Water electrolysis is the most promising method for generating clean hydrogen, but the use of expensive catalysts significantly hinders the integration of this technology into industrial processes.

A particularly relevant issue in this regard is the creation of synthetic systems that would be competitive in terms of efficiency, selectivity, and reproducibility compared to metallic analogs. It has been previously shown that increasing the efficiency of the catalytic process of hydrogen formation is possible by combining two pyridine-containing fragments in the ortho-position through altering the final stage of the reaction mechanism.<sup>1,2</sup>

Through a series of electrochemical methods, the electrochemical properties and electrocatalytic activity of hydroperchlorates of 2,2'-bipyridine were studied. It was demonstrated that in the reaction of molecular hydrogen formation in the presence of the investigated salts, the process occurs at the same potentials but through different mechanisms. In the case of the studied compounds, at a potential of -0.85 V, the mechanism is CECE, while at a potential of -1.25 V, the mechanism is ECEC.

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# COMPARATIVE STUDY OF THE PROPERTIES OF MASSIVE AND ALUMINUM OXIDE SUPPORTED OXIDES $\text{Ce}_{1-x}\text{Ni}_x\text{O}_y$

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Complex oxides, in which the cations of the catalytically active component are built into the structure of the oxide support, are promising catalyst precursors [1, 2]. For the development of methods for targeted regulation of the functional properties of materials by varying their structural characteristics, it is of interest to assess the influence of the carrier on the genesis and properties of complex oxides. The purpose of this work is a comparative analysis of the physicochemical and catalytic properties of bulk  $\text{Ce}_{1-x}\text{Ni}_x\text{O}_y$  oxides supported on aluminum oxide and the establishment of the correlation relationship “composition–structure–functional properties.” It is shown that after heat treatment in an oxidizing environment, the synthesized samples are mesoporous materials containing solid solutions based on cerium (IV) oxide. During the reduction activation for  $\text{Ce}_{1-x}\text{Ni}_x\text{O}_y/\text{Al}_2\text{O}_3$  samples compared to  $\text{Ce}_{1-x}\text{Ni}_x\text{O}_y$  samples, the temperature of formation of NiO particles increases (530 vs. 340°C), and their average size decreases (6.5 vs. 15 nm). After the methane reforming reaction, the textural and structural characteristics of the  $\text{Ce}_{1-x}\text{Ni}_x\text{O}_y/\text{Al}_2\text{O}_3$  samples are preserved. It has been established that at a Ni content of ~10 wt. %  $\text{Ce}_{1-x}\text{Ni}_x\text{O}_y/\text{Al}_2\text{O}_3$  catalysts provide higher values of methane conversion (96 vs. 65%) and  $\text{CO}_2$  (83 vs. 69%), hydrogen yield (95 vs. 74%) and resistance to deactivation in reactions of steam-carbon dioxide reforming of methane. The relationship between the characteristics of materials and their functional properties has been revealed.

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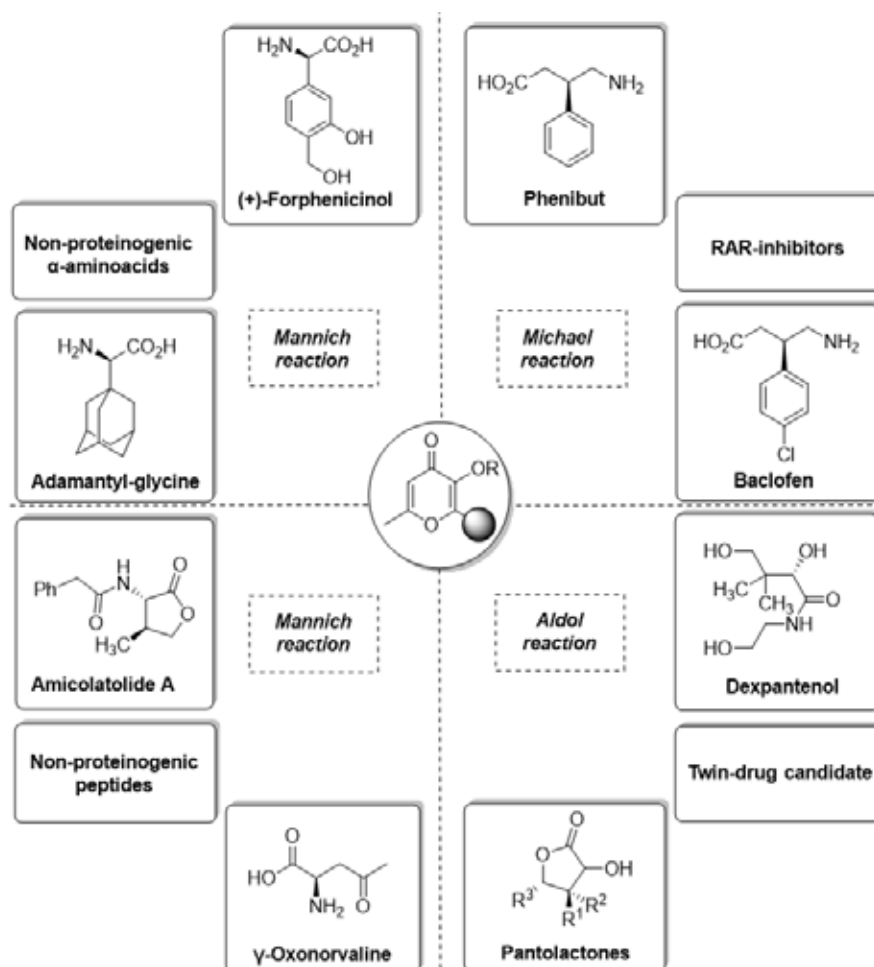
*This work was supported by the Ministry of Science and Higher Education of the Russian Federation within the governmental assignment for Boreskov Institute of Catalysis (project FWUR-2024-0033).*

# SYMBIOSIS OF ASYMMETRIC ORGANOCATALYSIS AND OXIDATIVE FRAGMENTATION: NEW APPROACH TO OPTICALLY PURE DRUGS

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# AMMOXIDATION OF PROPYLENE IN A FLUIDIZED BED OF CATALYST

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The synthesis of acrylic acid nitrile by oxidative ammonolysis of propylene remains the main industrial process for the production of AN, which consists of the oxidation of propylene and ammonia with atmospheric oxygen in a boiling layer of a multicomponent catalyst.

Along with acrylic acid nitrile, acetonitrile and hydrocyanic acid are afforded. The degree of conversion of the starting substances and the selectivity of oxidation are determined not only by temperature, pressure and the ratio of the components of the reaction mixture, but also by the activity of the catalyst.

The study of the mechanism of joint oxidation of propylene and ammonia indicates the need to form a catalyst surface that includes active centers of different natures responsible for the abstraction of propylene hydrogen in the allylic position, the adsorption of electron-excess ammonia, and metal oxide systems that generate oxygen as a result of their redox transformation.

The results of a study of the physicochemical state of modified bismuth-molybdenum systems on silicon oxide showed that the catalyst has a specific surface area of 30 m<sup>2</sup>/g and is characterized by a pore size of 40-100 Å.

X-ray phase analysis of the catalyst indicates the presence of the main phases: cerium(III) molybdate and a solid solution of nickel(II) and magnesium molybdates. Impurity phases are bismuth molybdates ( $\gamma$ -Bi<sub>2</sub>MoO<sub>6</sub>) and iron (III), bismuth hydroxide-molybdate hydrate BiMo<sub>2</sub>O<sub>7</sub>(OH)(H<sub>2</sub>O)<sub>2</sub>.

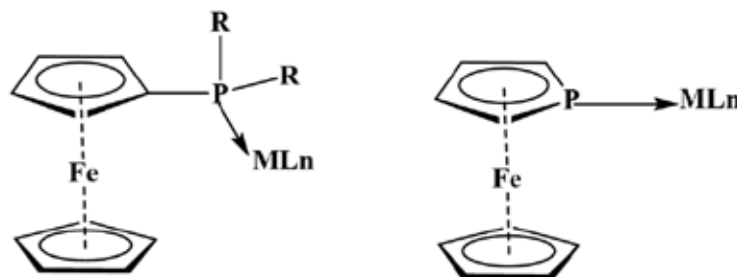
Analysis of the morphology indicates predominantly smooth, spherical particles with a diameter in the range of 5-50 μm. Elemental composition mapping shows that the catalyst particles operating in the process of propylene amnoxidation have protrusions in which silicon, oxygen, molybdenum and iron are concentrated. The chip of a destroyed particle has an increased iron content and a reduced silicon and oxygen content. The catalyst provides a total propylene conversion of up to 98%, with the yield of acrylic acid nitrile being 77% wt, hydrocyanic acid 5.5% wt, acetonitrile 2.5% wt.

# TETRAARYL-SUBSTITUTED PHOSPHACYANOFERROCENES AS LIGANDS FOR THE DESIGN OF REDOX-SWITCHABLE CATALYSTS

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Redox-switchable catalysts are designed using redox-active moieties. Thus, oxidation of ferrocene to ferrocenium cation leads to a more electron acceptor ligand and increases the electron density deficit at the catalytic centre, which in turn facilitates the reductive elimination step, accelerates the catalytic reaction and increases the product yield. In redox-switched ligands, the distance between the Fe atom in the ferrocene and the metal catalytic centre is three bonds (Fe-C-P-MLn), which somewhat reduces the influence of the electron-acceptor properties of the ferrocene cation due to the break of the conjugation in the exocyclic C-P bond. In this connection, a group of phosphorus-containing ferrocenes - phosphoferrocenes, in which the  $\eta^1$  type of coordination of the phospholyl ligand with the catalytic centre and the shortest possible distance between the  $\text{Fe}^{+3}$  atom and the metal catalytic centre (via 2 bonds (Fe-P-MLn) are realised, is of great interest. This fact allows us to hope for the most 'efficient' transfer of electronic effects, which will lead to more electron-deficient catalytic centres, thus accelerating the catalytic reaction and improving yields [1][2]



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# REDUCTIVE COUPLING OF NITROARENES WITH CARBOXYLIC ACIDS – A DIRECT ROUTE TO AMIDE SYNTHESIS

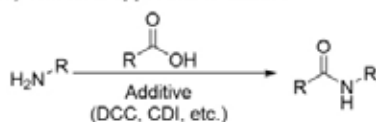
**Losev M.A., Kozlov A.S., Kharitonov V.B., Afanasyev O.I., Loginov D.A., Chusov D.A.**

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Amide bonds are one of the most important functional groups in chemistry and biology. They are found in a wide range of compounds, including peptides, proteins, polymers and drugs. The classical approach to the synthesis of amides implies modification of carboxylic acid with the release of appropriate reactive intermediate products, or in situ modification using certain additives<sup>1</sup>. Such modifications require the use of stoichiometric amounts of toxic activators, as a result of which equimolar amounts of waste are formed, and the atomic efficiency of the process decreases.

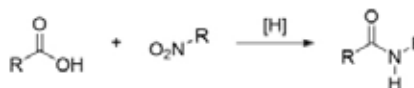
One possible way to overcome these problems is to use nitroarenes as a nitrogen source. The reduction of nitroarenes is a classic way to produce amines. Earlier, our research group developed a direct reaction of nitroarenes with carboxylic acids, using converter gas as a reducing agent<sup>2</sup>. In this work, we have developed a rhodium-catalyzed method using carbon monoxide as a reducing agent, allowing the synthesis of aliphatic and aro-matic amides with a wide variety of functional groups. This approach solves the main problems of the previously described methods of direct amidation with nitro compounds, such as the use of solid reducing agents, high loads of carboxylic acids and low selectivity.

a) Classical approach to amides



- ✗ Activating agents are required
- ✗ Low atom economy, toxic side products

b) Direct amidation by nitro-compounds



*This work:*

- ✓ No stoichiometric solid byproducts
- ✓ Higher atom efficiency
- ✓ Functional group tolerance

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# STUDY OF ELECTROCHEMICALLY SYNTHESIZED HEMATITE IN HETEROGENEOUS PHOTO-FENTON PROCESS

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The heterogeneous Fenton-like process is one of the most efficient methods of degrading wastewater components to non-toxic products. Iron oxides have minimal leaching of iron ions, are easily regenerated after wastewater treatment and exhibit high activity over a long period of operation. In this work, we have investigated a heterogeneous Fenton-like process using the iron oxide catalyst  $\alpha\text{-Fe}_2\text{O}_3$ .

The synthesis of iron (III) oxide was carried out as follows: electrolysis of 0.1 M aqueous sodium chloride solution was carried out using iron sludge as electrodes connected as anode and cathode at a current density of 0.1 A/cm<sup>2</sup>.

The obtained material was investigated in detail by XRD, SEM, DRS, RS, FTIR, XPS and vibrational magnetometry. The study of structure and morphology showed that  $\alpha\text{-Fe}_2\text{O}_3$  is a phase-pure highly crystalline powder with rhombohedral (hexagonal) structure having quasi-spherical morphology with a particle size of about 200-500 nm and crystallite size of 64 nm.

The catalytic activity of the synthesized powder was determined during the decomposition of rhodamine B in the photostimulated Fenton process. The dependence of the oxidation rate of rhodamine B on the amount of catalyst, hydrogen peroxide and dye were studied.

Optimal concentrations of catalyst, hydrogen peroxide and dye allowed achieving a high degradation rate of 0.506 min<sup>-1</sup> with a dye degradation rate of 99.15% in 12 min. The stability of the catalyst was investigated in 5 consecutive cycles.

The mechanism of the process was also investigated using active radical capture experiments. It was shown that photogenerated electrons reduce  $\text{Fe}^{3+}$  to  $\text{Fe}^{2+}$ , which, reacting with  $\text{H}_2\text{O}_2$  and  $\text{O}_2$ , leads to the generation of  $\bullet\text{OH}$  and  $\bullet\text{O}_2^-$  radicals, which are the main oxidizing agents of RhdB.

*The work was financially supported by RNF, project No. 22-73-10091.*



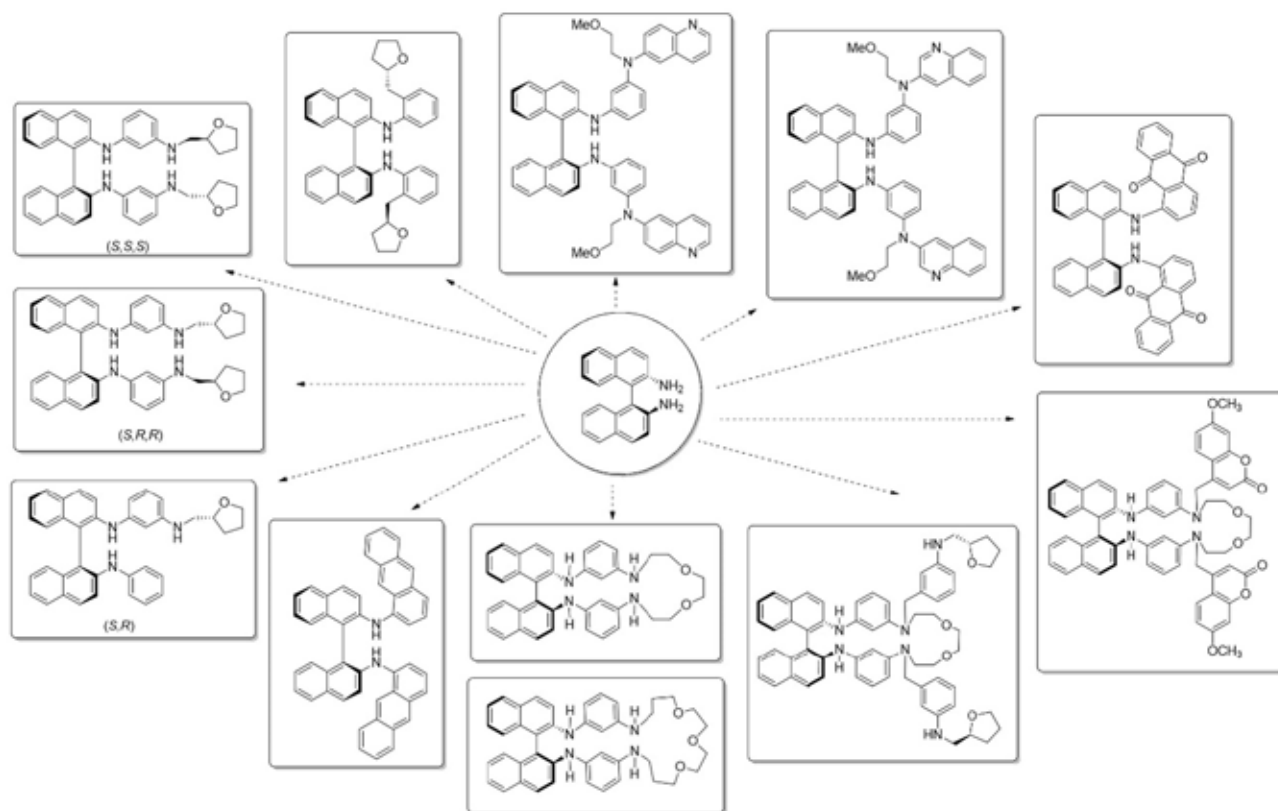
# BINAM DERIVATIVES FOR FLUORESCENT DETECTION OF AMINO ALCOHOLS AND METAL CATIONS

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Detection and quantitative analysis of optically active organic compounds is a key problem of modern chemistry, production of pharmaceutical and agrochemical substances. One of the most promising approaches deals with their fluorescence detection using enantioselective chemosensor molecules.

In this work, a number of new derivatives of 2,2'-diamino-1,1'-binaphthalene (BINAM), including macrocyclic compounds, were synthesized using Pd-catalyzed amination reactions. The resulting compounds are characterized by different length of the polyoxadiazine chains, the structure of exocyclic fluorophore groups (dansyl, coumarin, quinoline) and additional chiral substituents with nitrogen and oxygen heteroatoms. It was demonstrated that the obtained compounds can change their emission spectra in the presence of chiral amino alcohols and cations of several metals, which indicates the possibility of their implementation as fluorescent detectors.

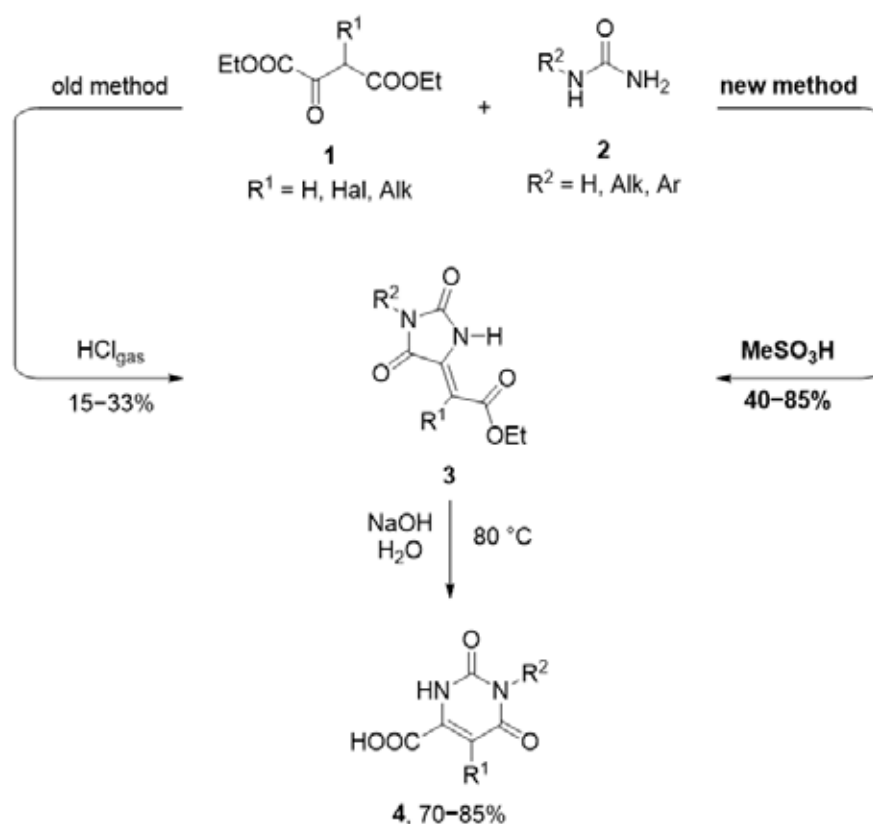


# NEW METHOD FOR 5-CARBOXYMETHYLIDENE HYDANTOINS SYNTHESIS

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5-Methylidene hydantoin is of great interest for medicinal chemistry due to their high bioavailability and ease of preparation<sup>1</sup>. 5-Carboxymethylidene hydantoin readily transforms into uracil-6-carboxylic acid under base conditions<sup>2</sup>. Here we present new method for 5-methylidene hydantoin synthesis without gaseous HCl and with improved yields.



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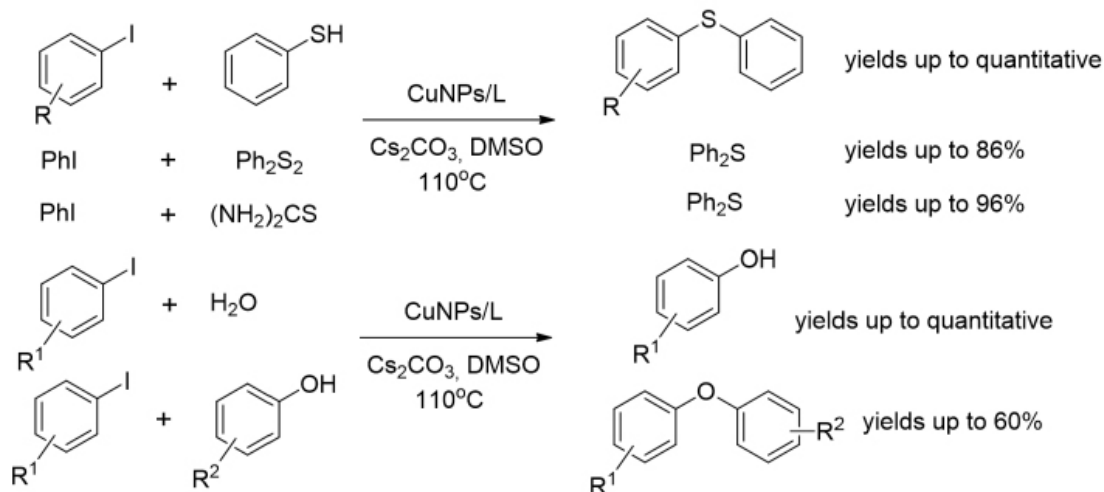
*The work was carried out with the financial support of the Russian Science Foundation, project 23-23-00207.*

# COPPER NANOPARTICLES IN THE CATALYTIC C-O AND C-S BONDS FORMATION

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An important trend in modern catalytic chemistry is associated with the use of nanoparticles as catalysts for the formation of carbon-carbon and carbon-heteroatom bonds. In this work, the formation of diaryl sulfides, phenols and diaryl ethers was investigated in the reactions of aryl iodides, respectively, with thiophenols, diaryl disulfides and thiourea to obtain compounds with C-S bonds, and with water, aliphatic alcohols and phenols to synthesize derivatives with C-O bonds. Commercially available free copper nanoparticles of various average sizes (25 nm, 10/80 nm, 72 nm, 86 nm), CuO nanoparticles (65 nm) were studied as catalysts, and a comparison was made with standard micro-sized Cu<sub>2</sub>O and CuO powders. The reactions were carried out in DMSO at 110°C in the presence of ligands (2-isobutyrylcyclohexanone, *rac*-BINOL). It was established that the yields of thiolation products were generally higher and often close to quantitative, primarily in the reactions of ArI with Ar'SH. In the case of the reactions with O-nucleophiles, the most efficient processes occurred with water, and more reluctant reactions ran with aliphatic alcohols. The influence of substituents in aryl iodides on the yields of reaction products was comprehensively studied. The induction periods of the reaction and the leaching of copper into solution were studied under various conditions.



*The work was supported by the RSF grant, project No 24-23-00149.*

# STUDY OF HYDROGENATION PROCESSES IN THE PRESENCE OF INFLICTED CATALYSTS BASED ON METALS OF VARIABLE VALENCE OBTAINED BY CHEMICAL REDUCTION

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The research is aimed at developing new efficient catalytic approaches to the synthesis of valuable chemical products. Hydrogenation reactions are one of the most important types of transformations in organic synthesis. Hydrogenation processes of practically important compounds require either harsh conditions using available nickel and copper catalysts, or the use of catalysts based on expensive metals (Pt, Pd, Ir, Rh). The development and introduction into the practice of organic synthesis of new environmentally friendly and economically feasible approaches to carrying out hydrogenation reactions on heterogeneous catalysts is not only of undoubted practical significance, but is an important fundamental task. The nature of the precursor and the method of synthesizing the active phase have a significant influence on the properties of supported metal catalysts. The use of chemical reduction of the precatalyst with sodium borohydride and/or hydrazine monohydrate makes it possible to obtain catalysts with a unique morphology, which makes it possible to significantly control the activity and selectivity of the resulting catalysts through the use of various carriers and precursors of the active metal phase.

The study is aimed at studying the patterns of hydrogenation processes in flow systems at atmospheric pressure of hydrogen of carbon-carbon double bonds, nitrile, nitro- and carbonyl groups in a wide range of practically significant compounds in the presence of supported nanostructured catalysts obtained by chemical reduction of salts or coordination compounds of variable metals valence. The use of this type of catalysts based on d-metals allows not only to intensify hydrogenation processes under mild conditions due to the size effect, but also to reduce the economic costs of catalyst production by replacing classical hydrogenation catalysts based on platinum group metals with more affordable ones without loss of activity of the used one.

# HIGHLY SELECTIVE AND STABLE CATALYTIC FILMS FOR THE HYDROGENATION OF 2-METHYL-3-BUTYN-2-OL IN MICROCAPILLARY REACTOR

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The semihydrogenation of alkynols to the corresponding enols is an important step in the industrial production of pharmaceuticals, agrochemicals and flavors.<sup>1</sup> Vitamin E synthesis involves enols such as 2-methyl-3-buten-2-ol (MBE), linalool and isophytol. Typically, these enols are prepared by selective hydrogenation of alkynols over palladium-based catalysts under mild conditions. Controlling the degree of hydrogenation and preventing complete hydrogenation of C≡C bonds to C–C bonds is key to achieving high yields of enols. Given the the growing market demand for enols, to obtain high-quality products, it is proposed to use continuous microcapillary reactors, the inner surface of which is coated with a highly selective, active and stable catalyst. This work is devoted to the development of highly selective catalytic coatings for the semihydrogenation of 2-methyl-3-buten-2-ol with an emphasis on the role of second metals (Zn, Ag), stabilizer of colloidal nanoparticles, catalyst supports based on pure TiO<sub>2</sub> and doped by Zr, Ce and Zn<sup>2</sup>, as well as the influence of reaction conditions and the study of the kinetics of the catalytic reaction to establish its mechanism and the main factors for increasing selectivity. Finally, a strategy for developing highly efficient and selective catalytic coatings for the solvent-free hydrogenation of alkynols in a microcapillary reactor is proposed.

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# Pd-Ag/TiO<sub>2</sub> CATALYTIC FILMS: PREPARATION THROUGH THE POLYOL PROCESS, CHARACTERISTICS AND REACTIVITY IN SELECTIVE HYDROGENATION OF 2-METHYL-3-BUTYN-2-OL

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Selective hydrogenation reactions have been used since the beginning of this century, and alkenols, which are the most important industrial products of the pharmaceutical and perfume industries, are mainly produced by selective hydrogenation of the corresponding alkyne alcohol. The Pd–Ag bimetallic composition is an effective catalyst for the selective hydrogenation of terminal and internal alkynes. Currently, the influence of the structure of Pd–Ag nanoparticles on the catalytic characteristics of this system in the liquid-phase hydrogenation of alkynols has not been sufficiently studied. The polyol process allows the synthesis of monodisperse, non-agglomerated precious metal particles in the nanometer range. In addition, this method is used to synthesize a single-atomic alloy (SAA) with a core-shell structure<sup>1</sup>, for this purpose a second metal (shell) is sequentially reduced on the surface of nanoparticles of the first metal (core). The purpose of this work is to use this process to obtain catalytic films based on monometallic (Pd) and bimetallic (Pd–Ag) nanoparticles with different structures; and comparison of the efficiency of catalytic films based on them in the liquid-phase hydrogenation of 2-methyl-3-butyne-2-ol. A 10-fold increase in productivity was shown for a bimetallic film with a Pd core–Ag–Pd shell structure compared to the Pd-core–Ag shell structure and selectivity of alkenols for a Pd<sub>33</sub>Ag<sub>67</sub>/TiO<sub>2</sub> bimetallic film (S=96%) with a Pd core–Ag–Pd shell structure compared to monometallic Pd/TiO<sub>2</sub> (S=89%) with 97% conversion and stable operation for 64 hours in a microcapillary reactor.

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*The work was carried out with financial support from the Ministry of Science and Higher Education of the Russian Federation within the framework of a state assignment from the Boriskov Institute of Catalysis SB RAS (project FWUR-2024-0033).*



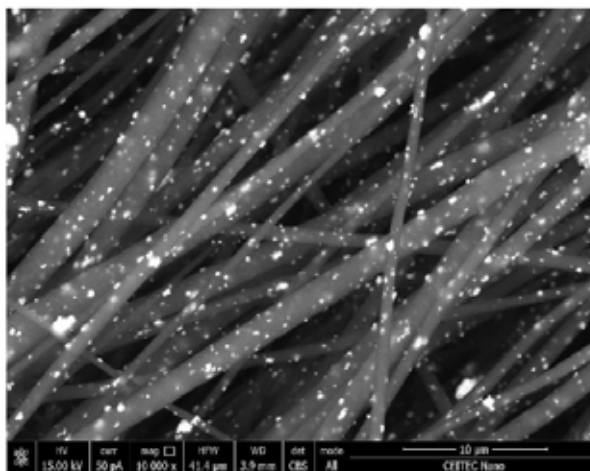
# SYNTHESIS OF HYBRID MAGNETO-PIEZOELECTRIC COMPOSITE MEMBRANES FOR CATALYTIC APPLICATIONS

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The urgent task for ecology is the creation of stimulus-sensitive smart catalysts capable of decomposing organic dyes with high efficiency. To effectively solve the problem of collecting mechanical vibrations and light energy, it is possible to combine the advantages of photoactive piezo-materials and ferroelectric polymers.<sup>1</sup>

Fiber membranes were synthesized by electrospinning method based on polyvinylidene fluoride (PVDF) and bismuth ferrite (BiFeO<sub>3</sub>/BFO). The samples underwent investigation using scanning electron microscopy (SEM) (refer to Figure 1), FTIR spectroscopy, X-ray photoelectron spectroscopy (XPS), and vibration magnetometry.



**Figure 1:** SEM image of PVDF/BFO fibers.

The results of piezophotocatalytic experiments on the decomposition of Methylene Blue (MB) dye indicate that the reaction rate increased when ultrasonic treatment and irradiation with both visible and UV light were combined, compared to photolysis, sonolysis, and piezocatalysis. To confirm the generation of piezoelectric potential under mechanical action or ultrasonic treatment, a piezoelectric nanogenerator was fabricated and tested.

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# OBTAINING OF MESOPOROUS PHOSPHATES WITH HIGH SPECIFIC SURFACE AREA BY THERMAL DEVOLATILIZATION METHOD

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Magnesium phosphates are of great interest as a group of substances that can be used in catalysis, electrocatalysis, as semiconductor materials and slow-release fertilizers<sup>1</sup>. There is a wide variety of forms of their crystallohydrates. The variety of compositions and, in some cases, structures of phosphates make it possible to regulate many of their properties, in particular the specific surface area, which is especially important in the production of catalysts.

The synthesis of mesoporous phosphates can be carried out by thermal devolatilization<sup>1</sup>. As the temperature rises, the precursor material gives off part, forming voids in the matrix of the basic substance, and this increases the specific surface area of the final material. This paper summarizes the results of the study of the role of the precursor material during thermal devolatilization in the production of materials (Table 1) with a highly developed surface.

Precursor	Mass loss during devolatilization, %	Specific surface area, m <sup>2</sup> /g	Average pore radius, nm
Mg <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> ·nH <sub>2</sub> O	24,7	74	5,23
MgNH <sub>4</sub> PO <sub>4</sub> ·6H <sub>2</sub> O	13,2	45	3,95

**Table 1.** An example of the results of thermal devolatilization of precursor materials at 90 ° C for 2 hours.

An important indicator is the share of mass loss during thermal treatment of the material, which correlates with the final increase in the specific surface area of the material and the decrease in the average pore radius. Further research provides the optimization of the conditions for the synthesis of precursor materials and the parameters of their temperature devolatilization during the formation of mesoporous materials with a high specific surface area as the basis of relatively inexpensive catalytic materials.

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# PALLADIUM CARBOXYLATES $[\text{Pd}(\text{RCO}_2)_2]_n$ AS CATALYSTS FOR THE OXIDATION OF ALCOHOLS: EFFECT OF A SUBSTITUTE IN THE CARBOXYLATE GROUP

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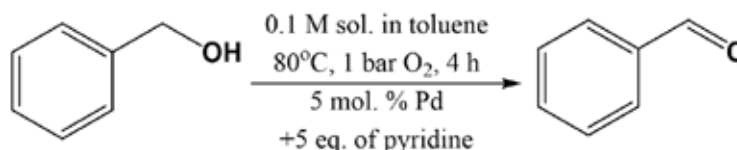
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Palladium carboxylates  $[\text{Pd}(\text{RCO}_2)_2]_n$  are well known as effective catalysts (or their precursors) for a wide range of transformations of organic substrates, including oxidative ones. One of these transformations is the oxidation of alcohols, which is an effective route to carbonyl compounds as important synthons of fine organic synthesis. Palladium acetate is most widely used as a basis for the design of catalytic systems for the oxidation of alcohols. In combination with coordinating bases such as pyridine, it provides efficient and selective oxidation of primary and secondary alcohols under relatively mild conditions (temperatures up to 120°C, oxygen pressure up to 10 atm.). Palladium trifluoroacetate under similar conditions demonstrates low activity, although it retains high selectivity.

Thus, we have shown that in the oxidation reaction of benzyl alcohol under the conditions shown in the diagram below, palladium trifluoro- and trichloroacetate provide a yield of 8-11% compared to 88% for palladium acetate:



However, the yield increases to 92% when using 15 mol. % palladium with the addition of 1.5 eq. pyridine. At the same pyridine content in the presence of 5 mol. % palladium yield is 75-83%. From this we can conclude that the influence of the substituent in the carboxylate ligand is not limited to the stability of the resulting active forms of palladium in general. Apparently, a test under identical conditions cannot always serve to assess the relative activity of palladium carboxylate complexes of similar composition and structure, but differing in substituents on the carboxylate groups.

*The work was carried out with the support of the Russian Science Foundation – project No. 23-73-00123.*

# SYNTHESIS AND CHARACTERIZATION OF CARBON NANOFIBERS OBTAINED BY THE PYROLYSIS OF TRICHLOROETHYLENE ON MICRODISPERSED Ni-M CATALYSTS

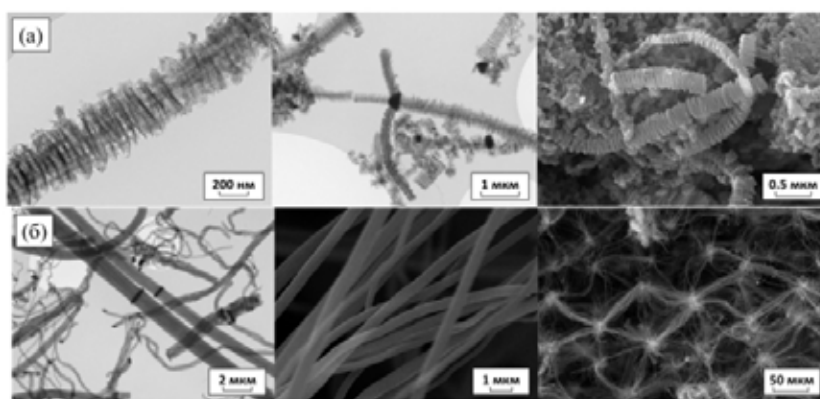
**Potylitsyna A.R.,<sup>a</sup> Rudneva Y.V.,<sup>b</sup> Popov A.A.,<sup>b</sup> Bauman Y.I.,<sup>a</sup>  
Shubin Y.V.,<sup>b</sup> Vedyagin A.A.,<sup>a</sup> Mishakov I.V.<sup>a</sup>**

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Carbon nanofibers (CNF) are nanosized fibrous structures consisting of graphene layers. The combination of high specific surface area, inertness, and good electrical and thermal conductivity makes these materials highly demanded in a wide range of applications.

In this work, carbon nanofibers were obtained by catalytic decomposition of trichloroethylene ( $C_2HCl_3$ , TCE) over bulk nickel and its alloys. The presence of chlorine in the substrate determines the unique segmented structure of the resulting product (Figure 1a). However, as shown in this study, the structural features of CNFs depend not only on the type of substrate to be degraded, but also on the catalyst composition. Fibers with segmented structure were obtained on Ni-Mo and Ni-W catalysts (Fig. 1a). At the same time, the material synthesized on Ni-Pd and Ni-Sn alloys is represented by long fibers that grow alongside and form a "net-like" macrostructure (Fig. 1b).



**Figure 1.** SEM and TEM images of carbon nanofibers obtained by TCE decomposition at 600°C  
(a) on 96Ni-4W catalyst; (b) on 99.75Ni-0.25Sn catalyst.

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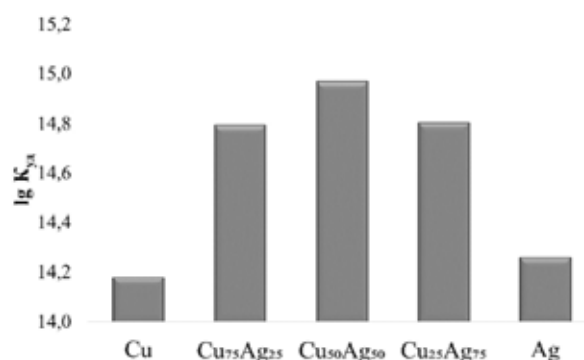
# SYNERGIC EFFECTS IN THE CATALYTIC PROPERTIES OF COPPER-SILVER BIMETALLIC NANOPARTICLES

Pshenitsyn M.B., Boeva O.A., Zhavoronkova K.N.

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Nanostructures are of interest to many scientific groups. This is due to their unique properties, which open up new applications for substances about which, as it seems to us, we know almost everything. One type of such structures is metal nanoparticles, which exhibit properties uncharacteristic for their element in the macroworld. The catalytic properties of mono- and bimetallic nanoparticles based on copper and silver will be discussed in this work.

The objects of research are nanoparticles deposited on  $\gamma\text{-Al}_2\text{O}_3$  with different ratios of copper and silver in the composition. The model reaction is ortho-para conversion of protium. The experiments were carried out at 77 K and a pressure of 0.5 Torr. The research results are shown in the figure below.



The catalysts showed high activity in relation to the isomeric conversion reaction of protium; the activity of bimetallic nanoparticles is 3-6 times higher compared to monoparticles, which cannot be explained by the addition of the properties of metals; therefore, the interaction of copper and silver in a nanoparticle leads to a synergy of catalytic properties.

*The work was carried out with financial support within the framework of the development program of the Russian Chemical Technical University named after D.I. Mendeleev "Priority-2030".*

# NANOSTARS AS A HIGHLY ACTIVE CATALYST IN MEMBRANE HYDROGEN PROCESSES

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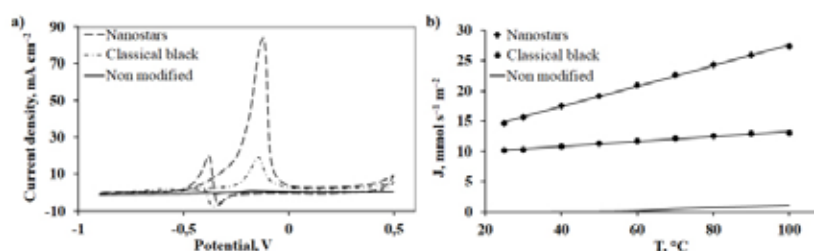
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Palladium-based catalytic systems are quite resistant to poisons, which makes them promising materials for use in hydrogen diffusion purification devices. The application of Pd-nanoparticles can intensify the transport of hydrogen through palladium-based membranes at low temperatures.<sup>1</sup>

During the study, two types of coatings on the surface of Pd-Ag films based on classical spherical nanoparticles and nanostars were synthesized by electrolytic deposition.



**Figure 1.** (a) Catalytic and (b) membrane studies of modified Pd-Ag films.

Nanostar-modified films have demonstrated excellent performance in catalytic and membrane processes, which may be due to increased surface adsorption activity. The use of nanostructured membrane materials will significantly intensify hydrogen transport and reduce the operating temperatures of the process.

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# DEVELOPMENT AND PREDICTION OF PROPERTIES OF COPPER-ZINC-ALUMINUM OXIDE CATALYSTS FOR LARGE-CAPACITY SYNTHESIS GAS PROCESSING PROCESSES

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High productivity and economic efficiency of production directly depends on the efficiency and stability of the catalysts at various stages of the technological process<sup>1,2</sup>.

The paper touches upon the actual problems of creating and further industrial implementation of CuO/ZnO/Al<sub>2</sub>O<sub>3</sub> catalysts for the process of low-temperature conversion of carbon monoxide (LTC) by water vapor in the production of ammonia and hydrogen. The presented report will reflect generalized data on the experience of the development of copper zinc aluminum catalysts carried out at ISUCT, including their production using resource- and energy-saving methods based on mechanochemical synthesis. Information on catalytic properties under conditions as close as possible to industrial ones (gas composition, process temperatures, pressure), as well as on the influence of process parameters on the activity and selectivity of these catalysts. For example, a change in selectivity depending on the pressure of the LTC process and the carbon monoxide content in the feed gas. The research methods and the results of evaluating the stability of the catalysts based on their forced deactivation are presented. In particular, data on changes in physico-chemical properties (active and specific surface area, porous structure, dispersion and particle size of the active metal) will be reflected and their relationship with activity and selectivity will be shown. The trends of changes in these properties during thermal decontamination are shown. Based on the analysis, conclusions are drawn on the stability of the catalysts and their service life.

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*The work was performed within the framework of the state assignment for research (Topic N FZZW-2024-0004)*

# DEVELOPMENT OF CATALYSTS FOR RESOURCE- SAVING CONVERSION OF METHANE INTO HYDROGEN- CONTAINING GAS

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The development of coal deposits is accompanied by the release of methane-containing gas, the capture and processing of which is critical to ensuring methane safety of mines and environmental protection<sup>1,2</sup>. In order to create effective catalysts for the resource-saving conversion of coal industry methane into hydrogen-containing gas, complex oxides supported on aluminum oxide were synthesized, the patterns of their formation and physicochemical properties were studied using a complex of physicochemical methods. To control the functional characteristics of catalysts in the target reaction, methods for designing catalytic systems have been developed, including the use of the effects of mutual enhancement of the action of metals and modification of the composition of the support. Mutual enhancement of the action of metals was achieved by modifying the Ni active component with a second metal (Me = Pd, Re, Mo) or by forming a surface solid solution with an oxide promoter (M = Ce, La, Zr, Mg), followed by its activation in a reducing environment. The developed catalysts were tested during the conversion of coal mine methane of various compositions and the “composition–structure–functional properties” relationship was established. The catalyst compositions and parameters of their synthesis that are most resistant to the formation of carbon deposits have been identified. Factors influencing the achievement of high process performance have been identified. The composition of the catalyst was revealed –  $20\text{Ce}_{0.2}\text{Ni}_{0.8}\text{O}_{1.2}/\text{Al}_2\text{O}_3$ , which, due to the combination of the thermal stability of modified  $(\gamma+\delta)\text{-Al}_2\text{O}_3$ , the strong interaction of the Ni–support and the anti-coking properties of  $\text{CeO}_2$ , provides high rates of methane conversion and  $\text{H}_2$  yield.

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# ROLE OF AMINO GROUPS IN POROUS COORDINATION POLYMERS FOR CATALYTIC CONVERSION OF CO<sub>2</sub>

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In the context of CO<sub>2</sub> conversion reaction, non-covalent interactions determine its adsorption and activation on the catalyst surface, leading to enhanced catalytic activity and selectivity. The analysis of non-covalent interactions becomes an important aspect of designing efficient electrocatalysts.

This work focuses on analyzing the influence of non-covalent interactions on the stereoselectivity of the synthesis and the electronic structure of the molecules. The main tool was various electrochemical methods with semi-differential method of treatment. They revealed that the introduction of an amine-containing group into ferrocenyl-R-phosphinate ligand, used in the synthesis of coordination polymers and catalysts for CO<sub>2</sub> reduction, has a significant effect on the electrochemical properties of the ligand and on the stereoselectivity of its synthesis. However, the use of ligands with amine-containing groups in CO<sub>2</sub> reduction reactions is not possible in all cases, so the process design requires consideration of nonspecific interactions.

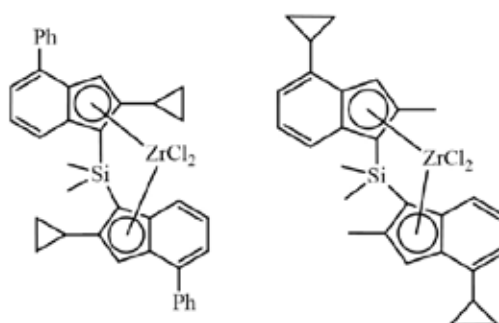
*This work was supported by the grant of the Russian Science Foundation № 22-73-10203.*

# OLEFIN POLYMERIZATION CATALYSTS BASED ON CYCLOPROPYL-SUBSTITUTED BIS(INDENYL) ZIRCONOCENE COMPLEXES OF $C_2$ -SYMMETRY

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$C_2$ -symmetrical ansa-complexes of Group 4 metals activated by MAO or perfluoroborate activators are highly efficient catalysts of stereoselective propylene polymerization, for which a reliable structure-properties correlation has been established.<sup>1</sup> One of the most successful examples are systems based on *ansa*-zirconocenes of  $C_2$ -symmetry bearing  $Me_2Si$ -bridge as well as alkyl and aryl substituents at the 2<sup>nd</sup> and 4<sup>th</sup> positions of the indenyl fragments, respectively. New complexes of this type containing cyclopropyl substituents in the indenyl fragments are reported here, for example:



Pd-catalyzed cross-coupling reactions involving halogen-substituted indenenes were employed to introduce the cyclopropyl substituent. The obtained cyclopropyl-substituted indenenes were used for the synthesis of  $Me_2Si$ -bridged ligands which were converted to the corresponding *ansa*-metallocenes. At the final stage of the research, the obtained complexes activated by MAO or perfluoroborate activator AB ( $PhNHMe^+[B(C_6F_5)_4]^-$ ) were shown to form highly active and stereoselective propylene polymerization catalysts with characteristics comparable to those of metallocene catalysts with common non-cyclic alkyl substituents.

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# STUDY OF PIEZO/PHOTOCATALYTIC PROPERTIES OF PVDF NANOFIBERS MODIFIED WITH MAGNESIUM NITRATE.

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With the growth of industrial capacities, the level of pollution and toxicity, including organic compounds, increases. One of the promising methods of cleaning is piezo/photocatalytic processes, which use two types of natural energy: solar energy for photocatalysis and mechanical energy for piezocatalysis<sup>1</sup>. In this work, a composite polymer membrane based on organic piezoelectric material polyvinylidene fluoride (PVDF) with addition of hydrated magnesium nitrate salt  $\text{Mg}(\text{NO}_3)_2 \times 4\text{H}_2\text{O}$  synthesized by electrospinning method<sup>2</sup> was used.

The obtained sample was investigated by scanning electron microscopy (SEM), X-ray diffraction (XRD), optical spectroscopy, X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy (RS). The catalytic properties were studied by decomposition of model dye methylene blue (MB) under irradiation with Visible and UV-visible light, and ultrasound at 18kHz was used as a source of mechanical stress. The composite material showed high photocatalytic activity. The results showed that under UV-visible irradiation, piezophotocatalysis exhibited the highest activity in MS decomposition (92% in 25 min), while in the absence of light irradiation, piezocatalysis (83% efficiency in 60 min), and photocatalysis showed 89% efficiency in the same time period. Using a visible light source, the photocatalysis and piezophotocatalysis activities were 44% and 74%, respectively. It is worth noting that neither the polymer nor the salt is photosensitive materials.

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# SYNTHESIS OF ZSM-5 ZEOLITE WITH LOW SODIUM CONTENT

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ZSM-5 zeolites are the most widely used as highly effective catalysts and adsorbents in many processes of the chemical and petrochemical industry. The interest in these zeolites is due to the presence of large cavities and a three-dimensional ring in the structure, as a result of which these materials have an increased diffusion capacity into the pores of the catalyst of large-molecular hydrocarbons, which significantly expands the scope of their use in technological processes<sup>1</sup>.

Due to the fact that the presence of sodium reduces the activity of the catalyst in many technological processes, this entails the requirement for almost complete removal of Na<sup>+</sup>, including by replacing it with NH<sup>4+</sup>. Thus, the development of a direct synthesis with a low sodium content is relevant.

The samples were prepared according to the deposition formula: Na<sub>2</sub>O·Al<sub>2</sub>O<sub>3</sub>·50C<sub>2</sub>H<sub>5</sub>ONH<sub>2</sub>·50SiO<sub>2</sub>·525H<sub>2</sub>O. Previously, the mixture of the initial components was subjected to microwave treatment for 10 min<sup>2</sup>, after which hydrothermal synthesis was performed in an autoclave with a volume of 250 ml for 24-72 hours at a temperature of 150°C.

As a result, the optimal parameters for the synthesis of zeolite ZSM-5 with a reduced content of Na<sup>+</sup> ions were determined, it was shown that after 48 hours the crystallization product was zeolite ZSM-5 with a crystalline phase content of 95%, no other phases were detected. An increase in the crystallization time led to the formation of an additional quartz phase in the area of the diffraction angle of 2θ: 25-27 degrees, which may be due to recrystallization of the product, and a decrease in time led to the production of a product with a high content of amorphous phase.

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# ALGINATES AS “GREEN” CARRIERS FOR IMMOBILIZATION OF CHIRAL ORGANIC CATALYSTS

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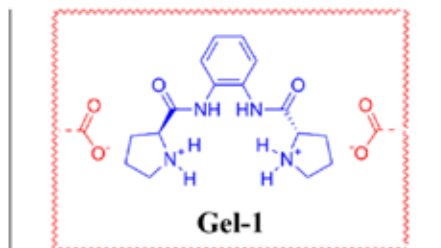
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Homogeneous catalysis is a successful area of modern chemistry. However, such catalysts are practically impossible to regenerate. At the same time, heterogeneous catalysts can be easily separated from the reaction mixture. Unfortunately, heterogeneous catalysts have significant disadvantages, such as inhomogeneous arrangement of active centers in space and inhomogeneity of the carrier surface.

This leads to low selectivity and efficiency of heterogeneous catalysis compared to homogeneous catalysis<sup>1</sup>. It seemed that the problem was solved by immobilization of homogeneous catalysts on polymeric solid carriers. Nevertheless, despite numerous attempts to solve this problem, such catalysts are practically not used in industry<sup>2</sup>. The reason for this is the high price and short life of such catalysts.

We propose a new type of immobilization of homogeneous chiral catalysts based on the use of available natural carriers without using expensive immobilization techniques. We have chosen a natural polysaccharide, alginic acid, as a carrier. By adding to it a catalytic particle containing several basic amino groups, we will carry out ionic immobilization of this catalyst with the formation of a chiral heterogeneous **Gel-1** framework.



This framework was used as a catalyst for the reaction of warfarin drug preparation, where it showed high efficiency and selectivity, which opens up a wide range of possibilities for the preparation of new drugs by asymmetric heterogeneous catalysis.

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# SYNTHESIS OF NEW NAPHTHYLTERPYRIDINE DERIVATIVES - POTENTIAL LIGANDS FOR METALORGANIC CATALYSIS

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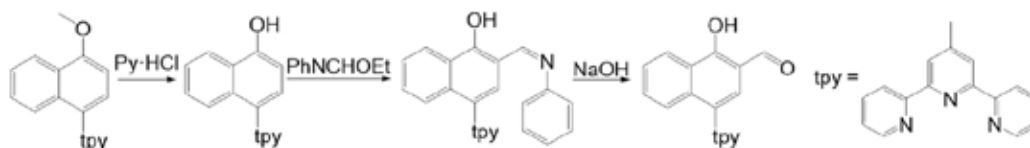
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The new derivatives of 2,2':6',2''-terpyridine ligands have attracted increasing attention from researchers caused by their wide range of practical applications in the fields of catalysis, chemosensing, optoelectronics, and supramolecular chemistry. This is due to their high chelating ability, as well as their propensity for  $\pi$ - $\pi$  interactions and the formation of strong hydrogen bonds.

4'-(4-Methoxynaphthalen-1-yl)-2,2':6',2''-terpyridine and 4'-(6-methoxynaphthalen-2-yl)-2,2':6',2''-terpyridine were synthesized using a known methodology through the Kröhnke pyridine synthesis with the aim of further functionalization. Subsequently, the 4,1 and 6,2 derivatives were subjected to reactions according to the scheme.



The obtained compounds are NNN-type ligands and may be of interest for Ni, Ru and Pd catalysis.

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# DEVELOPMENT OF IRON-BASED CATALYSTS TO PRODUCE TURQUOISE HYDROGEN BY METHANE PYROLYSIS

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The catalytic decomposition of methane is one of the promising methods of the turquoise hydrogen production, which is recognized as a pivotal future energy carrier<sup>1</sup>. However, the low efficiency and short lifespan of catalysts pose challenges in attaining the high hydrogen yields needed for industrial purposes, despite the absence of direct CO<sub>2</sub> emissions<sup>2</sup>.

The present study explored a new approach to obtain catalysts - aerosol spray pyrolysis for 10-30 wt. % Fe/Al<sub>2</sub>O<sub>3</sub>. Characterization of the catalysts with a set of methods (BET, XRD, TEM and SEM) proves homogeneous distribution of iron within amorphous spherical particles with size of 1 micrometer. The reaction was carried out at 700 °C – 800 °C in fixed bed reactor under CH<sub>4</sub>/N<sub>2</sub> atmosphere<sup>3</sup>. These catalysts showed methane conversion up to 8.6 % without H<sub>2</sub> pre-reduction. The investigation into the impact of catalyst calcination at temperatures of 400°C and 900°C reveals a reduction in reaction rates by a factor of 1.5. The carbon co-product characterization by TEM, Raman, TGA revealed the formation of multi-walled nanotubes (MWCNTs).

The current investigation examined the impact of incorporating cobalt as a promoter for iron on the catalytic performance. The results reveal that Co addition in 30% Fe/Al<sub>2</sub>O<sub>3</sub> has shown increased the H<sub>2</sub> yield and stability of the catalyst by 2 times. The maximum H<sub>2</sub> yield was obtained using 30% FeCo<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> catalyst at 700 °C. The methane to hydrogen conversion decreases by 2 - 4% at 700°C but leads to an increase in the lifetime of the catalyst.

The findings demonstrate encouraging prospects for employing the aerosol spray pyrolysis method in iron-based catalytic systems for methane decomposition reactions. This paves the way for accelerated process scaling and bring methane pyrolysis closer to becoming an industrial alternative way to produce turquoise hydrogen.

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# SYNTHESIS AND STUDY OF THE CATALYTIC ACTIVITY OF PHOTOACTIVE Pd/NHC SYSTEMS

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Photocatalysis is a valuable tool to significantly expand the potential of synthetic organic chemistry<sup>1</sup>. Researchers from around the world are using photocatalysts to build C-C and C-heteroatom bonds in substrates where traditional organic synthesis methods are inefficient<sup>1,2</sup>. However, they can rarely be regenerated at the end of a reaction, which raises questions about the stability of photocatalysts as well as possible unexplored processes in their evolution. Understanding the transformations of catalysts undergoing the reaction will enable the development of new high-performance catalytic systems<sup>3,4</sup>.

In this work, photoactive Pd/NHC (N-heterocyclic carbene) complexes were synthesized as an example of a dynamic photocatalytic system. Its catalytic activity was studied on a model photooxidative amidation reaction between aldehyde derivatives and secondary amines. A wide range of 28 different amidation reaction products in yields ranging from 26 to 92% were synthesized to prove the efficiency of the methodology.

In the next step, the behavior of the Pd/NHC complex in solution was studied. Reaction monitoring using mass spectrometry was used to study of the reaction mechanism and to show the presence of dynamic transformations of the Pd/NHC complex under amidation reaction conditions.

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# RESEARCH AND DEVELOPMENT OF HIGHLY EFFICIENT MOF-BASED CATALYSTS FOR ORTHO-PARA HYDROGEN CONVERSION

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In recent years hydrogen energy is one of the most actively developing areas of science and technology. The problem of hydrogen storage and transport is the key problem in the way of introducing hydrogen energy. Hydrogen liquefaction is the most simple and well-studied method to store hydrogen with high energy density. The key stage of this process is the ortho-para conversion of hydrogen. Under normal conditions, isomer concentrations are correlated as 1/3, while at the boiling point at equilibrium, hydrogen is almost entirely composed of the para-isomer. For this reason, preliminary ortho-para conversion is necessary to avoid spontaneous boiling and explosion of hydrogen. In industry, iron oxide catalysts (eg Ionex®) are commonly used for ortho-para hydrogen conversion. However, these materials have rather low porosity and availability of metal ions for hydrogen. On the other hand, the porosity, specific surface area, and accessibility of paramagnetic metal ions for hydrogen are much higher in metal-organic frameworks (MOF). In this regard, MOFs that have the potential for large-scale production should be considered, and shaping methods must be developed to obtain mechanically strong particles of the required size.

In this work, the efficiency of MOF-based ortho-para hydrogen conversion catalysts containing paramagnetic metal ions was studied. MOFs with high scaling potential and high efficiency in the process of ortho-para hydrogen conversion were selected as objects of study. The influence of activation and modification conditions by doping for some MOFs on the catalysis efficiency was also studied. Approaches to the shaping of the considered MOFs have been developed to obtain mechanically strong and catalytically efficient materials.

*"This work was supported by the Russian Science Foundation № 22-73-10239"*

# ADVANTAGES OF RETICULATED CATALYTIC SYSTEMS FOR GAS TREATMENT OF NITROGEN AND CARBON OXIDES AND VOLATILE ORGANIC COMPOUNDS IN ATMOSPHERIC EMISSIONS OF CHEMICAL AND METALLURGICAL INDUSTRIES

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LLC "Ecostream" creates catalytic systems based on reticulated catalysts with active components (platinum, palladium rhodium, ruthenium) applied using a special technology, for industrial atmospheric emissions gas treatment of chemical plants from the most typical pollutants - nitrogen (I, II, IV) oxides  $N_2O$ ,  $NO$ ,  $NO_2$  and carbon (II) oxides  $CO$ , as well as for the catalytic oxidation of volatile organic compounds (vapors of solvents, aerosols of paints and varnishes) in pollutions of metalworking plants. Reticulated catalyst systems operating on principle of heterogeneous catalysis are a highly efficient way to purify atmospheric emissions due to fact that catalytic interactions in catalysts of this type occur at the interface between the phase of convertible gas mixture and the catalyst. Interaction of convertible substances is ensured on developed surface of mesh catalysts created by applying active components to multilayer supports - silica fabrics (for low-temperature processes up to 500 °C) or mesh of heat-resistant alloys based on stainless steel, fehral, etc. (for high-temperature processes from 500 °C to 1000 °C), with formation of activated complexes in the form of intermediate surface compounds of catalyst and reacting substances, which then form catalysis products that restore the surface of catalyst.

The required weight, layer volume and packing density of reticulated catalysts for efficient gas treatment processes are determined on basis of experimental studies of activity performed in own laboratory pilot bench test unit. The volumetric velocity of gas mixture for reticulated catalyst systems based on multilayer silica fabric according to research results is up to 40000 hour<sup>-1</sup>, at which the highest efficiency of gas cleaning processes is achieved, which is 3 - 5 times higher than known block and granular catalysts.



# MIXED LN-AL (LN = LA, CE, PR) OXIDES: SYNTHESIS, STRUCTURE AND CATALYTIC PROPERTIES IN OXIDATIVE COUPLING OF METHANE

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Aluminates of rare earth elements (REE) of the general formula  $\text{LnAlO}_3$  and of perovskite structure are promising catalysts for the production of ethylene and ethane via oxidative coupling of methane (OCM). Comparing the properties of La, Ce and Pr aluminates, which differ in the ability to change the oxidation degree, is of interest in order to understand the mechanism of their catalytic action.

The regularities of formation of La, Ce and Pr aluminates are considered.  $\text{CeAlO}_3$  was obtained by treating a mixture of Ce and Al oxides in a stream of  $\text{H}_2$  at 800°C. It has low efficiency in the OCM process and decomposes in oxygen-containing media to form  $\text{CeO}_2$  and amorphous  $\text{Al}_2\text{O}_3$ .

Single-phase La and Pr aluminates were obtained by heating amorphous precursors at 900°C in air. Unlike  $\text{CeAlO}_3$ , Pr aluminate is stable in the reaction medium during methane oxidation and demonstrates higher activity and selectivity in the formation of ethylene compared to  $\text{LaAlO}_3$  due to the ability of the  $\text{Pr}^{3+}$  cation, unlike  $\text{La}^{3+}$ , to activate  $\text{O}_2$  molecules via electron transfer with a change in the Pr oxidation state and the formation of reactive oxygen species:



Ion-radicals  $\text{O}^-$  in oxide systems are known to play the role of active centers that conduct the formation of OCM products:



The possibility of changing the morphology, chemical and phase composition of the resulting systems using processing in water and water-ammonia fluid media is demonstrated. Such treatment of La-Al oxide precursors leads to the production of materials containing  $\text{LaAlO}_3$  and  $\text{La}_2\text{O}_3$  phases and demonstrating advanced efficiency in the OCM process.

*Acknowledgement.* The research was supported by the Russian Science Foundation grant No. 23-13-00360, <https://rscf.ru/project/23-13-00360/>.

# HYDRODEOXYGENATION AND HYDROISOMERIZATION OF RAPESEED OIL OVER ZEOLITE-CONTAINING $\text{MoS}_2$ CATALYSTS

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In the aviation industry, the use of hydrogen or electricity seems unlikely, therefore, jet fuel, the components of which are industrially obtained from esters or fatty acid triglycerides (FATs), in two stages, becomes the solution to the problem. First, a mixture of alkanes is obtained as a result of hydrodeoxygenation (HDO), then hydroisomerization/hydrocracking of alkanes is performed. The one-stage process of hydroprocessing of FATs into jet fuel components is more efficient; therefore, the development of polyfunctional catalysts that ensure the occurrence of several reactions simultaneously (HDO, hydroisomerization, and hydrocracking) is a promising area of research that has been actively developing in recent years.

For this purpose, alumina and composite granular supports (30 wt.% of zeolite/70 wt.%  $\text{Al}_2\text{O}_3$ ) were prepared. Mo catalysts were synthesized by incipient wetness impregnation by aqua solution containing precursors of active component, followed by drying at 110°C for 4 hours.

A comparative study of the prepared catalysts in the hydroconversion of rapeseed oil (RSO) was performed in a flow reactor at wide range of conditions (310 and 330°C, 3.0 and 5.0 MPa, 600 and 1200  $\text{Nm}^3/\text{m}^3$ , 18 and 36  $\text{h}^{-1}$ ). The liquid and gases products were quantified using gas chromatographs, Vario EL Cube was used to follow total O content.

Molybdenum sulfide supported on  $\text{Al}_2\text{O}_3$ -zeolite (ZSM-22, SAPO-11) provides high selectivity for the conversion of RSO via the direct "HDO" route (70-94% in depends on reaction conditions). Complete oxygen conversion was observed at all reaction conditions. Iso/n ratio was strongly affected by process conditions. Temperature and H/C ratio increase resulted in higher iso/n ratio. Increase in hydrogen pressure leaded to lower iso/n ratio. Probably it can be explained by the inhibiting effect of hydrogen disulfide (from dimethyl disulfide decompose to preserve sulfide state of catalyst) and minor content of produced CO. Higher pressure results in higher solubility of these gases in the liquid products and as result hydroisomerization was inhibited. It should be noted that amount of cracked product ( $<C_9$ ) was varied from 1 to 10 % in depends on process conditions and zeolite type.

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# CATALITIC ISOTOPE EXCHANGE BETWEEN CARBON DIOXIDE AND WATER VAPOR

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From the point of view of thermodynamics, one of the most promising methods for separating oxygen isotopes is chemical isotope exchange between carbon dioxide and water<sup>1</sup>. When using a heterogeneous catalyst, the process occurs in two stages: catalytic isotope exchange between carbon dioxide and water vapor and phase isotope exchange between water and its vapor. To implement a countercurrent separation process, it is necessary to prevent liquid water from entering the active centers of the catalyst, which can be achieved by using a hydrophobic catalyst or carrying out the process in devices in which the catalyst is spatially separated from the flow of liquid water<sup>2</sup>.

Table 1 presents the results of a study of the activity of catalysts based on oxides of various metals deposited on a carrier –  $\gamma$ - $\text{Al}_2\text{O}_3$ . The observed rate constant ( $k$ ,  $\text{s}^{-1}$ ) and the rate of isotope exchange ( $R_{\text{IE}}$ ,  $\text{mol}/(\text{m}^3 \cdot \text{s})$ ) were chosen as indicators of catalytic activity.

Catalyst	$\text{CuO}/\text{ZnO}/\text{Al}_2\text{O}_3$	$\text{Fe}_2\text{O}_3/\text{Al}_2\text{O}_3$	$\text{CoO}/\text{Al}_2\text{O}_3$	$\text{NiO}/\text{Al}_2\text{O}_3$	$\text{Ce}_2\text{O}_3/\text{Al}_2\text{O}_3$
$k$ , $\text{s}^{-1}$	$0.927 \pm 0.067$	$1.50 \pm 0.17$	$2.13 \pm 0.20$	$4.98 \pm 0.55$	$1.04 \pm 0.10$
$R_{\text{IE}}$ , $\text{mol}/(\text{m}^3 \cdot \text{s})$	$5.68 \pm 0.38$	$9.2 \pm 1.0$	$13.1 \pm 1.3$	$30.5 \pm 3.4$	$6.38 \pm 0.64$

**Table 1.** Activity of catalysts in the reaction of isotope exchange between carbon dioxide and water vapor at  $T=348 \text{ K}$ ;  $P=0.1 \text{ MPa}$ ;  $G_{\text{CO}_2}=1.2 \text{ mol/h}$ ;  $G_{\text{H}_2\text{O}}=0.3 \text{ mol/h}$

Of the catalysts studied, nickel oxide supported on aluminum oxide showed the greatest catalytic activity in the reaction of isotope exchange between carbon dioxide and water vapor. This sample showed twice the activity compared to the industrial catalyst NTK-10-2FM, which was studied earlier (under the same conditions  $k=2.35 \pm 0.35 \text{ s}^{-1}$ ;  $R_{\text{IE}}=14.4 \pm 2.2 \text{ mol}/(\text{m}^3 \cdot \text{s})$ ).

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*The work is performed in the framework of the development program "Priority-2030" of the Mendeleev University of Chemical Technology of Russia.*





SECTION 8

**POLYMERS AND POLYMERIC  
MATERIALS  
(INCLUDING 2<sup>ND</sup>  
INTERNATIONAL SYMPOSIUM  
“MODERN TRENDS  
IN DENDRIMER CHEMISTRY  
AND APPLICATIONS”)**

# PROSPECTIVE DIRECTIONS FOR THE DEVELOPMENT OF POLYMERS AND POLYMER MATERIALS

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The development of modern technologies requires the creation of a wide range of polymer and composite materials with various morphologies and adjustable physical-mechanical characteristics. Large-scale efforts are underway worldwide to develop and implement new materials across various industries. The focus is not only on developing new compounds but also on the high-tech utilization of traditional materials, including new processing methods and additive technologies. Numerical methods are widely used to effectively utilize existing material databases. Overall, the total funding for innovations in materials science reaches \$1 trillion. According to forecasts, special attention will be given to interdisciplinary research in high-modulus, high-strength carbide, carbon, metal oxide fibers and structures, materials for energy, secondary power sources, smart materials, piezo- and thermoelectrics, shape-memory materials, materials for flexible electronics, monitoring external conditions and parameters of various systems and human condition monitoring, metamaterials, and more. In the field of thermoplastics and reactoplastics, research is being funded to develop plastics with adjustable resistance, radio absorption, and magnetization, as well as high-temperature plastics with high sorption capacity for various components, including radioactive and toxic substances. Special emphasis is placed on developing materials based on natural raw materials, both structural and functional: sorbents, biofuels, physiologically active materials, including biodegradable ones. Research in these areas is typically conducted by international groups using advanced infrastructure.

In accordance with Presidential Decree No. 309 "On the National Development Goals of the Russian Federation for the Period up to 2030 and Beyond to 2036" dated May 7, 2024, targeted tasks have been set to ensure technological independence in the field of new materials and chemistry. The priority of technological policy is to achieve technological sovereignty – the presence of critical cross-cutting technologies of its own development in the direction of "new materials and substances technologies, their modeling, and development." Solving the assigned tasks in modern conditions is an extremely complex challenge and requires the identification of key priorities, which will be discussed during the talk.

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# MACROMOLECULAR NANO-OBJECTS: OUTCOMES OF THE EXTENSIVE DEVELOPMENT PHASE

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Macromolecular nano-objects or macromolecules-particles, a new (fourth) category in the general classification of polymers based on the structure of the main chain, are distinguished by their three-dimensional geometric shape and specific sizes. Emerging from idealized theoretical concepts, they have attracted researchers' attention with their perfection and combinatorial possibilities for creating real objects. All of them have appeared thanks to unique synthetic strategies: hyperbranched polymers (Flory), dendrimers (Tomalia, Frechet), multi-arm stars (Roovers, Vasilenko), nanogels (Meshkov, Muzafarov), and dense molecular brushes (Matyjaszewski, Schmidt, Sheiko). These new objects have led to an exponential growth in research, inspired by the prospect of obtaining materials with a unique set of properties.

The scientific schools of the Russian Academy of Sciences have made fundamental contributions to these studies. Through their example and consistent interest, focused on solving the critical task of identifying the structure-property relationship for each of the new macromolecular forms, they have safeguarded the main research direction from external applied influences, such as practical applications, forecasts, and assessments of prospects. This approach has led to significant results, confirming the presence of unique properties for each of the mentioned forms through targeted structural modifications. For example, dendrimers exhibited a qualitative transition from low to high generations and the ability to crystallize in the absence of specific interactions; multi-arm stars showed a globular nature and unique rheology; dense macromolecular brushes demonstrated fundamentally different intermolecular interactions compared to classical systems. Finally, for nanogels, the transition from macromolecule to particle was traced as the core-shell ratio changed.

In summary, the essential foundation has been laid, allowing for a critical review of the accumulated factual material, determining the prospects for further development in this field, and moving towards the targeted search for potential practical applications for these types of objects



# FUNCTIONAL MATERIALS FOR ORGANIC ELECTRONICS: YESTERDAY, TODAY AND TOMORROW

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Oligomeric and polymeric materials have been widely used in microelectronics for a long time as dielectrics, photoresists, protective coatings, as a part of highly filled polymer composites and their substrates. However, with the invention of soluble conductive polymers, the range of their applications has significantly expanded and led to the emergence of organic electronics, characterized by lightness, flexibility, transparency and a number of other valuable characteristics that distinguish it into a separate field of microelectronics.

The current state and prospects for the development of functional materials for organic electronics, among which conductive polymers<sup>1</sup>, organic semiconductors and luminophores are considered in the report. Most of them are linearly conjugated or annulated heterocyclic compounds<sup>2</sup> of oligomeric or polymeric nature. Depending on their physical-chemical characteristics, they can be used as various functional layers in a variety of organic electronics devices: organic field-effect<sup>3</sup>, electrochemical<sup>4</sup> and light-emitting transistors<sup>5</sup>, organic light-emitting diodes, organic photovoltaic cells<sup>6-8</sup>, various photo-, chemo- and biosensors<sup>9</sup>.

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# BOTTLEBRUSH NETWORKS: PROGRAMMABLE PROPERTIES EMPOWERED BY ARCHITECTURE

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Bottlebrush macromolecules are resourceful building blocks for constructing tissue-mimetic elastomers and gels with sought after combinations of elasticity, damping, swelling, and adhesion. Densely grafted side chains define physical properties in two ways: (i) they disentangle network strands and (ii) they increase strand persistent length. The first trait alleviates constraints for lowering the crosslink density, enabling supersoft and super-swelling polymer networks that closely match soft tissues like brain and jellyfish. The second trait, variable persistence length, controls elastic modulus, strain-stiffening, and relaxation times. By architecturally tuning the size and flexibility of brush-like network strands, we can create materials possessing oxymoronic property combinations, such as being soft-yet-firm, elastic-yet-dissipating, and stiff-yet-stretchable. Recently, we have explored brush macromolecules with active backbones that synergize with the passive side chains to generate novel materials such as super swelling-yet-resilient hydrogels and bottlebrush liquid crystals. In short, the design-by-architecture approach empowers programmable variations of a network's modulus, damping factor, swelling ratio, and Rouse time independently of one another, meeting the diverse needs of both medical and non-medical technologies.

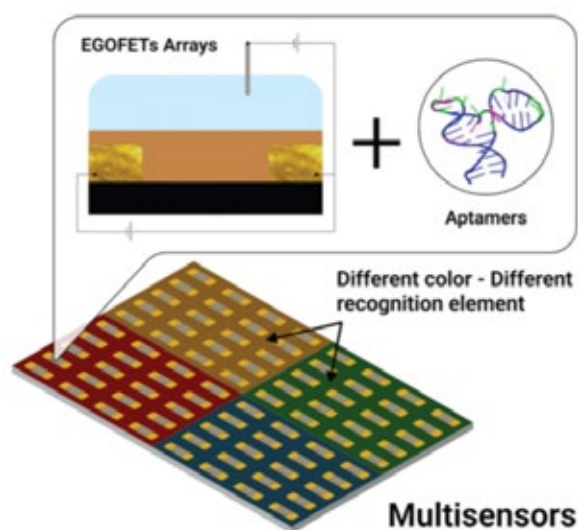
# MATERIALS FOR FUNCTIONAL AND RECEPTOR LAYERS OF LIQUID SENSORS BASED ON ORGANIC TRANSISTORS

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Recently, the field of multi-purpose biological and chemical analysis with parallel detection of one or more analytes using electrolyte-gated organic field-effect transistors (EGOFETs) has been actively developing.<sup>1</sup>

The presented report summarizes the results of researches devoted to the use of EGOFETs with an active layer of organic semiconducting materials and various recognition layers as a platform for biosensing (Figure 1).



**Figure 1** - Architecture of a multisensory system based on EGOFETs with a biorecognition layer based on aptamers<sup>2</sup>

The operation principles of EGOFETs, their advantages and disadvantages are considered in details, criteria for the selection of semiconducting and receptor materials, the causes of degradation and ways to eliminate them are given.<sup>3</sup> The most successful examples of multisensory devices based on EGOFETs for the detection of biological and chemical markers and analytes are demonstrated.<sup>2</sup>

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# POLYMER BASIS OF LITHOGRAPHIC MATERIALS: PROBLEMS AND SOLUTIONS

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The possibility of independent development of the domestic microelectronic industry is determined by the need to develop (including mandatory scientific research) and produce the entire complex of materials. Approximately a thousand of them are critical, i.e. those on which the characteristics of products depend and to which special requirements for cleanliness are imposed. Constraining factors for their production are small volumes of consumption and, as a consequence, long-term payback of costs or their unprofitability; lack of appropriate material base (infrastructure and equipment); lack of scientific and technical groundwork - a limited number of organizations have the competence to develop and produce modern materials.

Ways to overcome existing problems in the development of domestic production of highly pure materials for microelectronics, including such an important component of lithographic materials as polymers, may be the following:

- creation of technological chains (research institutes - applied institutes - manufacturing enterprises) for the development and development of new technological processes, specialized materials;
- organization of centers for conducting research and micro-tonnage production of materials for microelectronics in categorized clean production facilities on the basis of institutes of the Russian Academy of Sciences in order to ensure the technological sovereignty of Russia in the field of lithographic materials for existing (180-90 nm) and new (65-28 nm) technologies.

Using the example of an established and successfully operating technological chain (MERI JSC - FRC PCP MC RAS - JSC «NIOPIK» - LLC "Polyketon" - JSC "Mikron"), the report presents work on the research and development of polymers for anti-reflective coatings, photoresists and surfactants substances.

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# CRYSTALLIZATION OF HIGH-GENERATION DENDRIMERS: FROM SPACE FILLING TO DENSE PACKING

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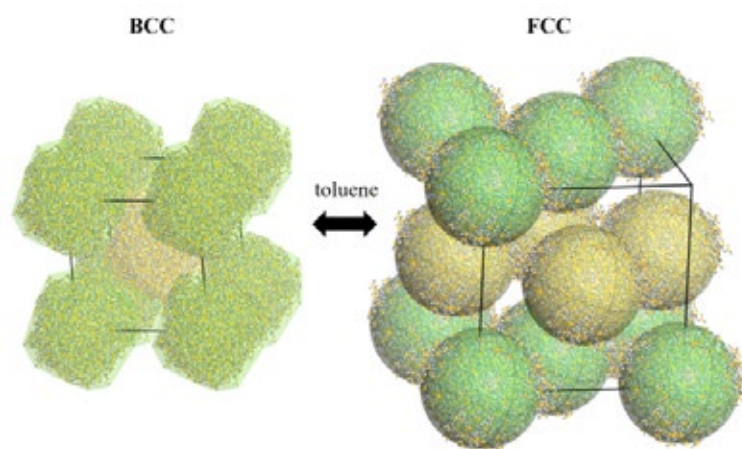
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Carbosilane dendrimers of high generation exhibit properties of both macromolecules and nanoparticles and can simulate the complex task of packing soft quasispherical objects into a well-organized three-dimensional structure. The article offers an original approach to crystallization of dendrimers of high generation using annealing procedure in solvent pairs<sup>1,2</sup>. Identifying the common mesophase features of dendrimers from multiple generation, including the formation of a densely packaged cubic FCC and transitions from primitive cubic BCC to FCC, allows understanding and revealing the overall properties of the crystallization process, which occurs as a result of symmetry breaking.



**Figure 1.** Molecular reorganization upon phase transition during solvent annealing of G6 dendrimer.

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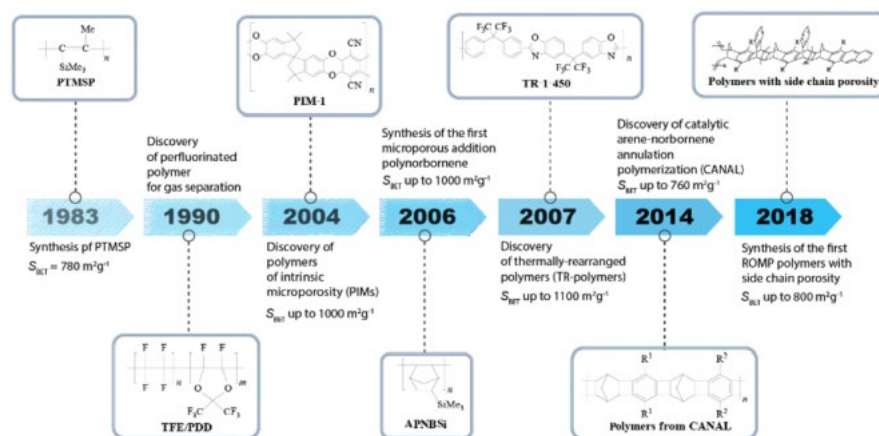


# MACROMOLECULAR DESIGN OF POLYMERIC MEMBRANE MATERIALS BASED ON SUBSTITUTED NORBORNENES: CURRENT STATE AND PROSPECTS FOR DEVELOPMENT

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The development of technologies and tightening of environmental requirements to industrial processes make the development of new membrane polymeric materials for gas separation, fuel cells, separation of enantiomers from the corresponding racemic mixtures, etc. in demand. A promising class of monomers for the creation of such polymers are strained cycloolefins, in particular norbornene derivatives, which have a number of significant advantages. The application of these monomers for the design of polymeric membrane materials opens up enormous opportunities to vary the structure of the monomer linkage and to establish valuable structure-property relationships. The report will review recent advances in the targeted synthesis of membrane materials based on norbornene derivatives, including optically active ones, in comparison with other polymer groups being developed for similar purposes (Fig. 1), including data from the scientific group of the authors.



**Figure 1.** Main classes of highly permeable glassy polymers.<sup>1,2</sup>

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# FULL FACTORIAL ANALYSIS IN DESIGN OF CHITOSAN SCAFFOLDS FOR 3D CELL CULTURING

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Cryogelation is a simple and cost-effective approach to fabrication of porous polymer materials, which can significantly overperform hydrogels of the same chemical composition in terms of mechanical stability, elasticity and permeability. Due to the structural similarity with glycosaminoglycans, one of the main components of extracellular matrix, chitosan and its derivatives remain in the focus of interest for development of 3D cellular models. In cancer research this interest is related to ability of chitosan to mimic tumor microenvironments and elevate the expression levels of cancer stem cell markers genes providing external signals to alter the fate of cancer cells and their chemoresistance. A number of studies have demonstrated recently that both surface charge and chemistry and mechanical properties are important for cell-matrix interactions and cancer stem cell differentiation using polymer scaffolds. Thus, to develop more realistic microtumor models for pharmaceutical tests it is crucial to control chemical and mechanical stimuli in polymer scaffolds independently.

Fabrication of chitosan cryogels via chemical cross-linking with glutaraldehyde has two significant limitations: increase of cytotoxicity with increasing cross-linking density and high rate of cross-linking reaction, which complicates prevention of gelation before freezing of the polymer solution. Diglycidyl ether of glycols (DGE), which are most important cross-linkers for hyaluronic acid, have been earlier used to cross-link chitosan only under heterogeneous conditions in alkaline media and elevated temperature.

Here using full factor analysis we have evaluated effects of solution viscosity, pH, DGE chain length and DGE:chitosan mole ratio on swelling, pore-size distribution, surface charge density, mechanical properties and susceptibility to enzymatic hydrolysis of chitosan cryogels. The cell-scaffold interactions have been investigated for colorectal cancer HCT 116 cell line cultured in chitosan cryogels and chitosan scaffold obtained via lyophilization and charge neutralization. It was shown that morphology of cell aggregates and cell circularity significantly depend on the scaffold characteristics.

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# REVERSIBLE DEACTIVATION RADICAL POLYMERIZATION: TASKS, IMPLEMENTATION AND PROSPECTS

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The renaissance of radical polymerization observed in recent decades is due to its new possibilities in the molecular design of polymers caused by the implementation of reversible reactions of chain deactivation. As a result, radical polymerization acquires the features of living anionic polymerization and can be used for the controlled synthesis of macromolecules of complex architecture, copolymers with the required distribution of monomer units along the chain and a given functionality, *etc.*

Reversible chain deactivation is achieved through the use of special compounds that suppress the termination reactions of propagating radicals and replace it with reversible termination and/or reversible chain transfer reactions. The first type includes polymerization processes involving low-activity and stable radicals and atom transfer radical polymerization (ATRP), the second type includes polymerization with reversible addition-fragmentation chain transfer (RAFT) and polymerization with degenerate chain transfer. The main difference between the listed options for controlled radical polymerization and live anionic polymerization is the coexistence of periods of "sleep" and "life" of macromolecules, which allow them to grow stepwise during polymerization and retain the ability to continue the chain growth after isolation of the polymer and its addition to a portion of a new monomer.

The choice of one or another activation method depends on the specific task being solved and, accordingly, on the chemical nature of the monomers. In recent years, ATRP and RAFT polymerization have been competing most actively with each other for leadership in the field of macromolecular design. This has led not only to the development of routine and easily scalable methods for the controlled synthesis of various homo- and copolymers, but also to the development of new approaches to the initiation of polymerization (PET – photo-induced electron transfer) and methods of its implementation (PISA – polymerization-induced self-assembly).

The result of these studies is the creation of numerous variants of smart polymers for different applications and the search for ways to commercialize controlled radical polymerization.

# THE USE OF SYNCHROTRON RADIATION FOR STRUCTURAL STUDIES OF FUNCTIONAL MATERIALS

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Modern synchrotron sources offer material scientists a wide variety of methods for studying the structure and self-organization processes in materials. The high intensity of X-ray beams achieved at third and fourth generation sources, as well as the ability to focus them to submicron sizes, allows for obtaining structural data with high spatial and temporal resolution.

One example of studying molecular self-assembly processes using nanofocused X-ray diffraction is described for the case of self-organization of wedge-shaped mesogens in the pores of a nanoscale aluminum oxide template<sup>1</sup>. The method allows for 2D scanning of the sample with a submicron step and quantitatively determining the degree of orientation of the columnar phase of the mesogens inside the nanoscale pores depending on the distance to the free surface of the membrane.

The combination of microfocused diffraction, grazing incidence diffraction, and in-situ ultrafast calorimetry enables detailed analysis of the structure, texture, and thermal behavior of functional materials with complex hierarchical organization<sup>2,3</sup>.

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# STRUCTURAL VARIABILITY AND FUNCTIONAL PROPERTIES OF CONJUGATED OLIGOMERS FOR ORGANIC OPTOELECTRONICS

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Symmetrical conjugated oligomers are of great interest as luminescent and semiconductor materials for organic optoelectronics.<sup>1</sup> In particular, co-oligomers based on phenylene, thiophene, furan and fluorene find their applications in organic light-emitting diodes, sensors, lasers and field-effect transistors.<sup>2</sup>

Materials based on oligoarylene-phenylenes demonstrated a lucky combination of high solid-state luminescence and charge transport. Introduction of heterocycles or terminal substituents,<sup>3</sup> directed crystallization,<sup>4</sup> polymorphism and molecular doping<sup>5</sup> were demonstrated to be the most powerful approaches for crystal structure, luminescence and semiconductor characteristics control. 9H-fluoren-9-ylidene derivatives,<sup>6</sup> including ((9H-(diazfluorene)-9-ylidene)methyl)arylenes, exhibit aggregation-induced emission, mechano- and thermochromism due to solid-state conformational rearrangements. The introduction of nitrogen atoms into the fluorene core also enhances electron-withdrawing properties and stability. Coordination polymers based on 1,4-bis((9H-(4,5-diazfluorene)-9-ylidene)methyl)arylenes have been shown to have porous structure, luminescence, and to be sensitive to dehydration.

Here, synthetic, crystal-engineering and physico-chemical approaches for both molecular and crystal structures variation and accordingly, the material functional properties tuning are discussed.

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# DIRECTED MODIFICATION OF CARBOSILANE DENDRIMERS AS A WAY TO CONTROL THEIR CONFORMATIONAL BEHAVIOR AT THE HYDROPHOBIC-HYDROPHILIC INTERPHASE BOUNDARY: ATOMISTIC SIMULATIONS

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Amphiphilic dendrimers with segments of different chemical nature are attracting great attention due to new possibilities of regulating their properties in the integral "composition-structure" space, thus expanding the range of their practical applications. By changing the nature of the end groups, which determine the solubility of dendrimers, it is possible to significantly influence the affinity of the dendrimer to different solvents. In this case, the tree-like structure of dendrimers can serve as an important factor in controlling their surface-active properties as well as self-assembly in solutions and at interfaces.

This talk will give an overview of the results of computer simulations of carbosilane dendrimers with varying fractions and distributions of hydrophilic groups of different chemical nature in the end segments. These objects represent ideal model systems due to the absence of groups with specific interactions in the carbosilane core, which makes it possible to study fundamental effects related to the structural features of these macromolecules. We discuss the results of the analysis of the size, shape, mobility and detailed distributions of various segments obtained in the framework of the atomistic modeling of single amphiphilic carbosilane dendrimers in toluene, water and at the water/air and water/toluene interfacial boundaries, depending on the structure and generation number of the dendrimers, as well as their surface activity depending on the fraction and distribution of hydrophilic groups.

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# EXAMPLE OF ABSTRACT SYNTHESIS AND MODIFICATION OF ORGANOSILICON MOLECULES USING THE CuAAC REACTION

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The work presents results on the introduction of organozide and acetylene fragments into the structure of organosilicon molecules, as well as their modification according to the mechanism of the azide-alkyne cycloaddition reaction (CuAAC). We have demonstrated that this approach makes it possible to effectively introduce alkoxysilanes into the structure,

polysiloxanes and carbosilanes are organic substituents containing various heteroatoms to form a triazole ring, which is difficult to achieve with other synthetic approaches. In addition, we considered various options for the catalytic and non-catalytic use of the CuAAC reaction.

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# ULTRA-HIGH MOLECULAR WEIGHT POLYETHYLENE. THE CURRENT STATE OF THE PROBLEM.

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Ultra-high molecular weight polyethylene (UHMWPE) is an engineering thermoplastic obtained by polymerization of ethylene. UHMWPE is resistant to concentrated acids and alkalis, extremely low temperatures (up to  $-120^{\circ}\text{C}$ ), is characterized by low moisture absorption, low coefficient of friction, as well as extremely high values of specific strength characteristics in a highly oriented state.

With the above advantages, UHMWPE has found application in a wide number of industries and end-user products: mechanical engineering and equipment manufacturing; battery separators; reinforcing grids of road surfaces and building retaining walls, fishing nets, ropes and slings; personal protective equipment; medical implants, etc.

The high molecular weight of UHMWPE causes the formation of a large number of intermolecular entanglements between adjacent macromolecular “coils” of the polymer, which excludes the possibility of using traditional methods of polymer processing such as extrusion or melt injection molding.

Despite the noted difficulties of processing, the volume of UHMWPE production worldwide is constantly growing, as well as the volume of its processing.

The purpose of this work is to analyze a number of new opportunities in the field of development, creation and production of a promising class of materials based on UHMWPE, including the use of new catalytic systems for its synthesis and non-traditional methods of its processing both in the world's leading UHMWPE producing countries and in the Russian Federation also.

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# NECESSITY OF A SYSTEMIC APPROACH TO THE PROBLEM OF PROCESSING POLYMER WASTE

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Pollution of the World Ocean by plastic waste is a pressing international problem. According to the most conservative estimates, millions of tons of plastic are thrown into the ocean every year, and the area of the Great Pacific Spot achieves 1.5 million sq. km.

Unfortunately, the international community today is being imposed by a number of approaches to solving such problem that do not have a serious scientific basis and are deeply contradictory at their core. The essence of the measures proposed by developed countries is to fix the current state of affairs, in which a small circle of countries have developed industry and technology (including the production of a wide range of polymer materials), and for the rest of the world such development is artificially restrained for environmental reasons.

The fundamental drawback of this approach is ignoring the fact that life on planet Earth is itself a phenomenon that has a polymer basis, that is incomparable in scale with the volumes of production of synthetic polymers, and therefore in the biosphere exists a set of effective paths for the disposal and processing of polymer materials within the framework of closed cycles, such as the large carbon cycle.

The only way out of this situation was the development of a systemic, sovereign concept of the Russian Academy of Sciences, aimed at solving the problem of polymer waste, and its further promotion both on the territory of our country and together with interested countries. The developed Concept involves solving the problem of polymer waste using biomimetic methods and technologies, choosing the most economical and safe ones. It is the result of a wide discussion among specialists in the field of polymer materials science and ecology.

The report will discuss the main conclusions and recommendations of the developed concept to guide action to solve the problem of polymer waste.

# REDOX-ACTIVE POLYMERS AS ELECTRODE MATERIALS FOR PROMISING TYPES OF BATTERIES

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Using organic redox-active polymers as electrode materials opens up principally new opportunities for the development of metal-ion batteries. First, organic materials are usually based on light elements (C, H, N, O, S) and, therefore, can enable much higher specific capacities than compounds of heavy transition metals. Second, organic materials are usually non-toxic and environmentally friendly. Third, polymeric materials are soft and, therefore, can operate at high charge and discharge rates in ultrafast batteries. Moreover, mechanical properties of polymeric cathodes and anodes enable their application in truly bendable batteries for emerging generation of portable electronics. Finally, amorphous nature and simple redox mechanisms of polymeric electrode materials make them almost non-specific with respect to the type of mobile ions. This unique tolerance of organic electrodes enabled successful demonstration of organic batteries operating with tens of different ions, in particular  $H^+$ ,  $Li^+$ ,  $Na^+$ ,  $K^+$ ,  $NH_4^+$ ,  $Mg^{2+}$ ,  $Ca^{2+}$ ,  $Sr^{2+}$ ,  $Zn^{2+}$ ,  $Al^{3+}$ , etc. Thus, using organic materials, in particular, redox-active polymers, paves a way to the development of multiple new types of batteries for a broad variety of applications.

In this talk, we will provide an overview of our recent results on the design of organic and metal-organic redox active polymers and their application as electrode materials in lithium, sodium and potassium batteries. In particular, we will present ultrafast potassium batteries (charging/discharging in less than a minute) delivering high specific capacities and energy densities of  $\sim 600\text{--}900\text{ W h kg}^{-1}$  for the best organic cathode components. The polymer-based devices also demonstrated good cyclability with no capacity decay after a few thousand of charge-discharge cycles.

The obtained results suggest that organic electrode materials, while being at the infancy of their development, start to show commercially interesting performances thus attracting continuously growing attention to the new generation of post-lithium metal-ion battery technologies.

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# POLYMER WASTE: PROBLEMS AND PROSPECTS

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Polymer materials are designed to have a limited service life. Therefore, the problem of minimizing polymer waste and its disposal is becoming increasingly urgent. This can be achieved either through recycling, requiring separate collection and sorting, or through the development of zero-waste, closed-loop technologies. The final disposal of polymers occurs when burned in an incineration plant or when buried in a landfill. The life cycle of a landfill ends with its reclamation and the formation of fertile soil on the surface of the landfill. To combat wind and water erosion, accompanied by the destruction of the top layer, polymer soil stabilizers are used, including interpolymer complexes - products of the interaction between oppositely charged ionic polymers. This technology allows the adjustment of the stabilizer properties to the composition of soil to be treated.

# THERMAL, FLAME RETARDANT AND CRYO-RESISTANT POLYMER COMPOSITE MATERIALS FOR ADVANCED TECHNOLOGIES

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Multifunctional, lightweight, and durable thermal, fire and cryo-resistant polyimide-based composite materials are of significant interest to high-speed transport in terms of improving vehicle design and fuel economy. They can be used in aviation, automotive, construction as a finishing material, as well as in shipbuilding. An important area of application is thermal and flame-retardant vibration protection coating, as well as electrical insulation materials. In the production of polyimides (electrical insulating films, binders for composites, fibers, cryo- and heat-resistant foams, etc.) and the monomers necessary for this, Russian Federation is decisively behind the United States, Western European countries, Japan, and China. Polyimides, along with excellent mechanical characteristics and higher heat resistance compared to conventional engineering plastics (polyamides, polyesters, polysulfides), have additional useful properties: the highest fire resistance combined with high impact resistance and unique stability of physical, mechanical, and dielectric properties in the temperature range from cryogenic to +400°C.

The lecture presents new approaches to the production of composite materials based on partially crystalline thermoplastics, using aqueous solutions of polyamide acid salts, as well as by modifying the chemical structure of polyimide by varying the structure of the dianhydride and diamine fragments of the polymer chain. These approaches are aimed not only at the use of commercially available monomers necessary for the synthesis of polyimides and partially produced in the Russian Federation, but also at obtaining one-, two- and three-dimensional products based on them using modern additive technologies and environmentally friendly solvents.

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# VESICLES FORMED BY SUPRAMOLECULAR COMPLEXES CONTAINING MONODENDRON LIGANDS

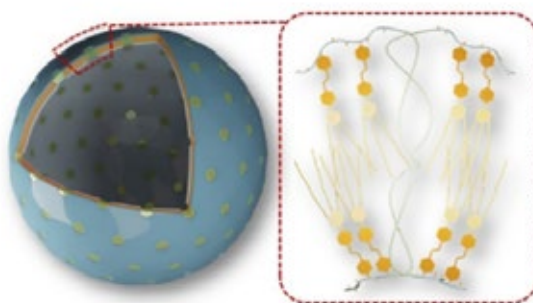
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Vesicles are spherical structures containing an inner aqueous compartment separated from the external water phase by one or more surfactant bilayers. Polymersomes, i.e. vesicles made up of amphiphilic block copolymers, have a high potential for applications in artificial organelles, nanoreactors and drug delivery due to their high stability and resistance to rupture.<sup>1</sup> It was shown by us previously that vesicles could be formed by supramolecular complexes of a polybase and monodendron amphiphilic sulfonic acid molecules at low degree of neutralization (DN).<sup>2</sup> In these vesicles, amphiphilic sulfonic acid molecules form bilayers and the polymer backbones are sandwiched between them. In contrast to classical polymersomes, where the polymer chains are preferably perpendicular to the interface, the backbones in this case are oriented parallel to the vesicle surface.

In this work, a block copolymer containing a polybase block and a thermoresponsive poly(*N*-isopropylacrylamide) (PNIPAAm) block was used to prepare supramolecular complexes with photochromic monodendron amphiphilic sulfonic acid molecules. These complexes can also form vesicles, and the complex block builds up the vesicle wall and the other block forms channels embedded in the bilayers. Depending on the chemical structure of the monodendron molecules, the complexes form either vesicle-in-vesicles or unilamellar vesicles. The thermal as well as photo responsiveness of these vesicles has been clearly demonstrated by temperature dependent dynamic light scattering measurements as well as optical microscopy.



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# FEATURES OF SYNTHESIS OF STYRENE-ACRYLIC DISPERSIONS FOR SURFACE SIZING OF PAPER AND CARDBOARD

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Paper and cardboard are widely used in almost all industries. One of the main consumer properties of paper is its resistance to moisture. Untreated paper has high water absorption, which often leads to an almost complete loss of strength of the paper sheet. This problem is solved by sizing sheets, which can be either intra-mass, when a sizing agent is added directly to aqueous suspension of cellulose, or surface, by applying sizing agents to the surface of the product.

At this moment, surface sizing has become a universal technological process for controlling the properties of paper and cardboard: hydrophobicity, general and surface strength, porosity and others. At present time, to increase the efficiency of surface sizing, emulsions of alkenyl succinic anhydride, alken ketene dimer, anionic and cationic emulsions based on copolymers of styrene with maleic anhydride, nitrile or acrylic acid esters are used. Difficulties in the production of such dispersions at domestic manufactures are due to the fact that the nature of such products and the technology of their synthesis differ significantly from the widespread styrene-acrylic dispersions of a similar monomer composition, used, for example, in the production of paint-and-lacquer materials. Moreover, the main distinguishing feature of such products is the multicomponent nature of their composition, when the dispersion of a hydrophobic additive consists of at least two polymers and some of special additives.

In the presented work, the features of the synthesis of anionic styrene-acrylic dispersions for surface sizing of paper and cardboard were studied. The influence of the monomer composition and molecular weight of the polymer, the concentration and nature of the anionic surfactant on the effectiveness of the resulting sizing agents was assessed. The influence of natural starch-based polymers introduced into the reaction system on the quality of the resulting product was studied. It has been shown that graft copolymers obtained from natural polymers act as colloidal stabilizers of styrene-acrylic dispersions.

# PREPARATION OF FUNCTIONALE ORGANOSILONE MOLECULES OF DIFFERENT STRUCTURES BY THE CUAAC REACTION IN THE PRESENCE OF A HETEROGENEOUS CATALYST

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Organosilicon molecules of both individual and polymer structure are an integral part of modern knowledge-intensive industrial production and high technology. The creation of simple methods for their synthesis must meet modern environmental and economic standards.<sup>1,2</sup>

This work demonstrates the possibility of creating a range of functional organosilicon molecules from organoalkoxysilanes to polydimethylsiloxanes and carbosilane dendrimers using a Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC) reaction in the presence of a heterogeneous catalyst. All processes were carried out under solution-free conditions at a relatively low temperature of 60 °C. An important result of the work is the study of copper leaching from a heterogeneous catalyst into the final polysiloxanes and the assessment of their potential toxicity to biological cells.<sup>3</sup>

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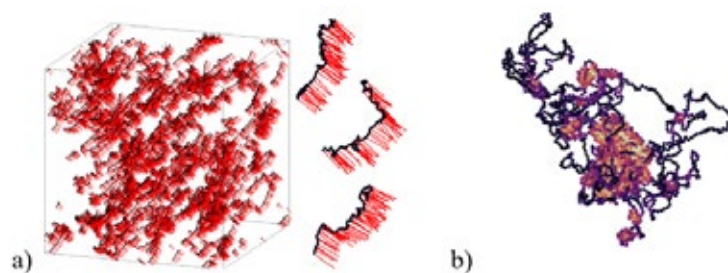
# SELF ORGANIZATION IN POLYMERS WITH ACTIVE UNITS

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Active matter is a new and rapidly developing field of chemical physics that describes systems with active agents that can convert the energy of the medium into their own motion. In such systems, there is no usual thermodynamic equilibrium and unusual effects of self-ordering and stratification can be observed.<sup>1</sup> Such systems can be found on different spatial and temporal scales, ranging from bacteria and molecular motors to flocks of birds and swarms of fish.

But what happens if the active agents form polymer chains? Polymers are poor in entropy, and therefore more prone to self-ordering and structuring, compared with low-molecular weight systems. Using examples of several models of polymers with active units, their features and unusual properties will be demonstrated, including the ability to co-directional collective movement<sup>2</sup> and partial collapse under the influence of activity, see Figure 1.



**Figure 1.** Examples of polymer systems with active units: spontaneous unidirectional motion in polymer solution (a) and partial collapse in a single swollen chain (b)

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# SYNTHESIS OF COMPOSITE MATERIALS BASED ON CALCIUM PHOSPHATES AND SODIUM ALGINATE-CHITOSAN POLYELECTROLYTE COMPLEX

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Currently, special attention of researchers is paid to a new class of biopolymers—polyelectrolyte complexes (PEC). Often, PEC biopolymers have physicochemical and biological properties that differ from the properties of the original polymers.

It is known that sodium alginate enters into a polyelectrolyte reaction with chitosan. The formation of the complex occurs through the mechanism of electrostatic interaction between oppositely charged functional groups of polyelectrolytes.

This is evidenced by a decrease in the hydrodynamic properties of sodium alginate with the addition of chitosan gel, which can be explained by the blocking of negatively charged carboxyl groups of alginate by positively charged amino groups of chitosan. In this case, the dynamic viscosity of the resulting PEC takes an intermediate value between the viscosities for sodium alginate and chitosan, which indicates the formation of a non-stoichiometric water-soluble complex with a predominance of acidic functional groups.

The introduction of a mixture of FA into the resulting polyelectrolyte gel leads to a rapid increase in the viscosity of the system as a result of the formation of a more rigid structure, and with an increase in the filler content, to a complete loss of fluidity. Which indicates the mechanism of composite formation, similar to sodium alginate and a mixture of FA, namely the cross-linking of polymer polysaccharide chains by calcium ions.

The results of X-ray diffraction of the composite material indicate that the introduction of powder material into the PEC matrix does not change its component composition.

The BET method has established that the specific surface area of a composite material characterized by a filler/matrix ratio of 30/70 decreases compared to powder material from 23 m<sup>2</sup>/g to 18 m<sup>2</sup>/g, but at the same time occupies an intermediate value between the data obtained for similar composite materials, in which the matrix was sodium alginate - 37 m<sup>2</sup>/g and chitosan - 6 m<sup>2</sup>/g. It is important to note that an increase in the drying temperature of the sample from 25 to 200°C promotes an increase in the specific surface area to 27 m<sup>2</sup>/g.

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# CURRENT STATE OF DEVELOPMENT OF ADHESIVE MATERIALS FOR AVIATION TECHNOLOGY IN THE RUSSIAN FEDERATION

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Modern aviation technology uses a number of structural and functional adhesive materials. Structural materials include such materials as: structural epoxy film adhesives, cold-curing epoxy adhesives; phenolic rubber film adhesives, adhesive prepregs for PCM for structural purposes <sup>1-2</sup>.

Functional ones include: foaming adhesives, heat-resistant adhesives, rubber adhesives, adhesives with special properties (conductive and others).

PCMs obtained from adhesive prepregs based on glass fiber fillers and carbon fiber fillers have a wide range of properties depending on the physical and mechanical characteristics of the adhesive binders and reinforcing fillers used for their production.

A distinctive feature of adhesive prepregs is that they make it possible to implement a highly efficient technology for assembling glued, highly loaded honeycomb structures from non-metallic materials of single and complex curvature, during which the molding of the skin and its gluing with the honeycomb core occurs in one technological operation <sup>3</sup>.

The report examines in detail the properties of previously developed adhesives and adhesive prepregs used in modern aviation technology, as well as new developments by the Kurchatov Institute Research Center - VIAM in this area.

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# HIGH-PERFORMANCE POLYMERS AND TECHNOLOGIES AS KEY ELEMENTS OF FUTURE MEDICINE

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The development of 3D and 4D printing technologies based on polymer and composite materials is changing the healthcare industry at a global level, enabling the production of medical instruments, surgical templates, scaffolds for tissue engineering, and personalized implants.

Despite significant progress in polymer additive technologies, the main limiting factor for the further success of this area in medicine is the lack of domestic certified materials.

At the same time, for the application of high-performance polymers and technologies in medicine, it is important to critically evaluate and characterize new materials in terms of structural, mechanical and thermal behavior, with particular attention to the biocompatibility provided by the chemical structure, molecular weight and supramolecular organization of the polymer, rather than its shape.

The report discusses the problems of using synthetic polymers and composites as implants. Particular attention is paid to high performance polymers and composites based on them, which, in combination with 3D and 4D printing, significantly expand the possibilities for obtaining personalized implants<sup>1</sup>. The results of the development of high performance polymers for medical purposes at the Center for Advanced Materials and Additive Technologies of KBSU are discussed. New approaches to modifying polymers to enhance their osseointegration, regulate mechanical properties and supramolecular structure to obtain high-quality and safe products with properties similar to human bone tissue are presented. The issue of medical purity of the polymer is being considered.

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# SYNTHESIS AND PROPERTIES OF ANIONIC COPOLYMERS AND MICROGELS FOR BIOMEDICAL ADHESIVES

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High-adhesive materials are widely used in many fields: in the creation of composite materials, the manufacture of paints and adhesives, and in various biomedical applications. For example, polymer-based medical adhesives are used to connect tissue during injuries and incisions. Such materials not only speed up the process of closing the incision, but also reduce the risk of injury and the spread of infectious diseases. When choosing a composition, it is important to pay attention to the fact that adhesives used in regenerative medicine must be biocompatible and have high adhesion without interfering with tissue growth.

One way to solve this problem may be to use adhesives obtained by forming dynamic non-covalent bonds between components. In this work, under conditions of radical polymerization, a number of anionic water-soluble polymers of various compositions and structures were synthesized for further use as one of the components of medical glue. The following were obtained: a) linear polymers, b) branched polymers and c) microgels, which included hydrophilic, hydrophobic, and anionic monomer units.

Reversible chain transfer polymerization in aqueous or organic media has been used to synthesize linear and branched polymers. Water-soluble copolymers of acrylic acid (AA) with N-isopropylacrylamide (NIPAM), sodium styrene sulfonate with NIPAM, and AA with styrene were prepared and characterized. The synthesis of microgels was carried out by precipitation polymerization in water. Microgels based on copolymers of NIPAM and AA, and NIPAM and sodium styrene sulfonate were obtained and characterized. Next, using the dynamic light scattering method, the features of the thermo- and pH-sensitive behavior of polymers in aqueous solutions were studied to determine the optimal compositions for further inclusion in the adhesive composition.

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# NEW APPROACHES TO THE FUNCTIONALIZATION OF CHITOSAN

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Until recently, the chemistry of the natural polymers chitin and chitosan was largely limited to traditional approaches of classical organic chemistry. The use of new approaches of click chemistry, sonochemistry, microwave irradiation and other methods of intensifying chemical reactions is an important and urgent task of modern BMC chemistry. New polymer analog reactions in the chemistry of chitin and chitosan make it possible to synthesize a number of new derivatives of these polysaccharides with attractive physicochemical, mechanical and pharmacological properties.

In our scientific group, research in this area is carried out in two directions: (1) ultrasound-promoted new polymer-like derivatives of chitin and chitosan and (2) electrochemical polymer-like transformations of chitin and chitosan. As a result of the development of these directions, we introduced ultrasonic thiol-yne and phenol-yne addition, nitron-nitrile 1,3-dipolar cycloaddition, electrochemical direct N-arylation into the chemistry of chitin and chitosan, obtained new highly active antibacterial polymers, films and food coatings on them basis, nanoparticles and drug delivery systems. This report will be devoted to these and our other recent achievements in the chemistry of chitin and chitosan.

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# NEW ORGANIC SEMICONDUCTORS BASED ON DONOR-ACCEPTOR OLIGOMERS FOR ORGANIC AND HYBRID OPTOELECTRONICS

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Donor-acceptor (D-A) conjugated oligomers and polymers are of great interest because their properties can be fine-tuned over a wide range for a specific type of application. This talk will present the molecular design, synthesis and comprehensive study of the properties of a new series of D-A compounds (small molecules, oligomers, polymers) of diverse chemical structures having oligothiophene links as a conjugated spacer. The obtained materials have valuable properties and can be used in organic solar cells<sup>1-3</sup>, photodetectors<sup>1</sup>, photo- and electroluminescent devices<sup>4-6</sup>, hole-transport layers of perovskite solar cells<sup>7,8</sup>, etc.

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# GELATION IN PROCESSES INVOLVING QUATERNARY AM-MONIUM COMPOUNDS

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Quaternary ammonium monomers, such as N,N-diallyl-N,N-dimethylammonium chloride and acrylic acid, were used as study objects for hydrogel formation. The polymerization procedure was carried out in aqueous solutions using crosslinking agents such as quaternary ammonium monomers, commonly used N,N-methylene bisacrylamide, tetra- and triallyl monomers, and tetraallylpiperizidium chloride<sup>1</sup>. It has been discovered that for many processes, polymerization begins with the generation of soluble products up to specific conversions, and with considerable transformations of the monomer into the polymer, highly swelling polymer products are produced in water. Many polymers, including acrylic acid, can be crosslinked by quaternary ammonium monomers. The examination of the kinetic patterns of polymerization processes revealed that in all situations, increasing the monomer concentration reduces the induction period and increases the polymerization rate. The curves of the conversion dependency on time are acquired and straightened in logarithmic coordinates, confirming the first order of the monomer of the reactions that occur. The synthesis of water-soluble polymers is observed up to a particular conversion point, which can be explained in the examined systems using the classical scheme of radical polymerization, additional initiation, and chain growth leading to crosslinking. Thus, at the first stage of polymerization and under particular conditions, many gelation processes manifest as a radical process with a noticeable gel effect, and the structure of the subsequent hydrogels is heterogeneous and heavily dependent on the conditions of their synthesis.

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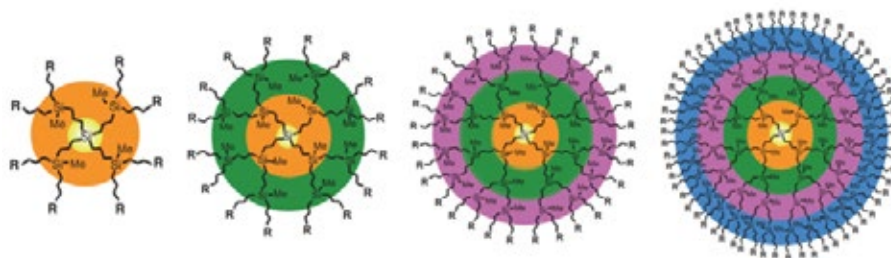
# THERMODYNAMICS OF CARBOSILANE DENDRIMERS AS A FUNDAMENTAL BASIS FOR THE CREATION OF NEW TYPES OF POLYMERIC MATTER

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Dendrimers are a class of macromolecular nanoobjects with multifunctionality and unique properties. High possibilities of modifying the structure of dendrimers make them very promising molecules for the practical application in nanotechnology, materials science and engineering, catalysis, biomedicine, and photonics. Currently, carbosilane dendrimers (Figure 1) are of great interest and particular importance owing to the thermodynamic stability, low polarity and high strength of the Si–C bond.



**Figure 1.** Structures of carbosilane dendrimers of the first–fourth generations (G1–G4) with different functional end groups (R)

A comprehensive study of the series of carbosilane dendrimers of various generations with different nature of the outer layer is carried out by methods of precise calorimetry and thermal analysis. A set of fundamental thermodynamic characteristics of the studied compounds is determined. The use of methods of chemical thermodynamics made it possible to establish the "structure vs. property" relationships, which are the fundamental basis of the development of technology for producing new dendrimeric materials.

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# USING AMMONIA AS A REACTION MEDIUM – A NEW APPROACH TO SILICONE SYNTHESIS AND RECYCLING

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Silicones are widely used in various industries. Due to the peculiarities of their chemical structure, they are distinguished by a number of properties that allow them to occupy a special place among rubber elastic materials.

The development of modern technologies requires more careful control over the properties of the resulting products. One way of realizing this is the use of narrowly dispersed polymers. Such compounds allow for tuning the properties of the products by varying the molar mass and architecture of macromolecules in a controlled manner. Another pressing issue of modern silicone chemistry is the recycling and disposal of waste. Due to their high thermal stability and chemical inertness, silicone rubbers are difficult to recycle using conventional methods.

Thus, today we can distinguish two main tasks in this area of research: 1 – search for new effective approaches to obtaining silicones of a strictly specified structure; 2 – development of technological methods for processing waste from the silicone industry.

In this work, we propose a universal approach for the synthesis and recycling of silicones in an ammonia environment. By varying the reaction conditions, it is possible to both obtain narrowly dispersed functional polymers of various architectures and recycling waste silicone products into cyclic and linear monomer products.

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# FROM MOLECULAR BRUSHES TO MOLECULAR FILLERS

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In recent years, molecular brushes (MBs) have gone from being exotic research objects that demonstrated the power of polymer theory and progress in the development of synthetic approaches to unexpectedly turning into unique materials that are fundamentally different from the usual polymeric matter in the mechanism of intermolecular interaction. Nano-size, elongated worm-like shape of the molecular brush molecule, variability of chemical modification, based on the needs of the polymer matrix, are the optimal candidates for the use of molecular brushes as anisometric molecular fillers. Since the elongated conformation of the molecular brush molecule is achieved under the condition of a high degree of polymerization of the main chain and a high grafting density of side chains, which, in turn, depend on the synthesis method used, these two factors are mandatory when using molecular brushes as anisometric fillers.

This work will present an analysis of the synthetic procedures used to synthesize molecular brushes in terms of their efficiency and scalability potential, and their potential for use as anisometric fillers for molecular composites.

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# STRUCTURE FORMATION IN MULTICOMPONENT REACTIVE POLYMER SYSTEMS

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Increasing requirements of industry to the performance characteristics of materials are accompanied by increasing complexity of composite formulations. For example, to improve physical-mechanical and technological properties of thermoset binder carbon plastics use modification with thermoplastics and active diluents. In such multicomponent systems as a result of chemical reaction of curing there is a decrease in thermodynamic compatibility of components with the formation of a complex heterogeneous structure that determines the properties of the composite. In this regard, an urgent task of modern materials science is the development of approaches to the control of structure formation in multicomponent polymer systems and, as a consequence, the creation of materials with the required complex of properties.

In this work, approaches to the control, qualitative and quantitative prediction of phase organization in multicomponent curing polymer systems were developed and tested by means of complex studies of bi- and three-component diaminodiphenyl sulfone curing systems of epoxy oligomer with polycaprolactone, as well as with polysulfone and active diluent alkyl glycidyl ether.

By methods of optical interferometry, scanning and optical microscopy, IR spectroscopy and differential scanning calorimetry the complex studies of mixing of components of the systems before and during chemical reactions, as well as the evolution of phase organization during curing were carried out. Based on the results of the study, a technique for determining the concentration ranges of all possible types of phase organization in cured mixtures was developed using the example of a bicomponent system. Qualitative trends are shown, and quantitative dependences of the influence of mixture parameters on the sizes of phase structures in the cured composition are constructed on the example of the studied system. An approach for quantitative determination of compositions of coexisting phases is proposed. Much attention is paid to the study of structure formation in the phase reversal region of the phase diagram. The systems formed in this region have a structure of the type of interpenetrating phases and are characterized by a jump-like change of some properties. The developed approaches and the obtained regularities have been tested on the ternary system and are universal.

# STUDY OF THE INFLUENCE OF SINTERING MODES OF POLYETHERETHER KETONE AND POLYPHENYLENE SULPHONE POWDERS ON THE MECHANICAL PROPERTIES OF SAMPLES

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Today, among the many ways to process materials and produce products, methods based on the process of sintering powders are of great interest. In particular, we can highlight powder injection molding and 3D printing by selective laser sintering. Metal, ceramic or polymer powders can be used as raw materials for sintering, which are consolidated using thermal or laser radiation.

Sintering conditions can have a significant impact on the final properties and geometry of the products. In this regard, thermoplastic powders of polyetherether ketone (PEEK) and polyphenylene sulfone (PPSU) were sintered at different temperatures. Powders with different melt viscosities were taken for the study: PEEK with a viscosity at a shear rate of  $92 \text{ s}^{-1}$  and a temperature of  $380^\circ\text{C}$  equal to 603, 2175 and 6130 Pa·s and PFSU with a viscosity of 472, 996 and 2650 Pa·s at a temperature of  $350^\circ\text{C}$ .

Sintering of PEEK at temperatures of 340, 350, 360 and  $370^\circ\text{C}$  for 1 hour showed that the volumetric shrinkage of the samples largely depends on the bulk density of the powders - the higher the bulk density, the lower the shrinkage. At  $360^\circ\text{C}$ , the shrinkage becomes constant for all PEEK powder samples. Also, porosity is reduced to minimum values. For PEEK powder with the highest bulk density ( $0.43 \text{ g/cm}^3$ ), the shrinkage was 36 % and the porosity was 1.2 %. It was found that the powder with the highest viscosity exhibits better retention of sample shape. PPSU powders, due to their low bulk density, demonstrated significant shrinkage and geometry distortion. For the PPSU sample with the highest bulk density ( $0.3 \text{ g/cm}^3$ ), a minimum porosity of 7 % was achieved at  $270^\circ\text{C}$ , while the volumetric shrinkage was 62 %.

The study of mechanical properties showed that with increasing sintering temperature, an increase in mechanical properties occurs. The highest values are naturally achieved by samples with the lowest porosity. It is noteworthy that the properties of samples obtained by sintering reach the properties of samples obtained by injection molding.

Thus, the most optimal sintering temperatures for PEEK and PPSU powders can be considered 360 and  $270^\circ\text{C}$ , respectively. Under these modes, a good combination of mechanical properties and product geometry is achieved.

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# PRINCIPLES OF CREATING FIBERS REINFORCED PLASTICS WITH INCREASED CRACK RESISTANCE BASED ON HYBRID MATRICES POLYEPOXIDE-THERMOPLASTICS

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Products made of fibers reinforced plastics (FRP) have a low specific gravity and high strength characteristics, due to which they are used for the manufacturing of products with high weight perfection. Epoxy compositions remain the most common matrices for reinforced plastics. However, they are characterized by low crack resistance. The greatest effect of increasing the crack resistance of matrices and FRP is achieved when using rigid-chain thermoplastic polymers. With such modification, the heat resistance of the materials does not decrease.

At the Laboratory of Reinforced Plastics of the FRCCP RAS, systematic research is being carried out aimed at creating an FRP based on multicomponent hybrid epoxy polymer matrices. Based on the research results, the principles of creating an FRP have been developed, which consistently including all stages of creating a composite material. The integrated approach makes it possible to obtain FRP with the specified strength properties <sup>1-3</sup>.

Depending on the type and amount of thermoplastics polymers in the epoxy matrix and curing conditions can increase the fracture toughness of epoxy matrices from  $\sim 0.3$  to  $\sim 2.0$  kJ/m<sup>2</sup>. The effect of growth crack resistance is retained for FRP. The fracture toughness of glass fibers reinforced plastics and organo fibers reinforced plastics can increase from  $\sim 1.0$  to  $\sim 2.0$  kJ/m<sup>2</sup>, for carbon fibers reinforced plastics – from  $\sim 0.3$  up to  $\sim 0.6$  kJ/m<sup>2</sup>.

The results obtained are of practical significance for the creation of products from polymer composite materials based on hybrid mixed binders with directional control of their final structure, providing increased values of crack resistance.

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# POLYMER PHOTOSENSITIZING SYSTEMS FOR ANTIMICROBIAL PHOTODYNAMIC THERAPY

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Treatment of purulent wounds remains one of the most difficult problems of modern medicine, despite the advances in clinical practice and pharmacology. This is due to the fact that, on the one hand, purulent wounds and burns are among the most common types of traumatic lesions, on the other hand, the treatment strategy for purulent-inflammatory diseases of soft tissues remains not fully developed. The situation is so serious that in 2014, the WHO warned in a release that humanity is inexorably approaching a “post-antibiotic era” and identified a group of five pathogens (*Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa* and *Enterobacter*) that can lead to the development of superinfections that are resistant to all known antibiotics. In recent years, there has been growing interest in antimicrobial photodynamic therapy (APDT) as a complete alternative to antibiotic therapy in the treatment of local infectious processes. The search in this direction is associated with the development of new conjugates based on both porphyrin photosensitizers (PS), traditionally used in PDT, and dyes with PS properties. In this work, the comparative effectiveness of the use of model wounds in rats, the porphyrin PS - Photoditazine (a drug currently used in PDT practice), and the dyes Bengal pink and methylene blue at the early stage of the wound process in APDT was studied. All PSs were used in combination with amphiphilic polymers (polyvinylpyrrolidone, Pluronic F127, polyethylene glycol), which, as previously shown, increase the effectiveness of PDT and reduce the toxic effects of radiation on blood vessels (hemorrhagic reaction). It turned out that complexes of all photosensitizers with Pluronic are most effective in these processes. At the same time, Photoditazine is quickly deactivated during photoirradiation, and methylene blue and Bengal pink are practically not subject to photodestruction. Moreover, in all three cases, regenerative processes in the wounds are observed - the growth of fibroblasts and the formation of new capillaries.

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# INVESTIGATION OF THE INFLUENCE OF MODIFIED FILLERS ON FLAME RETARDANT PROPERTIES OF POLYVINYLCHLORIDE PLASTISOL

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Nowadays, the production of plastisols for various purposes has increased due to the technical and economic advantages of this technology.

The presence of modified aluminium hydroxide and modified magnesium hydroxide reduces the temperature on the unheated side by 10.3 °C (modified aluminium hydroxide with amidophosphate) and by 31.8 °C (modified magnesium hydroxide with amidophosphate). The formed coke has a low value of thermal conductivity coefficient and high thermal resistance, which leads to a decrease in the exit of combustible products into the gas phase, reducing the flow of combustible gases to the flame. Thus the blowing coefficient increases 11 times with the addition of modified aluminium hydroxide and 10 times with the addition of modified magnesium hydroxide.

The results of tests on determination of coke residue at temperature 750 °C and exposure time 30 minutes correlate with the above data, so coke residue increases by more than 20% (modified aluminium hydroxide amidophosphate) and by more than 30% (modified magnesium hydroxide amidophosphate).

The presence of modified aluminium hydroxide improves the adhesion strength by 1.6 times and the addition of modified magnesium hydroxide improves the adhesion strength by 1.5 times.

At carrying out research of the received polyvinylchloride plastisols by method of electron microscopy it has been established that at modification of aluminium and magnesium hydroxide reduction of agglomeration of filler particles is observed that promotes its better distribution in a matrix of polymer. Also by the increase of phosphorus peak it is possible to draw a conclusion about the detection of phosphorus on the surface of filler particles - aluminium and magnesium hydroxide, that testifies to the carried out surface modification of fillers that increases their antipyretric abilities.



# HYBRID INORGANIC-ORGANIC NANOBIOCOMPOSITES AS PROMISING PLATFORMS FOR INTERDISCIPLINARY RESEARCH AND TECHNOLOGY

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A methodology for obtaining water-soluble, aggregatively highly stable, biocompatible nanocomposites, which are nanoparticles of zero-valent metals, chalcogens, metal-chalcogenides, other chemical elements and their compounds, as well as organic substances, encapsulated in polymer macromolecules, has been developed<sup>1</sup> and continues to be expanded<sup>2-14</sup>.

The report will discuss the synthesis, structure, physicochemical, biological properties of new nanobiocomposites and their promising areas of application as magnetic, optical, catalytic materials, as well as means of parallel multichannel therapy and diagnostics (theranostics).

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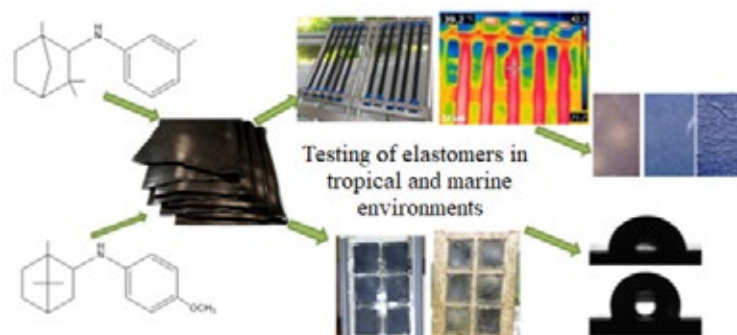
*The work was carried out with the financial support of the RCSI (RFBR), project 20-53-44002\_Mong\_a.*

# DEVELOPMENT AND RESEARCH OF PROPERTIES OF NEW ELASTOMERIC MATERIALS WITH INCREASED RESISTANCE TO THE EFFECTS OF THE TROPIC ATMOSPHERE AND THE MARINE ENVIRONMENT

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In a tropical climate, elastomeric products are exposed to intense solar radiation, ozone and high temperatures along with high humidity. In addition, the specifics are the effects of fungi and microorganisms on rubbers and rubber products. As a result, rubbers must have increased resistance to thermal, light and ozone aging, as well as resistance to biological effects.



The report presents generalized data on the results of long-term field tests conducted at the Con Zo and Dam Bai climate stations in the territory of the Socialist Republic of Vietnam.

The purpose of the work is to create elastomeric materials that provide a multiplicative effect in improving the efficiency of equipment and machinery operated in a tropical climate and marine environment.

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# AMPHIPHILIC HOMOPOLYMERS: FEATURES OF SELF-ORGANIZATION IN GRAFTED LAYERS AND SOLUTION

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Amphiphilic homopolymers are macromolecules, part or all of whose monomer units contain significantly different (hydrophobic and hydrophilic) groups. Amphiphilic homopolymers include macromolecules with amphiphilic monomer units, comb-like macromolecules, polymeric surfactants, macromolecules with micelle-forming units, etc. Amphiphilic homopolymers have effective external activity, forming a unique structure with a characteristic nanometer scale. A feature of the self-organization of amphiphilic homopolymers is sensitivity to the position of groups with different affinities in monomer units, which in some cases can lead to the emergence of specific entropic-driven attraction.

The talk will describe how this entropy-induced attraction affects the morphology of amphiphilic homopolymers solution and the structure of their dense grafted layers [1-4].

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*The work was carried out with financial support from the Russian Science Foundation, project No. 19-73-20104-P.*

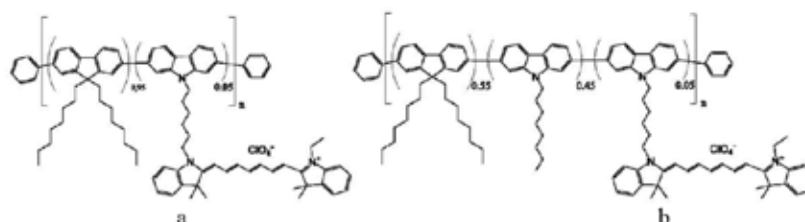
# POLYFLUORENES WITH COVALENTLY ATTACHED CYANINE DYES: SYNTHESIS AND APPLICATIONS IN OPTOELECTRONICS

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New copolyfluorenes containing covalently attached fragments of cyanine dyes have been synthesized, which are widely used in LED devices,<sup>1</sup> optical,<sup>2</sup> and chemical sensors.<sup>3</sup> It has been shown that the use of CPF-1 (Fig. 1a) as a material for the light-emitting layer of laboratory samples of organic light-emitting diodes makes it possible to obtain fairly intense and almost white electroluminescence (CIE color coordinates  $x=0.328$ ,  $y=0.343$ ).



**Figure 1.** Structures of CPF-1 (a) and CPF-2 (b).

The absorption and luminescence spectra of copolyfluorenes in acidic (pH=1.65) and alkaline (pH=9.18) buffer solutions were studied. It was shown that in the luminescence spectrum of copolyfluorene CPF-2 (Fig. 1b) with the same cyanine dye as in CPF-1, the emission band of the cyanine dye at 680 nm appears only in an acidic medium.

Thus, the studied copolyfluorenes are promising for use in optoelectronics and chemosensory.

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# FEATURES OF THE SYNTHESIS OF EASILY DEGRADABLE POLYMERS WITH THE PARTICIPATION OF CYCLIC KETENE ACETALS

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Most commercially produced polymers are carbon-chain polymers synthesized by radical polymerization. Such objects are usually resistant to external influences (hydrolysis, biodegradation, photolysis, etc.) Radical polymerization of cyclic ketene acetals (CKA) with ring opening has acquired particular interest due to the relevance of obtaining easily degradable polymers. In the course of CCA polymerization, a sequential opening of the double bond and the acetal ring occurs. As a result, ester links are included in the carbon chain, that provides the subsequent hydrolytic or enzymatic decomposition of the polymer.

Despite the increased interest in these processes, the mechanism and kinetics of radical polymerization of CKA have almost not been studied. According to our and literary data, they have features that are not typical of the common radical polymerization of vinyl monomers.

In this report, we plan to present previously unknown especial features of radical polymerization of CKA using the example of polymerization of 2-methylene-1,3-dioxepane and 5,6-benzo-2-methylene-1,3-dioxepane. In particular, the questions of auto-inhibition during the reaction, higher orders of polymerization rates in respect to the monomer and initiator concentration, high values of the heat of polymerization and activation energy of the process, an unusual mechanism of initiation, propagation and restriction of the chain will be discussed.

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# COPOLYMERS BASED ON POLYETHER KETONES FOR 3D PRINTING

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In recent years, polymer materials used in additive technologies have been of particular interest. High-tech molding of parts with complex configurations using 3D technologies places high demands on polymer materials in terms of consumer characteristics and manufacturability. Among such materials, a special place is occupied by polyether ketones, which combine high mechanical properties with heat resistance, fire resistance, and resistance to aggressive environments.

In this regard, an extremely important task is to identify the main factors that determine the production of polyether ketones with a macromolecular structure, which will provide a combination of high performance properties (thermal and heat resistance, deformation-strength characteristics) with high manufacturability for processing into products using 3D printing.

The report presents the results of a study of the relationship between the patterns of synthesis of polyether ketones and their rheological, thermal properties, molecular weight distribution, which made it possible to develop a method for the synthesis of polyether ketones with improved performance characteristics for use in various 3D printing methods - selective laser sintering and layer-by-layer deposition of molten polymer filament.

Previously unstudied copolyether ketones based on 1,4-dihydroxybenzene and 4,4'-dihydroxybiphenyl, which have a set of necessary properties for use in 3D printing, have been studied. It has been shown that reducing the degree of crystallinity of polyetheretherketone by introducing 4,4'-dihydroxybiphenyl into its structure leads to a significant increase in the quality of 3D printing using the FDM method. Testing of printed samples from the synthesized copolymer showed that the modulus of elasticity in bending and tension, as well as tensile strength, are high and close to the properties of samples obtained by injection molding.



# ON THE CATALYTIC HYDROGENATION OF POLYMERS

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Hydrogenation of polymers, including synthetic rubbers, is one of the modification methods that ensures their resistance to oxidation, exposure to aggressive media, as well as improved mechanical properties, which determines their use in particularly critical areas [1-3]. Despite the demand for some polymers, there are no technologies implemented in the Russian industry for obtaining their hydrogenated derivatives.

This is due not only to the difficulties of implementing the catalytic hydrogenation stage directly, but also to the existence of the problem of isolating the catalyst and its reuse.

If we consider the hydrogenation of a polymer obtained in latex, then the most acceptable is to carry out the process in latex in the presence of a homogeneous catalyst, or in solution on a heterogeneous catalyst. In the second case, the polymer must be isolated from latex, cleaned of auxiliary components, and then dissolved in a suitable solvent, hydrogenated and the polymer isolated again. All this naturally increases the cost of the hydrogenated polymer.

The hydrogenation of latex in the presence of a homogeneous catalyst fits into the general scheme of obtaining a commercial product, only the hydrogenation stage is added, but the problem arises of isolating the catalyst, which, as a rule, complexes based on precious metals are used. The most attractive solution is the recycling of an aqueous phase containing a dissolved catalytic complex, however, other known methods of separating homogeneous catalysts are also possible.

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# POLYSACCHARIDES AS POSSIBLE CARRIERS FOR PHOTSENSITIZERS IN ANTIBACTERIAL PHODYNAMIC THERAPY

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Formation of heterogeneous photosensitizing systems for medical purposes (for example, for use in the treatment of wounds using antibacterial photodynamic therapy, APDT) requires the use of biocompatible, bactericidal and non-toxic carriers. Natural polysaccharides meet these requirements – chitosan (ChT), sodium alginate (SA), hyaluronic acid. In particular, chitosan has proven itself well as a bactericidal polymer carrier for photosensitizers (PS) in APDT both in vitro and in vivo for the treatment of infected wounds. Due to its wound healing and hemostatic properties, sodium alginate is used in clinical practice, since its use in the treatment of skin and tissue damage accelerates the rehabilitation of patients. Interest in polysaccharides is also due to the fact that wound coverings based on them can remove excess exudate, while keeping the wound surface moist, provide gas exchange, prevent mechanical trauma to tissue, and also provide the possibility of non-contact visual monitoring of the wound.

In this work, we studied the photocatalytic activity (in the model reaction of tryptophan photooxidation in water) and photosensitizing properties in the generation of singlet  $^1O_2$  oxygen of porphyrin and non-porphyrin PS immobilized on polysaccharide xerogels, as well as on a water-insoluble polyelectrolyte complex ChT/SA. Examples of the use of photosensitizer/polysaccharide systems in the treatment of model wounds in laboratory animals using APDT are also shown.

*The work was carried out with the financial support of the Russian Science Foundation, project 24-43-00084.*

# INVESTIGATION OF THE INFLUENCE OF SPACER'S TYPE ON THE PHYSICAL AND CHEMICAL PROPERTIES OF POLYCARBORANESILOXANES

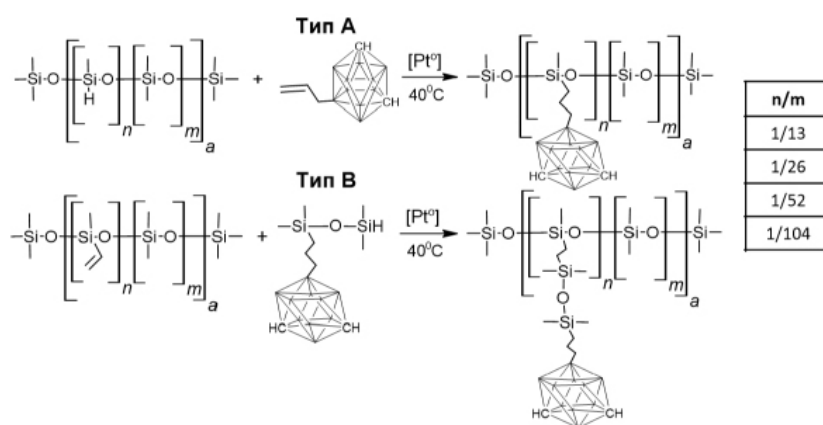
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Polydimethylsiloxanes (PDMS) have unique physico-chemical properties such as low glass transition temperatures, stability at high and low temperatures, etc. Currently the approach involving the incorporation of organoelement groups into the structure of siloxane polymers in order to give them new properties is developing quickly. Previously, a series of new polycarboransiloxanes (type A) were prepared at INEOS RAS. It was found that microphase separation of siloxane and carboranyl components occurs in such systems<sup>1</sup>. This work is a continuation of this research and represents the synthesis of polycarboransiloxanes which differ in the spacer structure between siloxane and carboranyl components (type B), as well as a comparative analysis of the physico-chemical properties of two different types of polycarboransiloxanes.



**Figure 1.** Scheme for the synthesis of polycarboransiloxanes type A and type B

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# SYNTHESIS AND PROPERTIES OF POLY(L-LACTIDE-CO- $\epsilon$ -CAPROLACTONE) FOR BIOMEDICAL APPLICATIONS

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Shape-memory materials are widely used in medicine for development of various products, including «smart» medical devices, ensuring rapid minimally invasive implantation. Recently, researchers have become interested in the biodegradable copolymer poly(L-lactide-co- $\epsilon$ -caprolactone) (PLCL), which can be used for devices changing their shape in a programmed manner when heated to  $\sim 37^\circ\text{C}$ . It is known that the properties of PLCL can be finely adjusted by changing the ratio of L-lactide (LA) and  $\epsilon$ -caprolactone (CL) units. Additionally, copolymers with the same composition may have different properties due to differences in the microstructure of the polymeric chain. Therefore, to synthesize PLCL for biomedical applications, it is necessary to determine the effect of reaction conditions on the characteristics of the synthesized polymers.

The copolymers with an LA:CL ratio of 70:30 were synthesized by ring-opening polymerization (ROP) at a temperature of  $160^\circ\text{C}$  in the presence of the catalyst tin 2-ethylhexanoate (II) and the 1,12-dodecanediol. It was found that increasing the concentration of 1,12-dodecanediol from 500 to 10000 ppm led to a decrease in the time required to reach equilibrium monomer conversion from 360 to 120 minutes. The molecular weight characteristics of the synthesized polymers were investigated using GPC, showing that the average molecular weight of the polymers ranged from 30 to 110 kDa. The parameters of microstructure of the polymeric chain were calculated from NMR spectra, including the average length of the monomer sequences of LA and CL, as well as the randomness character ( $R$ ). It was demonstrated that increasing the concentration of 1,12-dodecanediol led to a copolymer with a more random distribution of monomeric units, as evidenced by the decrease of  $R$  from 0.7 to 0.5. The dependence of thermal properties on the type of microstructure was evaluated by the DSC. Hydrolytic degradation profile showed that copolymers with higher molecular weight degrade over a longer period, the degradation period ranges from 14 to 30 days.

*The work was supported by the Ministry of Education and Science of the Russian Federation (government assignment No. FFSM-2022-0003).*

# MECHANICAL PROPERTIES OF COMPOSITE HYDROGEL MATERIALS BASED ON POLYACRYLAMIDE REINFORCED WITH CHITIN NANOCRYSTALS

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Composite hydrogels find various applications in biomedicine. The introduction of filler provides such advantages of the material as the ability to fine-tune mechanical properties and to achieve higher strength and Young modulus compared to unfilled systems, as well as increased biological activity, namely, improved cell proliferation, differentiation and migration.

One of the popular fillers is chitin nanocrystals, which have a high characteristic ratio and elastic modulus ranging from 41 to 220 GPa. In addition to reinforcing properties, this filler has anti-inflammatory and wound healing effects, which makes it promising for use in biomedicine.

In this work, composite hydrogel materials based on polyacrylamide (Acros Organics, Belgium) filled with chitin nanocrystals of different nature were prepared and their physicochemical and mechanical properties were investigated depending on the concentration, polymorphic modification ( $\alpha$ - and  $\beta$ -chitin) and the method of nanocrystal extraction.

Chitin nanocrystals were synthesized by TEMPO-oxidation, acid hydrolysis and exfoliation methods in the presence of ascorbic acid. Composite hydrogels were prepared by free-radical polymerization of acrylamide and N,N'-methylenebisacrylamide in the presence of an initiator - ammonium persulfate. Ascorbic acid acted as a catalyst. The amount of filler was varied in the range from 1 to 3 wt.%.

The morphology of the synthesized materials was investigated by scanning electron microscopy. Mechanical properties, including hysteresis loss, of composite hydrogels were studied in indentation tests.

*The work was carried out within the stage assignment of NRC "Kurchatov institute".*

# HIGHLY EFFECTIVE BACTERICIDAL COMPOSITIONS BASED ON CHITOSAN WITH SILVER NANOPARTICLES

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Silver nanoparticles (NPs), due to their effective antibacterial and antifungal activity, are of active interest to researchers due to the growing antibiotic resistance of microorganisms and the development of resistant bacterial strains. Silver NPs are able to physically interact with the cell surface of various bacteria, adhering, accumulating on it and causing structural changes that eventually lead to necrosis of the bacterium. NPs with sizes  $< 30$  nm are able to penetrate inside the bacteria and affect it from the inside. It is promising to use biocompatible, biodegradable polysaccharide chitosan as a stabilizer of NPs due to its unique sorption and chelating properties due to the presence of amino and hydroxyl functional groups.

Silver NPs were formed in situ in the solution of chitosan stabilizer during UV-induced reduction of  $\text{AgNO}_3$  dopant. It was shown that the change in the molecular weight of chitosan allows to regulate the average size of silver particles, and the size of the latter decreases with increasing molecular weight of polysaccharide. Silver NPs dispersions with particle size  $\sim 8$  nm, formed in chitosan solutions with higher molecular weight, show a pronounced bactericidal activity, which is especially clear for *Escherichia coli* bacteria (Gram-negative bacteria). Increasing the size of silver particles only up to 12 nm leads to a sharp decrease in bactericidal activity. On the basis of dispersions of silver NPs stabilized with chitosan, homogeneous and transparent films with strength up to 90 MPa can be obtained.

The obtained results can be applied in the creation of bactericidal, styptic, wound-healing materials and functional materials based on chitosan in the form of solutions, gels, sponges and films.

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# THE SYNTHESIS AND PROPERTIES OF HYBRID DENDRIMERS COMPOSED OF A CARBOSILANE CORE AND AROMATIC SHELL BY CUAAC

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Dendrimers and structures based on them typically consist of blocks of the same type. Previously, our group demonstrated the possibility of synthesizing core/shell dendrimers by combining hard polyphenylene and soft carbosilane blocks <sup>1,2</sup>. The advantage of the Cu-catalyzed core-shell azide-alkyne cycloaddition reaction is total conversion and the absence of many side processes.

Our research is focused on the synthesis and study of the properties of carbosilane dendrimers of the different generation with a polyphenylene dendrons in a shell <sup>3</sup>. A spacer of various lengths between the carbosilane core and the polyphenylene shell was used. We study the effect of a change in the length of the spacer, as well as the presence of a rigid triazole fragment, on the different ordering of hybrid systems. The influence of the number and density of hexaphenylbenzene groups in the dendrimer shell on the degree of crystallinity of macromolecules and the packing density in the crystal structure, as well as the phase and thermal behavior, is shown.

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# SYNTHESIS OF POLY(D,L-LACTIDE-CO-GLYCOLIDE) 50/50 WITH PREDETERMINED MOLECULAR STRUCTURE

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Poly(lactide-co-glycolide) is one of the synthetic biodegradable polymers widely used in medicine and pharmaceuticals due to its biocompatibility and the absence of toxic decomposition products. Lactide-based polymers have a wide range of properties that can be adjusted by changing the composition (the ratio of lactide and glycolide units), molecular weight, the nature of the end groups, etc. It is important to control these characteristics when developing systems for targeted delivery and prolonged release of drugs based on polymer micro - and nanoparticles. Poly(lactide-co-glycolide) used in pharma is subject to high demands on the accuracy of the composition, the type of end groups, and the residual content of monomers and solvents. Therefore, an important task is to study the effect of reaction conditions on the properties of polymers.

The main goal of the work is to study the effect of the concentration of 1,12-dodecanediol and 90% L-lactic acid as activators in the copolymerization reaction of D,L-lactide and glycolide (50:50) on the characteristics of polymers. Ring-opening polymerization was carried out at temperatures from 140 to 220 °C using tin 2-ethylhexanoate as a catalyst. The concentration of COOH-groups in the polymers was determined by spectrophotometry using a buffer solution of rhodamine 6G. It has been shown that polymers with a high content of carboxyl groups can be synthesized using 90% L-lactic acid as an activator. Using <sup>1</sup>H-NMR, the degree of monomer conversion and the composition of the copolymers were calculated. The microstructure of the polymer chain was studied using <sup>13</sup>C-NMR. It was found that its type determines the solubility of the resulting polymers. The influence of the nature of the end groups on the rate of hydrolytic degradation of copolymers is shown. In terms of their characteristics, the synthesized polymers are not inferior to analogues, produced abroad.

*The work was supported by the Ministry of Education and Science of the Russian Federation (state assignment No. FFSM-2022-0003)*

# OBTAINING POLYDIMETHYLSILOXANES WITH URETHANE FRAGMENTS IN THE MAIN POLYMER CHAIN BY THE CuAAC REACTION FOR 3D PRINTING

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**Krupnin A.E.**,<sup>4</sup> **Buzin A.I.**,<sup>1</sup> **Khanin D.A.**,<sup>5</sup> **Kostrov S.A.**,<sup>1,6</sup> **Bakirov A.V.**,<sup>1,4</sup>  
**Drozdov F.V.**,<sup>1,2,3</sup> **Chvalun S.N.**,<sup>1,3</sup> **Muzafarov A.M.**,<sup>1,5</sup> **Kramarenko E.Y.**,<sup>1,6</sup>  
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Studies have been carried out on the generation of polydimethylsiloxane (PDMS) copolymers with the inclusion of dynamic urethane fragments by the reaction of azide-alkyne cycloaddition catalyzed by a salt of monovalent copper (CuAAC). This approach is characterized by ease and a high level of control in reaction. The resulting copolymers have high potential due to dynamic interactions between the injected fragments into the polymer chain, which affects the performance characteristics of the final material.

The paper presents the results of obtaining such copolymers and investigates their physicochemical properties. It was also demonstrated the production of composite materials based on them by introducing particles of radio-technical carbonyl iron.

It is confirmed that the obtained thermoplastic materials can be used for 3D extrusion printing.

*The synthesis and modification of copolymers were carried out with the financial support of the Russian Science Foundation (Grant no. 23-43-00057).*

The study of the properties of copolymers was carried out with the financial support of L.N. Tolstoy TSPU, the "Priority 2030" program (Agreement No. 073-03-2022-117/7)

# THE INFLUENCE OF RIGID BLOCK STRUCTURE ON THE CHARACTERISTICS OF ESTER-TYPE URETHANE THERMOPLASTS

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Among the variety of polyurethane materials, thermoplastic polyurethanes (TPU) occupy a special place. A valuable set of performance characteristics combined with manufacturability determine the competitiveness of TPUs in the polymer market and demand in various industries.

TPUs are a block-polymers consisting of a soft and hard segments. The characteristics of the polymer are affected by the nature of each of these segments.

The purpose of this research is to study the dependence of TPU properties on the type of the hard segment.

The objects of this research were TPUs derived from oligobutylene glycol adipate (OBA) with a molecular weight of 1850, 4,4'-diphenylmethanediisocyanate (MDI) and low molecular weight chain extenders, namely, aromatic diol - 2,2'-[propane-2,2-diylbis(n-phenylenoxy)]diethanol (DFP-2) and aliphatic diol – 1,4-butanediol (BD). Thus, the soft segment in these TPUs was OBA, and the hard segment was formed due to the interaction of MDI and the above-mentioned diols.

The sample, the hard segment of which is formed with the participation of DFP-2, is amorphous and shows no remaining deformation after breaking, while the use of BD leads to the formation of a crystallized polymer showing residual deformation. Regarding deformation-strength characteristics and hardness, TPUs based on BD are superior to those obtained by using DFP-2. This is due to a decrease in the degree of separation of the soft and hard segments in the TPUs based on DFP-2 due to the presence of aromatic fragments, flexible ether bonds and side methyl substituents. The above stated leads to the weakened crystallization ability of the oligoester block, while the elastic recovery ability of the macromolecules of the unloaded sample is improved.

*The work was carried out with the financial support in the form of grant subsidies for academic leadership program "Priority 2030".*

# AROMATIC AMINOPOLYOL SYNTHESIS AND POLYURETHANE PAINT COATING BASED ON IT

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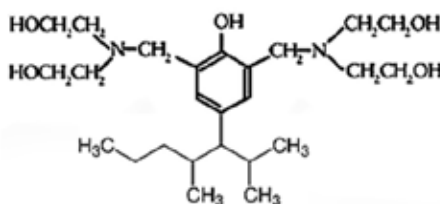
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The increasing demand for polyurethane (PU) products in the Russian market is often met through foreign supplies. This is due to the complete absence of isocyanate production in the country and a shortage of hydroxyl-containing compounds, including polyols. Due to sanctions in Russia, it is urgent to synthesize new polyols using domestic raw materials and develop technology for obtaining PU material based on them.

The objective of this work is to synthesize an aromatic aminopolyol for the purpose of obtaining a PU paint coating.

The synthesis of the aromatic aminopolyol was achieved through the Mannich reaction, which involved the condensation of nonylphenol, diethanolamine, and formaldehyde at 60°C, followed by water distillation.

The structure of the resulting product was identified through IR spectroscopy, MALDI-TOF mass spectrometry, and chemical analysis, which confirmed the formation of an aromatic aminopolyol with the following structure:



The aromatic aminopolyol was used to synthesize PU paint coatings along with hydroxyl acrylic resin, hexamethylene-1,6-diisocyanate-biuret and toluene. The resulting formulation produced a composition that yielded a PU coating with high hardness, adhesion, and resistance to impact loads.

*The research was funded by a grant from the academic leadership program 'Priority 2030', which received subsidies approved by the Government of the Russian Federation in 2021 under Resolution No. 72729.*

# PREPARATION OF SILICON OXYNITRIDE FILMS FROM INORGANIC POLYSILAZANE FOR ENCAPSULATION OF FLEXIBLE SOLAR CELLS

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Inorganic polysilazane is a precursor polymer to produce silicon oxynitride ceramic. Silicon oxynitride films produced from polysilazane are used to encapsulate flexible organic solar cells due to the possibility of a low-temperature UV-induced curing process. Silicon oxynitride films are also a material for multilayer antireflective coatings.

The chain structure of inorganic polysilazane affects the properties of the resulting films. The branching of the polymer chain depends on the ratio of silicon and nitrogen Si:N in the oligomer chain. Thus, chain branching affects the amount of film shrinkage during polymerization. Inorganic polysilazane with a branched structure, in which the Si:N ratio is close to 3, has the minimum shrinkage value. In this work, the influence of the parameters of the polysilazane synthesis process on the molecular weight and structure of the polymer chain and on the properties of silicon oxynitride films obtained from inorganic polysilazane was experimentally studied.

In the IR spectrum of the sample obtained at the maximum consumption rate of ammonia in the ammonolysis reaction of dichlorosilane (4 g/min), the region corresponding to the absorption of N–H bonds ( $3380\text{ cm}^{-1}$ ) is recorded. In the IR spectrum of the sample obtained with a minimum ammonia consumption (0.5 g/min), this region is not detected. The observed effect can be explained by the fact that at low ammonia consumption, an excess of dichlorosilane appears in the reaction zone, which leads to ammonolysis with the formation of branched chains by replacing N–H bonds with N–Si. The weight loss of the inorganic polysilazane film measured by thermogravimetric analysis was 1.2% in the temperature range from 70 to 180 °C, which means low shrinkage of the silicon oxynitride film.

*This work was financially supported by the Ministry of Science and Higher Education of the Russian Federation project number FSWR 2022-008.*



# SYNTHESIS AND INVESTIGATION OF PROPERTIES LADDER POLYPHENYLSILSESQUIOXANES OF VARIOUS MOLECULAR WEIGHTS OBTAINED IN AN AMMONIA MEDIUM

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Ladder-like polyphenylsilsesquioxanes (l-PPSQ) are a class of organosilicon polymers with a complex of valuable physico-chemical properties. The most commonly used method for the synthesis of l-PPSQ is the high-temperature polymerization of phenyltrichlorosilane hydrolysis products - a multistage method requiring the use of a catalyst, a large amount of organic solvents, as well as conducting the reaction under harsh conditions.

Previously, we developed an effective method for the synthesis of l-PPSQ by condensation of *cis*-tetraphenylcyclotetrasiloxanthetraol (*cis*-tetrol) in an ammonia medium. The advantage of this approach is that in this case ammonia acts as both a solvent and a catalyst for the condensation process. In addition, the resulting polymer does not need to be cleaned, since during decompression of ammonia, the active medium is instantly removed from the reaction zone.

In this paper, it will be shown how, by changing the synthesis temperature, it is possible to obtain l-PPSQ and films based on them with specified and variable molecular weight characteristics over a wide range, which cannot be achieved by alternative methods. We have obtained a wide range of l-PPSQ with molecular weights from 2 to 250 kDa. These polymers can act as promising building blocks in the production of various block copolymers, for example, analogues of Lestosil and Blocksil.

*The work was carried out with the financial support of the Russian National Fund, project 23-79-10256.*

# FREEZING PROCESS OF POLYMER SOLUTIONS FOR THE CREATION MATERIALS WITH A SPECIFIED MORPHOLOGY

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When developing artificial tissues, the pore architecture of the scaffold should imitate the structure and properties of the native matrix. Freeze casting is a promising method for creating three-dimensional material to replace damaged tissue.<sup>1</sup> It allows control of the structure of the resulting materials by controlling the thermodynamic conditions of the freezing process.<sup>2</sup> Although there is a good understanding of the physical basis of the method, many of the details of the processes occurring in it are not fully understood.

In the work we used a 2% solution of chitosan in a 2% aqueous solution of acetic acid. The study also used solutions of chitosan with the addition of carbon black (CB, Vulcan XC 72R) as a model system, in weight concentrations (based on the polymer weight) from 1 to 80 wt.%. Next, the prepared solutions were frozen in a developed installation using a Peltier element. The dependence of temperature on time was recorded using a Termodat-1.3M sensor. Then the samples were lyophilized in a Martin Christ Alpha 2-4LSC dryer to study the morphology of the materials using scanning electron microscopy on a Phenom XL instrument (ThermoFisher Scientific, USA).

As a result of the work, the dependence of the freezing rate and the degree of supercooling of the polymer solution on the filler concentration and cooling power was obtained. A comparison was made with the constructed mathematical model. When studying the morphology of materials, it was discovered that a layer of ice nucleation is formed in the region of the beginning of the freezing front. Its thickness depends on the filler concentration and cooling power. Further along the volume, ice is formed with a predominant anisotropic growth mechanism.

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*The work was carried out with the support of the state assignment of the National Research Center "Kurchatov Institute". The authors thank the resource center (RC) "Optics" and the RC for additive and virtual technologies ORC KK NIBKS-PT for studying the morphology of the samples and assistance in manufacturing the experimental setup.*

# FABRICATION SILICON CARBIDE FIBERS FROM A NEW TYPE OF PRECURSORS

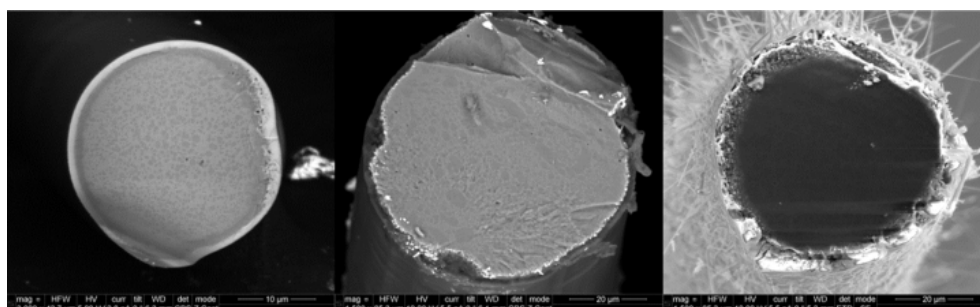
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Silicon carbide (SiC) ceramic fibers have a number of unique properties: strength, hardness, low thermal conductivity, low coefficient of thermal expansion, resistance to oxidation, high temperatures, chemical and radiation exposure. Fibers can serve as a reinforcing frame in composite materials used in many industries, particularly in the space and aviation industries.

There is a technology for creating SiC fibers by pyrolysis of an organosilicon polymer precursor. After spinning, polymer fibers must be cross-linked to prevent them from melting during pyrolysis. In this work, SiC fibers were obtained by pyrolysis of a new type of precursor capable of spontaneous cross-linking. This property of the precursor avoids the negative impact on the properties of the material by cross-linking with oxygen or the expensive process of electron irradiation. The resulting fibers were studied by electron microscopy, elemental and X-ray diffraction analysis.

The possibility of modifying fibers depending on pyrolysis conditions has been shown. Fibers coated with a silicon oxide shell, a carbon shell, and coated with nanorods were obtained.



**Figure 1.** SiC fiber shell, from left to right: silicon oxide, carbon, nanorods.

*The work was carried out within the framework of the state assignment of the National Research Center "Kurchatov Institute".*

# DESIGN OF NEW MATERIALS WITH ADJUSTABLE FLUORESCENT PROPERTIES BASED ON SILOXANES OF DIFFERENT ARCHITECTURE AND ORGANIC FLUOROPHORES

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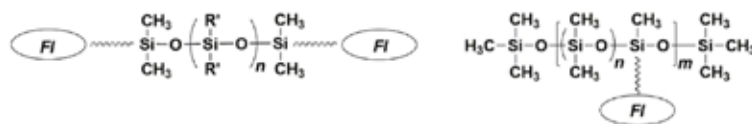
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A current area of research is the creation and study of the properties of materials that combine the unique properties of siloxane matrices (thermal and chemical stability, wide operating temperature range, high flexibility, optical transparency, inertness and biocompatibility) and organic fluorophores (fluorescence, sensory properties, interfluorophore interactions). Such combined systems make it possible to obtain new unique fluorescent materials that can be used in various fields of science as probes for the detection of various cells and organelles, as sensors for temperature and polarity of the environment, in optics and in OLED technologies as components for generating "white light", and in materials science – as fluorescent coatings capable of responding to changes in pressure and temperature.

In this work, bis- and multichromophoric systems with monomer-excimer fluorescence were obtained based on various fluorophores (boron difluoride dibenzoylmethanate, perylene diimide) and siloxane matrices of linear, cyclic and polymer structure (Fig. 1)<sup>1-3</sup>.



**Figure 1.** Bis- and multichromophoric systems

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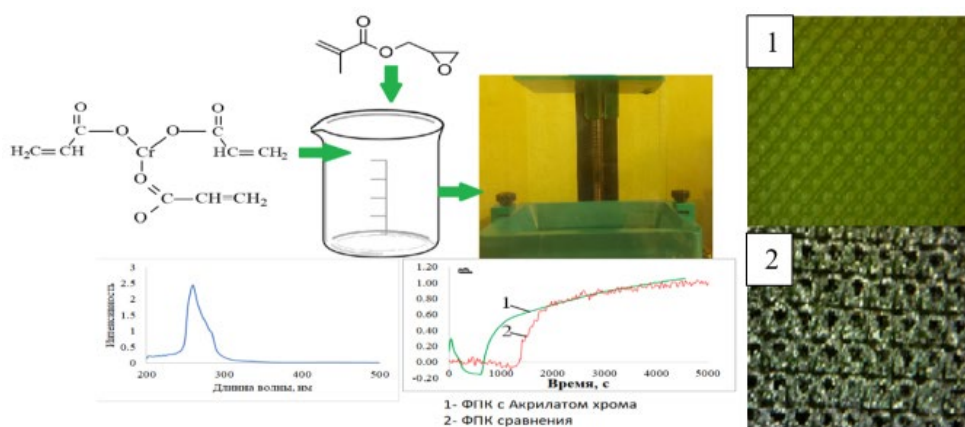
# PHOTOPOLYMERIZING COMPOSITION FOR 3D PRINTING MODIFIED WITH CHROMIUM ACRYLATE

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A directional change in the properties of polymer materials is possible due to the introduction of coordination compounds into the main macromolecular chain, which include metal-containing monomers. Well known works aimed at the synthesis of acetates, acrylates and (met)acrylates of d-metals of variable valence (nickel, cobalt, chromium, etc.), as well as the production of polymer materials based on them<sup>1</sup>. Due to the multiple bond in this type of compounds does not participate in coordination with the metal atom, their use as a component of photopolymerizable compositions (PhPC) has opened up new possibilities in stereolithography<sup>2</sup>. An important feature is that organometallic complexes can act as a UV adsorber in the formulation of PhPC.

The report presents data on the modification of PhPC based on glycidyl methacrylate and a photoinitiator with a chromium acrylate complex.



**Pic.** The scheme of the additive manufacturing process using FPC modified with chromium acrylate

The results of studying the kinetics of the photopolymerization process, evaluating the physico-mechanical properties and accuracy of 3D printing of products made of PhPC modified with chromium acrylate are discussed.

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# PHYSICOCHEMICAL AND BIOACTIVE PROPERTIES OF THE ARCTIC BROWN ALGAE PHLOROTANNINS

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Arctic brown algae, including the species *Fucus vesiculosus*, are a valuable, rapidly renewable source of a unique complex of antioxidant polyphenols (phlorotannins, PTs). These compounds have potential for use in broad-spectrum pharmaceuticals due to their increased activity, which is attributed to their physicochemical properties, conformational features, and structural organization.

Phlorotannins were isolated from the algae *F. vesiculosus* using a scheme developed by the authors.<sup>1</sup> The extract was purified and fractionated by solid-phase extraction (SPE) to obtain the active PT subfraction, which had a purity of 98%, a mass of 21.4 kDa, and an activity of 862 mg of ascorbic acid/g of extract. The key structural and functional characteristics of the isolated fraction were established using various techniques, including chromatography, NMR, molecular hydrodynamics, IR spectroscopy, oxometry, and potentiometry. The bioactive effect of phlorotannins on human blood cells appears to be influenced by the high concentration of free -OH groups. It has been observed that the tested fraction meets the criteria for selecting substances with antiseptic properties. The interaction between phlorotannins and cell membranes has been observed to increase the functional activity of immune cells, as demonstrated in an experiment with the blood of patients diagnosed with lymphocytic leukemia. It is worth noting that this interaction does not result in lysis, as has been shown in previous studies. This suggests that PTs have an immunostimulating effect, which could make the isolated drug a potential agent for antitumor therapy.

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*This project has been granted financial support from the Ministry of Science and Higher Education under the FSRU-2023-004 project.*



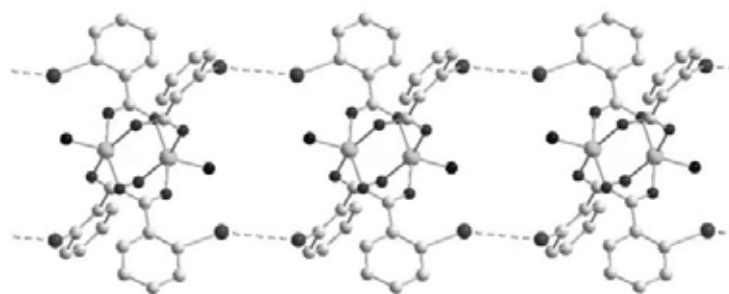
# IODINE-SUBSTITUTED AROMATIC CARBOXYLATES OF Cu(II) AND Zn(II): SYNTHESIS, STRUCTURE AND PROPERTIES

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The chemistry of Cu(II) and Zn(II) carboxylate complexes has been studied for a long time, but there has been no systematic study of compounds based on iodo-substituted aromatic carboxylic acids as building blocks for halogen-bonded (HB) systems.

In this work, we obtained complexes of Cu(II) and Zn(II) with anions of iodine-substituted acids, namely 2-iodobenzoic (HIBA), 3,5-diiodosalicylic and penta-iodobenzoic, as well as a wide range of additional N-donor ligands<sup>1-7</sup>. Data on the structural features, thermal stability, spectroscopic and magnetic characteristics of the obtained complexes are presented.



**Figure 1.** Structure of the  $[\text{Zn}_2(3\text{-MePy})_2(\text{IBA})_4]$  complex and its HB system  $\text{I}\cdots\text{I}$ .  
Pyridines are reduced to N atoms.

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# POLYHYDROXYL SILSESQUIOXANES. SYNTHESIS AND APPLICATION FOR SURFACE MODIFICATION OF DIFFERENT MATERIALS

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Creation of wear-, moisture-, and fire-resistant materials requires compounds possessing hydrophobic properties, i.e. ones with low surface energy<sup>1</sup>. Examples of such compounds can be various polyorganosiloxanes.

Polyorganosilsesquioxanes represent one of the most important classes of polyorganosiloxanes. Depending on the method of preparation, silsesquioxanes with different structures can be obtained: framework, ladder, random, etc.<sup>2</sup>. The structure of polyorganosilsesquioxanes determines their properties and applications.

Polymethylsilsesquioxanes with high content of hydroxyl groups are of great interest due to reactivity of these groups, what allows grafting of polymethylsilsesquioxane to the different surfaces such as glass, fabric, metal etc<sup>3</sup>.

The aim of the present work was to compare hydrophobising efficiency of polymethylsilsesquioxanes on various materials depend on its structure.

Polymethylsilsesquioxanes synthesised using hydrolytic polycondensation of methyltriethoxysilane in neutral conditions under pressure<sup>4</sup> were used as hydrophobisers.

The results of the investigation of the selected hydrophobisers will be presented. The level of surface hydrophobicity, adhesion strength, and vapour permeability for cotton fabric will be discussed. In addition, the effect of hydrophobisers structure and heat treatment on the level of surface hydrophobicity will be shown.

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# SELF-ASSEMBLY OF FIBRILLAR GELS IN SOLUTIONS OF AMPHIPHILIC COMB-LIKE MACROMOLECULES

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Fibrillar gels are polymer networks with elongated supramolecular structures formed during the self-assembly of individual macromolecules act as subchains. Such structures are widespread in biological objects, and the main example is the extracellular matrix, in which the composition and morphology of the gel directly determines the mechanical properties of tissues, transport properties, cell adsorption and their ability to differentiate. Understanding the formation processes of such objects and creating their synthetic analogues is one of the most important tasks at the intersection of polymer science and biology.

In this work, using coarse-grained computer modeling methods, a comprehensive study of the processes of spontaneous ordering of amphiphilic macromolecules with amphiphilicity at the level of a repeating unit was carried out in dilute and concentrated solution modes [1,2]. Predictions of possible morphologies of supramolecular fibrillar gels in single and binary solvents, as well as features of transitions between structures, are discussed. It has been shown that the self-assembly of fibrils of amphiphilic macromolecules is determined not only by the balance of volumetric and surface energy, but also by a special entropic attraction associated with the orientation of the lateral pendants. The areas and conditions of transitions between single fibrils and fibrils - aggregates of laterally connected fibrils - have been determined.

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# SYNTHESIS OF CONJUGATED POLYMERS BASED ON TRIPHENYLAMINE WITH VARIOUS SIDE ELECTRON-WITHDRAWING GROUPS AND THEIR APPLICATION IN HYBRID PHOTOVOLTAICS

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Currently, a wide range of organic hole-transport materials have been developed for use in perovskite solar cells<sup>1</sup>. Among them, due to the presence of such properties as high thermal stability, high glass transition temperature, good solubility in organic solvents, improved adhesion to the substrate, special attention is paid to polymers based on triphenylamine derivatives (TPA). Polymers with a donor-acceptor (D-A) structure are among the most promising materials. By introducing various electron-withdrawing groups into the structure of polymers, it is possible to effectively regulate the optoelectronic properties of materials: light absorption region, energy of HOMO and LUMO levels, charge mobility, and thus improve the output parameters of organic perovskite solar cells<sup>2</sup>.

The simplest method for the synthesis of polymers based on TPA is oxidative polymerization with  $\text{FeCl}_3$ <sup>3</sup>. The work presents the synthesis by oxidative polymerization of new polymers based on TPA D-A structure, describes their properties, and also presents primary data collected during the study of materials in optoelectronic devices.

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# SYNTHESIS OF COORDINATELY LINKED POLYURETHANES

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Polyurethanes are polymers on the basis of which it is possible to create materials with a wide range of performance characteristics: increased hardness, high modulus of elasticity, high elasticity, resistance to abrasion, solvents, oils and high strength. Segmented polyurethanes (SPU) are promising in terms of areas of application, the possibility of repeated processing and the effect on the supramolecular structure [1,2]. Such polyurethanes can be used as thermoplastic elastomers or in a dissolved state.

In this work, the effect of metal complex binding on the supramolecular organization and the resulting physical, mechanical and electrophysical properties of SPU were investigated. The products of the interaction of copper (II) chloride with N,N'-diethylhydroxylamine (DEHA) and copper (II) chloride in the form of its solution in tetrahydrofuran (THF) were used as coordinating centers. The features of the interaction of CuCl<sub>2</sub> with DEHA and THF were previously studied.

It turned out that the nature of the used metal complex systems has a significant impact on the supramolecular structure of the SPUs modified in this way (MCSPU). Thus, the use of CuCl<sub>2</sub> – DEHA even at 0.1 wt.% leads to a significant increase in the microphase separation of rigid and flexible MCSPU blocks. As a result, there is a significant increase in their strength, elasticity, heat resistance, temperature of the onset of segmental mobility and a decrease in the specific volumetric electrical resistance by 10,000 times. In the case of MCSPU obtained using CuCl<sub>2</sub> in the form of its solution in THF, loosening of rigid-chain supramolecular formations is observed.

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# MICROPOROUS BLOCK COPOLYMERS AS ANALYTICAL SENSORS FOR HEAVY METAL IONS

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Sensor membrane materials are widely used for the determination of cations and anions. The structure and morphology of the membrane are the basis that determines the rapid ion exchange at the membrane/solution interface. Block copolymers (BCs) are promising as sensor membranes. An important feature of BC is their ability to form a wide variety of supramolecular structures. The order and size of such supramolecular formations are determined by the chemical structure, molecular masses of the blocks, the ability of the blocks to segregate, and reaction conditions. To create new supramolecular architectures with specific self-assembly behavior, controlled synthesis of BS is promising.

Based on Pluronic terminated with potassium alcoholate groups ( $M_w = 4200$ , content of oxyethylene units 30%) and 2,4-toluene diisocyanate (TDI), nanoporous optically transparent block copolymers (OBC) were synthesized and studied. Reaction conditions were established under which polyisocyanates of acetal nature (O-polyisocyanates) are formed in OBC. To improve microphase separation, OBCs were modified with self-condensation-resistant bound Cu(II) silicas (ASiP-Cu). A structural feature of ASiP-Cu is the existence of polyoxyethylene branches in their structure. It was found that the use of ASiP-Cu makes it possible to strengthen the structure of O-polyisocyanate blocks and enhance the microphase separation of OBC.

To create analytical sensors based on microporous block copolymers, test systems were obtained by applying a selective layer of OBC to the surface of a polyethylene terephthalate film. The resulting test systems were studied as analytical sensors for the determination of heavy metal ions.

*This work was supported by the Russian Science Foundation (grant no. 23-23-10012).*



# SYNTHESIS OF 2,2'-DITHIODIETHANOL AT ATMOSPHERIC PRESSURE

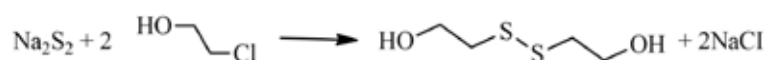
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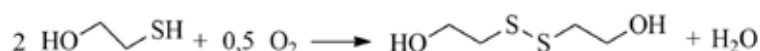
The industrial production of liquid thiols through the reaction of organic chlorine-containing compounds with sodium polysulfide generates a significant amount of wastewater, causing serious environmental concerns.

Therefore, the search for alternative methods to synthesize sulfur-containing polymers is a pressing issue.

The literature<sup>1</sup> describes a method for producing 2,2'-dithiodiethanol by reacting sodium disulfide with ethylene hydrochloride in a solvent medium – isopropyl alcohol in order to exclude the hydrolysis process of the product:



In this study, a method was employed to synthesize 2,2'-dithiodiethanol through the oxidation of 2-mercaptoethanol using anhydrous manganese acid salt and tri(n-butyl)amine as a tertiary amine under laboratory conditions at normal temperature and pressure, in accordance with the following reaction scheme:



According to the above scheme, the conversion rate of 2-mercaptoethanol exceeds 99% and water is generated as a byproduct. The extent of conversion of 2-mercaptoethanol has been determined by iodometry based on the content of sulfhydryl (SH) groups, as their presence is indicated by the residual level of 2-mercaptoethanol. The structure of the resultant 2,2'-dithiodiethanol has been verified using <sup>13</sup>C and <sup>1</sup>H nuclear magnetic resonance (NMR) techniques.

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# NOVEL PERVAPORATION MIXED MATRIX CHITOSAN MEMBRANES FOR ENCHANCED DEHYDRATION

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Pervaporation is the most promising membrane method for separating liquid mixtures of low molecular weight substances. It is also actively used for dehydration of various organic solvents. Hydrophilic polymers such as polysaccharides and polyvinyl alcohol are commonly applied as membrane materials for pervaporation dehydration. Among all the hydrophilic polymers, chitosan is a biopolymer derived from chitin and currently of interest for membrane development due to its film-forming properties, biodegradability, high water selectivity and thermal stability. However, low stability in dilute solutions and permeation flux are the main disadvantages of pervaporation membranes from chitosan for industrial applications.

In this work, bulk (volume) modification was carried out by introducing graphene oxide carbon nanoparticles into a chitosan matrix to develop mixed matrix pervaporation membranes with improved performance for the dehydration of alcohols. Structural and physicochemical changes in the developed composites and membranes from them were studied by spectroscopic and microscopic methods, measurements of contact angles and swelling degree, etc. The transport characteristics of membranes were evaluated in pervaporation dehydration of alcohols (ethanol, isopropanol, etc.).

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# ELECTROSPUN HYBRID MATRICES BASED ON CHITOSAN, CERIUM OXIDE, AND HALLOYSITE FOR BIOENGINEERING APPLICATIONS

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Biopolymer nanocomposite materials based on polysaccharides doped with organic and inorganic fillers have great potential in the development of tissue-engineered scaffolds<sup>1-3</sup>. In this work, cerium oxide nanoparticles and halloysite nanotubes were incorporated into electrospun chitosan-based matrices. The resulting nonwoven materials consisted of nanofibers with average diameters of 443±201 nm (chitosan), 151±63 nm (chitosan+halloysite), 175±76 nm (chitosan+cerium oxide), and 233±86 nm (chitosan+halloysite+cerium oxide). The samples were characterized by a uniform distribution of ceria nanoparticles and halloysite nanotubes. The introduction of nanofillers into the chitosan matrix increased the Young's modulus, yield stress and ultimate strength of the materials due to both the reinforcement of the polymer matrix with stiff nanotubes and the interaction of the positively charged chitosan with the negatively charged halloysite. A smaller increase in the stiffness of the material caused by the introduction of ceria nanoparticles into the same polymer matrix was a result of the formation of additional bonds between the polymer macromolecules and the nanoparticle surface. At the same time, inorganic fillers reduced the ultimate deformation characteristic of polymer-inorganic hybrid materials.

In vitro cultivation of mesenchymal stem cells showed that the developed hybrid matrices have good biocompatibility; in vivo experiments also demonstrated their pronounced regenerative potential.

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# THE POLYMER MEMBRANE MODIFIED BY 4'-AMINO-BENZO-15-CROWN-5-ETHER FOR LITHIUM EXTRACTION

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Lithium is an important component for electronics and power generation, and demand for it is steadily increasing. The price of lithium has increased by 320% over the past three years, and demand is expected to continue to outstrip supply. One promising method of lithium extraction is its extraction from oil and gas condensate field associated waters (brines) using DLE (direct lithium extraction) technology, which involves passing formation water through a membrane<sup>1</sup>.

A cellulose acetate-based polymer membrane was modified using 4'-amino-benzo-15-crown-5 ester (4AB15C5), which has a unique ability to bind lithium ions. This makes it an ideal candidate for lithium separation. There are many crown ethers with different sizes and functional groups, allowing the best option to be chosen for a particular application, in this study 4AB15C5 demonstrated good Li<sup>+</sup> selectivity in solution<sup>2</sup>. A suite of techniques including Fourier transform infrared spectroscopy, ion chromatography and scanning electron microscope were applied to study the properties of the 4AB15C5-modified membrane<sup>3</sup>. The 4AB15C5-modified membrane retains lithium, which allows efficient lithium extraction and reduces the energy consumption of the process.

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*The Priority 2030 Federal Academic Leadership Program for infrastructural support.*

# SYNTHESIS OF HYDROGEL MEMBRANE BASED ON GELATIN MODIFIED WITH A SILYLATING AGENT FOR CHEMICAL SENSORS

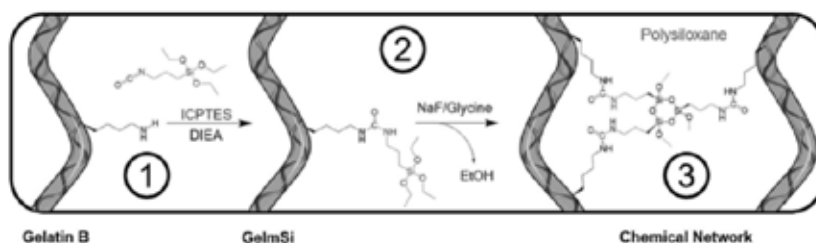
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Hydrogels are cross-linked three-dimensional polymer networks capable of swelling significantly in water and forming insoluble structures<sup>1</sup>. This work deals with the synthesis of hydrogel membrane based on modified gelatin.

(3-isocyanatopropyl)triethoxysilane is used as a gelatin modifier. The synthesis is carried out from (3-aminopropyl)triethoxysilane.

(3- Isocyanatopropyl)triethoxysilane interacts with the lysine side chains of gelatin in the presence of N,N-diisopropylethylamine to form a polymer with siloxane side groups. Crosslinking is carried out in the presence of sodium fluoride<sup>2</sup>.



**Figure 1:** Scheme of hydrogel synthesis

It is important to note that type B gelatin, characterized by low blooming force and low content of endotoxins, which are cytotoxic lipopolysaccharides, was chosen for the work.

Due to the formation of siloxane bonds, a rigid hydrogel was obtained. The obtained material is characterized by biocompatibility, which makes it possible to use this material as a medical sensor membrane.

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# SYNTHESIS OF POLYMER SORBENTS IMPRINTED WITH KANAMYCIN USING NON-COVALENT MOLECULAR IMPRINTING WITH THE SELF-ASSEMBLY APPROACH

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Kanamycin is a broad-spectrum antibacterial antibiotic for medical and veterinary applications, obtained by microbiological synthesis using the radiant fungus *Streptomyces kanamyceticus*. The culture fluid contains four types of kanamycin, which differ in their structure by radicals. Therefore, there is a need for highly selective extraction of the medical form of kanamycin A from a multi-component medium.

For this purpose, a method was developed for the synthesis of selective granular polymer sorbents based on 2-hydroxyethylmethacrylate, methacrylic acid, and ethylene glycol dimethacrylate by emulsion polymerization in the Pickering emulsion using a free-radical initiation mechanism and non-covalent molecular imprinting with a self-assembly approach.

The effect of the number of matrix molecules and the dispersion rate of the polymerization mixture on the porosity, uniformity, and structural stability of kanamycin A-imprinted polymers was studied in detail. It is established that the introduction of 6 mol.% of template molecules leads to the formation of polymer granules with a rigid, uniform structure. It is shown that the dispersion rate of the polymerization mixture of 300 rpm is optimal for creating imprinted polymer sorbents with the same permeability and porosity, regardless of the amount of template, by emulsion polymerization in a Pickering emulsion formed by selenium-poly(vinylpyrrolidone) nanocomposites.



# CYTOTOXIC EVALUATION OF COMPOSITE MATERIALS HYDROXYAPATHITE – HYALURONIC ACID

**Gerk S.A.<sup>a</sup>, Nashchekina Yu.N.<sup>b</sup>, Golovanova O.A.<sup>a</sup>**

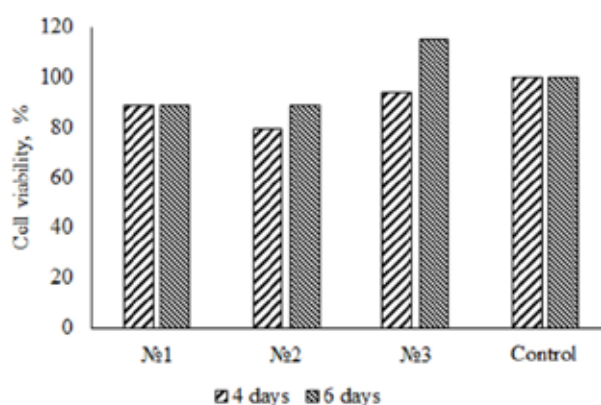
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Promising materials for bone grafting are composites based on hydroxyapatite and external biopolymers. Hyaluronic acid has a positive regenerative effect.

Hydroxyapatite powders were obtained from model human synovial fluid according to the author's method [1] using the method of hyaluronic acid in the form of sodium salt ( $M_r = 2.0 \cdot 10^6$  Da) of different structures, weight. %: 0.1 – sample No. 1; 0.2 – No. 2; 0.6 - No. 3. The cytotoxicity of the composites was tested using the MMT test on the FetMSC cell line (incubation time - 4 and 6 days). The supplies were previously sterilized with ozone for 90 minutes.

It has been established that the viability of cells when incubated with powder particles is 79 – 94% and depends on their properties.



**Figure 1.** Viability of FetMSCs with particle composites.

Composite No. 1, which is well resorbed under physiological conditions, exhibits a stable positive effect on cells. The absence of cytotoxicity to FetMSC was revealed after 6 days of incubation of the most crystallized powder No. 2. The most amorphized sample No. 3 did not have a negative effect on the cells for 4 days; further, an overestimated value of the viability index was noted, possibly due to partial contamination of the sample.

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*The work was carried out with the financial support of the Russian Science Foundation, project No. 23-23-00668.*

# MORPHOLOGICAL CHARACTERISTICS OF HYDROXYAPATITE-HYALURONIC ACID COMPOSITES OBTAINED FROM SYNOVIA PROTOTYPES

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A detailed study of the processes of crystallization of hydroxyapatite from supersaturated solutions, close in chemical composition to human intercellular fluids, will make it possible to obtain new osteoconductive materials with the desired biodegradation in vivo.

In this work, composites were synthesized from prototypes of human synovial fluid (synovium), containing high molecular weight hyaluronic acid from 0.05 to 0.80 wt. %. The micromorphology of the powders was studied using scanning electron microscopy (XSP-104).

The following morphological features of the powders were revealed. Hydroxyapatite-hyaluronic acid (HA-HHA) composites obtained from weakly viscous solutions (< 0.2 wt. %) are amorphized and are represented by loose oval-scaly aggregates that do not have clear boundaries, similar in porosity to particles of pure HA. At average viscosity values of the mother solution (0.2 – 0.4 wt.%), the aggregates have a more round shape and clear boundaries; formed crystals in the form of thin plate-like formations are visible on their surface. Composites made from gel-like solutions (> 0.4 wt. %) consist of amorphized round, densely structured conglomerates, with a homogeneous and low-porosity surface due to the resulting hydrated layer of polysaccharide-H<sub>2</sub>O. Composite materials synthesized from reaction mixtures containing ≤ 0.4 wt.% hyaluronic acid have a developed surface (S<sub>sp</sub> = 110 - 125 m<sup>2</sup>/g). Low porous compositions are formed from gel-like solutions (>0.4 wt %); their average specific surface area is ~ 47 m<sup>2</sup>/g.

A number of powders have been compiled according to changes in the type, shape and porosity of aggregates (wt.% polysaccharide - form): HA-pure - scaly, porous; HA-HHA (< 0.2) – loose, oval-scaly, porous; HA-HHA (0.2-0.4) – round with thin plates, porous; HA-HHA (> 0.4) – dense, voluminously rounded, slightly porous. Thus, composites synthesized from media containing 0.2-0.4 wt. % hyaluronic acid, are close in morphological characteristics to human bone tissue crystals.

*The work was carried out with the financial support of the Russian Science Foundation, project No. 23-23-00668.*

# ORGANOSILICATE HEAT-RESISTANT AND WATER-RESISTANT ELECTROINSULATING COATINGS BASED ON ORGANOSILOXANES OF LADDER STRUCTURE

**Glebova I.B.,<sup>a</sup> Ivanova A.G.,<sup>a</sup> Poletaev K.A.,<sup>a</sup> Sokolov G.S.,<sup>a</sup> Selivanov S.I.,<sup>a</sup>  
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Organosilicate coatings (OSC) based on organosilicon varnishes and highly dispersed fillers have corrosion resistance and high heat resistance (up to 350-400 °C). However, they are not resistant to water. To overcome this drawback, we for the first time chose polyphenylsilsesquioxane (PPSSO) as a binder for OSC, which, due to its ladder structure, forms a dense organosilicon matrix, and that provides not only heat resistance, but also resistance to water.<sup>1</sup> However, while using PPSSO as a binder, we encountered a problem - the excessive fragility of the resulting OSC. To overcome this problem, we carried out research work on optimizing the synthesis conditions of PPSSO and the synthesis of polymethylphenylsilsesquioxane (PMPSSO) containing methylphenylsiloxane units. Using NMR, XRF, SEM, DSC and SAXS methods, the resulting polyorganosiloxanes and OSCs based on them were studied. The influence of the synthesis conditions of PPSSO and PMPSSO and the heat treatment modes of OSC on the structure and physical and mechanical properties of the coatings was established. The resulting OSCs are dielectric ( $R_v > 10^{10} \text{ Oh}\cdot\text{m}$ ), adhesion – 1 point, hardness ~0.4 relative units, heat resistance up to 400 °C, and they withstand contact with sea water (>48 hours).

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# POLYMERIC MATRICES IN PREPREGS FOR PLASTIC SKI PRODUCTION

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Nowadays polymeric composite materials are highly-demanded in many branches of human activity, with each passing year the spheres of their application are expanding and production volumes are increasing. Widespread epoxy binders have found application for manufacturing prepregs for structural purposes.

The rapid development of the ski industry has led to the replacement of wooden skis by plastic (composite) skis, one of their components is prepreg. A modern plastic ski is composed of functional layers that are joined together in the process of moulding at optimal technological modes:  $120 \pm 2^\circ\text{C}$  for  $7 \pm 1$  min. The branch "Telekhany" of the State Enterprise "Belarustorg" is the only enterprise of the Republic of Belarus, where the production of plastic skis is carried out. For this purpose prepregs with a long shelf life - up to 6 months - are used.

The development of prepregs involved creation of a material that allows to produce high-quality plastic skis according to the selected technological process. The formulation of promising epoxy binders includes, wt. %: 37,4-40,3 epoxy resin based on bisphenol A, 25,0-26,9 canifoletperenomalein resin, 8,5-9,2 polymer modifying additives (polyvinyl butyral or acrylic copolymer), 22,5-27,5 organic solvents (acetone and acetic acid ethyl ester), 1,2-1,7 epoxy resin curing catalyst. Mixing of resins and polymer additives with solvents takes place at  $55 \pm 5^\circ\text{C}$ ; curing accelerator is introduced after homogenisation of all components of the epoxy binder. With the use of the proposed binders prepregs are obtained by the "wet" method. On the basis of the research results the patent for invention BY 24242 "Epoxy binder and prepreg on its basis for production of sports and running plastic skis" was obtained.

*The study was supported by the framework of separate R&D projects of the National Academy of Sciences of Belarus: "Development and research of operational properties of epoxy composition for prepreg manufacturing" (SR № 20190722, 2019) and "Development of prepreg fleece for plastic skis manufacturing" (SR № 20190722, 2020).*

# PREPARATION OF CROSS-LINKED POLYMERS BASED ON POLYSILOXANES

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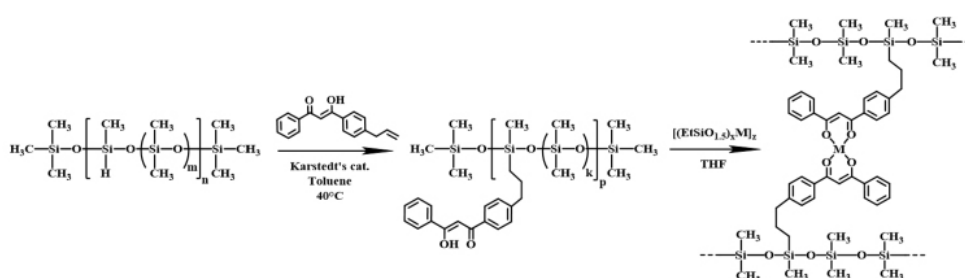
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At present, polymers cross-linked by interactions between metals and ligands are a promising class of high-molecular compounds that exhibit unique physical and chemical properties<sup>1</sup>. Such systems can be used in the field of smart materials<sup>2</sup>. In this study, polysiloxanes were used as a polymer matrix, as they have high heat and gas permeability, as well as biocompatibility<sup>3</sup>. Oligoorganometallosiloxanes acted as sources of metal ions and crosslinking agents. They contain ethyl substituents that ensure the compatibility of the oligomers with the matrix.

In this work, coordination-cross-linked polymers were obtained by the interaction of organometalsiloxanes with organic ligands, which are statistically distributed along the polysiloxane chain. The obtained materials were characterized by a set of physical and chemical methods.



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# MODIFICATION OF STRUCTURE AND PROPERTIES OF COMPOSITE POLYIMIDE FIBERS BY INTRODUCTION OF CARBON NANOPARTICLES

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Crystallizing polyimides have a significant advantage over amorphous materials, because there is a possibility to increase the limiting temperature of their operation, which in this case will no longer depend on the glass transition temperature  $T_g$  of the amorphous phase, but on the melting temperature of the crystalline regions that is essentially higher than  $T_g$ . The aim of this work was to obtain and to study in detail the structure and properties of heat-resistant nanocomposite fibers based on partially crystalline thermoplastic polyimide R-BAPB and carbon nanoparticles of anisodiametric shape (carbon single-walled nanotubes). Carbon nanotubes (SWCNTs) were introduced during a synthesis process at a PAA stage at concentrations of 0.05, 0.1 and 0.2 wt.%. The synthesized polyamide acid R-BAPB was subsequently subjected to chemical imidization. Fibers based on R-BAPB polyimide were obtained by melt extrusion, followed by high-temperature orientation drawing to various drawing ratios and crystallization annealing.

The influence of the introduction of single-walled carbon nanotubes into the R-BAPB matrix, as well as orientation drawing and crystallization annealing on the structure, thermal-physical and mechanical properties of composite fibers was studied. It was revealed that the use of SWCNTs initiates the heterogeneous nucleation of crystallites in the polyimide matrix on the surface of the nanoparticles. The introduction of SWCNTs leads to a significant increase in the rate of crystallization and a decrease the oriented fibers shrinkage during additional annealing, which ultimately makes it possible to get crystallized polyimide fibers with modified mechanical properties.



# INVESTIGATING SURFACTANTS AND PACKING TYPES FOR THE HYBRID CARBOSILANECYCLOSILOXANE DENDRIMERS

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Due to the hybrid carbosilanecyclosiloxane dendrimers' unique properties, which include their rigidity and changing molecular shape while maintaining a nearly unaltered chemical composition, they are promising candidates for application in a variety of fields. This is in addition to their inherent amphiphilicity. Early dendrimer generations should be expected to exhibit classical behavior, such as stabilizing emulsions during emulsion polymerization processes<sup>1</sup>. However, as the number of generation's increases and intramolecular rearrangements at the interface become more difficult to accomplish, a significant shift in surface activity must be anticipated.

The phenomenon of the dendrimers of high generations crystallizing with the polybutylshell<sup>2,3</sup> were discovered through the study of dendrimers as polymer systems with a very particular packing. These findings were validated by the data of the hybrid carbosilanesiloxane dendrimers study<sup>4</sup>. The results of research on hybrid carbosilane-cyclosiloxane dendrimers with surface-active characteristics will be discussed in this paper, in addition to X-ray diffraction data suggesting the potential for the formation of compact densely packing structures in a condensed state in the composition close-packed phase.

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# SYNTHESIS AND PROPERTIES OF NON-ISOCYANATE POLYSILOXANURETHANES

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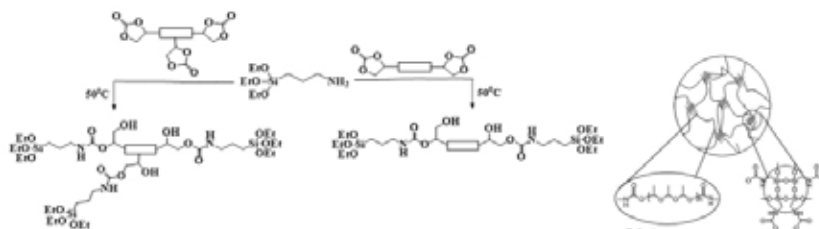
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The universality of polyurethanes makes it possible to create a variety of multifunctional materials based on them. The introduction of a siloxane block into the polyurethane structure gives materials and products based on them a number of unique characteristics - high abrasive resistance and cyclic bending load, and also imparts hydrophobicity, gas permeability and increased heat resistance<sup>1</sup>.

One of the main tasks of modern polymer chemistry is the development of environmentally friendly and safe ways to synthesize industrial polyurethanes. The most promising synthesis method, which eliminates toxic isocyanates, is the reaction of cyclic carbonates with primary amines.

We studied the process of aminolysis of cyclocarbonates of various structures and functionality with silanes and oligodimethylsiloxanes containing both  $\gamma$ -aminopropyl and ethoxyl substituents (Figure 1). Based on them, new cross-linked non-isocyanate polysiloxaneurethanes were obtained and their physicomechanical (tensile strength range was 0.5÷52 MPa, relative elongation range was 1.5÷66%) and thermal characteristics (thermal decomposition processes begin at temperatures above 200°C)<sup>2</sup>. It has been shown that based on the obtained oligomers, new polymer binders - sealants, glue, and adhesives - can be created.



**Figure 1.** Scheme of aminolysis of cyclocarbonates

## Literature

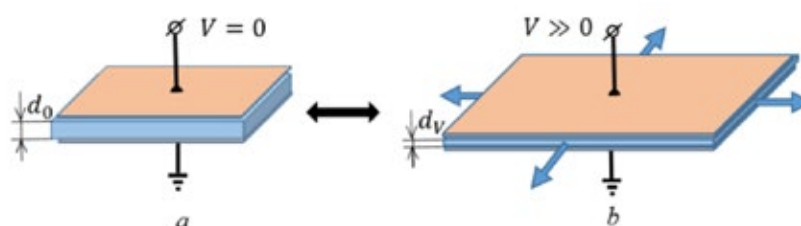
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# PDMS/MQ COMPOSITES – PROMISING MATERIALS FOR DIELECTRIC ELASTOMER ACTUATORS

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Recently, research in polymer chemistry has focused on the development of new soft, responsive materials for use in soft robotics. One of the actively developed and demanded materials in polymer robotics are dielectric elastomeric actuators (DEA).<sup>1-3</sup>



**Figure 1.** Operating principle of DEA

It was previously demonstrated that the performance of DEA depends on the ratio of the dielectric constant of the elastomer material to the Young's modulus  $\frac{\epsilon_r}{Y}$ .

In this work we will present the results of a study on the use of molecular composites based on high molecular weight polydimethylsiloxane rubber (PDMS) and MQ-copolymers as DEAs. It is found that despite the low dielectric constant, these composites demonstrate the best values of the parameter  $\frac{\epsilon_r}{Y}$  in comparison with other unmodified silicone materials, including commercially available ones, which, together with the wide possibilities of modification of PDMS/MQ composites, determines the prospects of their further use as a basis for the creation of DEA with low value of the actuation voltage.

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# METALLO-SUPRAMOLECULAR CROSS-LINKED POLYSILOXANES: SYNTHESIS AND PROPERTIES

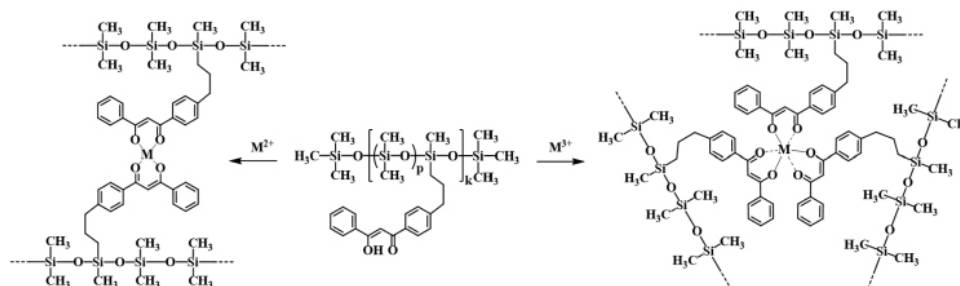
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Synthesis of polymers, cross-linked by metal-ligand interactions, is the new trend in modern polymer, organic, organometallic chemistry and materials science. Introduction of coordination compounds to polymer matrices provides the formation of supramolecular systems demonstrating specific properties, such as shape-memory<sup>1</sup>, sensor properties<sup>2</sup> and other. One of the common polymers used for the preparation of such systems is polysiloxanes<sup>3</sup> due to their valuable physical and chemical properties.

A new route based on the introduction of dibenzoylmethane derivatives into polydimethylsiloxanes was developed in this work. A reaction of these systems with different metals leads to formation of cross-linked polymer structures. In this work the effect of metals nature and their source on the structure and properties of target polymers was investigated as well as polymers' mechanical, rheological, thermal, optical and other properties.



**Figure 1.** Chemical structure of polysiloxanes, cross-linked by metals of different valency

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# DETERMINATION OF THE STRUCTURE OF SULFUR-CONTAINING POLYMERS OBTAINED BY REVERSE VULCANIZATION METHOD BY MALDI-TOF SPECTROMETRY

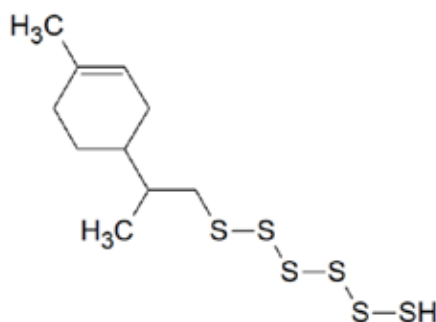
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Inverse vulcanization is the process of formation of polysulfides from elemental sulfur and small unsaturated organic molecules when heated above 159 °C<sup>1</sup>.

Polymer materials that have been produced using the inverse vulcanization method can selectively absorb mercury and some other heavy metals<sup>2,4</sup>, are promising replacements for mid-infrared lenses, and can be used as capsules for fertilizers and for the production of Li-S batteries<sup>3</sup>.

Despite the huge amount of scientific literature, it is still necessary to more accurately characterize the structure of sulfur-containing compounds (Fig. 1) and also their physicochemical properties. The MALDI-TOF mass spectrometry method is excellent for research.



**Fig. 1.** Fragment of a sulfur copolymer with limonene terminal scheme

The results of the interpretation of the MALDI spectra of a sulfur-limonene copolymer obtained by inverse vulcanization allowed us to determine the structure of the formed molecular fragments, which indicates the high potential of MALDI-TOF spectrometry as an analysis method for identifying the structural features of such polymers.

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# MODIFICATION OF POLYPROPYLENE FIBERS BY COMPOSITE MATERIALS WITH METAL-CONTAINING NANO-PARTICLES

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Polypropylene fibers are valued for their unique properties, which are in demand in many industries. Due to the increasing demands on materials, there is a growing interest in obtaining modified fibers with new functions. The most promising, from the point of view of functionality and quality of the materials obtained, are nanoparticle-based modifiers. However, traditional methods of combining fibers and modifying additives are ineffective in the case of nanoscale objects. The problems of aggregation of nanoparticles and their connection with a polymer fiber can be overcome with the help of a second polymer acting as a stabilizer<sup>1</sup>. Such materials can have new antimicrobial properties while maintaining durability and chemical resistance. The composites are characterized by strength, elasticity, electrical conductivity, biocidity, and improved tribological characterisation<sup>2</sup>.

In our work, two-component systems based on polypropylene filaments with a coating based on polyethylene or polytetrafluoroethylene modified with metal-containing nanoparticles were obtained and studied. This method is simpler and more economical than traditional ones, which makes it attractive to industry. Nano-composites act as a protective coating, increasing the strength and reducing the electrical resistance of the filaments, providing antimicrobial protection. Such filaments are suitable for the production of packages, geotextiles, medical devices and other goods, helping to prevent the spread of microorganisms.

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SELF-CATALYZED HYDROLYSIS OF TRIAZOLE-  
CONTAINING ALKOXYSILANES

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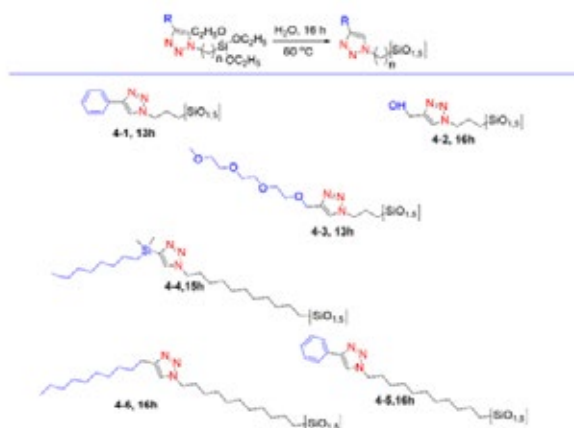
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Organotrialkoxysilanes are unique compounds that play an important role in modern science and industry.<sup>1</sup> In our work, we present an original approach to the preparation of organotriethoxysilanes starting from azidoalkyltriethoxysilanes and various types of substrates containing a terminal triple bond through the azide-alkyne cycloaddition (CuAAC) mechanism without the use of solvents, catalytic ligands and amines. The self-catalyzing effect of the triazole fragment formed as a result of azide-alkyne cycloaddition in the reaction of hydrolysis and condensation of alkoxy groups was also discovered, which made it possible to obtain a number of silsesquioxane products only by adding water, without the use of catalysts. As a result, a new original scheme has been constructed for the production of organosilicon trialkoxysilanes of a monomeric structure with their subsequent conversion into silsesquioxane polymers under “green” conditions.



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# NEW POLYMERIC MATERIALS FOR TISSUE ENGINEERING: COMPOSITES BASED ON ALIPHATIC POLYESTERS AND CELLULOSE DERIVATIVES

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Regeneration of tissue defects formed as a result of various types of injuries or surgical intervention in the treatment of various diseases is an actual problem of modern medicine<sup>1</sup>. This motivates chemists and material scientists to create polymeric materials that provide an opportunity to generate three-dimensional scaffolds from them by 3D printing, which can act as supporting media for cell proliferation and tissue regeneration<sup>2</sup>. Unfortunately, materials based on only one polymer are usually limited to conceptual use and prototyping because they have unsatisfactory mechanical properties. In addition, they usually fail to induce crucial biological processes, namely cell adhesion and differentiation. The combination of several polymers to obtain interpolymer composites is an important task to achieve suitable material characteristics through synergistic effects.

In the presented study, we obtained interpolymer composites combining the relatively hydrophobic poly(lactic acid) and poly(caprolactone) with the more hydrophilic hydroxypropyl cellulose. A method for combining the two polymers into a single material suitable for 3D printing was developed. The hydrophilic-hydrophobic and mechanical properties of the obtained samples were studied.

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# SOFT CORE-SHELL NANOPARTICLES BASED ON POLY(LACTIC ACID) AND POLYELECTROLYTES

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Despite significant advances in the past, tuberculosis is still a dangerous and fairly frequent disease. The development of new therapeutic approaches for the treatment of tuberculosis represents an important challenge for modern medicinal chemistry. To win the fight against this disease, the development of not only novel antibiotics but also drug delivery systems capable of enhancing the efficacy of both known and prospective molecules is required<sup>1</sup>.

A promising option for the use of pharmaceutical compositions based on suspensions of micro- and nanoparticles for local treatment of pulmonary tuberculosis is the use of nebulizer. In this case, of interest are "core-shell" particles capable of co-encapsulating various drugs in the core and shell of particles, as well as adhere to lung tissues due to the selected composition of the "shell" <sup>2</sup>.

In this work, we have obtained nanoparticles based on poly(lactic acid) and formed a shell on their surface using biocompatible polyelectrolytes. Poly(lysine) and chitosan were used as polycations, and heparin and hyaluronic acid were used as polyanions. First, the polycation was covalently bound on the surface of the nanoparticles followed by oppositely charged polyanions layering. Further layer-by-layer addition of polyelectrolytes allowed us to control the shell thickness and stiffness of the particles. We studied the effect of charge and shell thickness on the biocompatibility of the particles. We also performed the first experiments on co-encapsulation of drugs of different nature, which showed that the obtained nanocompositions are able to retain both hydrophilic and hydrophobic molecules.

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# SOY LECITHIN LIPOSOMES FOR PROTEIN DELIVERY

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Liposomes are biocompatible, chemically inert and biodegradable delivery systems for a variety of biologically active substances. This delivery system allows to include both hydrophilic and hydrophobic compounds simultaneously, as well as control their release in human body environment. In addition, liposomes are able to penetrate the biological barriers of the body. Currently, the task of preserving the activity and integrity of proteins during their passage through the gastrointestinal tract after oral administration remains urgent. Therefore, the development of methods for obtaining chemically stable liposomes with a high level of protein inclusion is a promising task in pharmacological development.

The aim of this study was to obtain a liposomal delivery system from soy lecithin for green fluorescent protein, as well as to study the kinetics of its release and distribution in the body under in vivo conditions.

To obtain liposomes, the most protein-friendly method was chosen - the hydration/rehydration of a thin film method. Soy lecithin was dissolved in hexane, and the solvent was evaporated on a rotary evaporator to form a thin film on the walls of a round-bottomed flask. Then, green fluorescent protein (GFP) dissolved in 0.01M phosphate buffer (pH 7.4) was poured into the flask. The obtained liposomes were studied by confocal microscopy. The particle size was 1-3 microns. The obtained samples were injected intragastrically into mice and after 20, 60, 180 minutes, the distribution of GFP in the blood, stomach and intestines was evaluated by gel documentation.

It has been shown that this system is effective for protein delivery. The method allows to achieve effective inclusion of proteins of different molecular weights and with different sharpening. Soy lecithin liposomes effectively protect protein from destruction in the acidic environment of the stomach and can be used for oral delivery of proteins and peptides.

# DESIGN, CALCULATION AND MANUFACTURE OF PERSONALISED BIODEGRADABLE PRODUCTS USING ADDITIVE TECHNOLOGIES

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The paper presents modern approaches to the design, calculation and manufacturing of personalized biodegradable products using additive technologies from thermoplastics and elastomers. The process of creation of personalized products for traumatology and surgery based on the results of computed tomography of patients, the procedure of manufacturing with the use of additive technologies and subsequent mechanical tests are considered.

The problem of constructing models of viscoelastic behavior of porous materials manufactured using 3D printing is considered. Approaches based on solutions of integral equations of hereditary mechanics and approaches based on structural rheological models are used.

*The work was carried out within the state assignment of NRC “Kurchatov institute”.*

# IN VITRO AND IN VIVO TOXICITY ASSESMENT OF CURCUMIN-LOADED AMPHIPHILIC POLY (N-VINYLPYRROLIDONE) NANOPARTICLES

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Curcumin is a natural polyphenol obtaining antitumor activity. However, curcumin has low bioavailability that limits its effectiveness in cancer therapy. Encapsulation of curcumin in polymer nanoparticles will overcome this disadvantage.

Curcumin-loaded amphiphilic poly(N-vinylpyrrolidone) nanoparticles (PVP-Cur NPs) were prepared by an emulsification method. The core of the curcumin-loaded particles was formed by hydrophobic n-octadecyl polymer moieties.

Morphology	Average Hydrodynamic Diameter (nm ± SD)	ζ- Potential (mV ± SD)	Polydispersity index	Degree of curcumin encapsulation, %
Spherical	200 ± 10	-5,0 ± 0,9	0,1 ± 0,02	95

**Table 1.** Main properties of the PVP-Cur NPs

PVP-Cur NPs exhibited significant cytotoxic activity in vitro against human glioblastoma cell lines T98G and U87 compared with free curcumin. Also, the nanoparticles obtained low cytotoxicity for normal fibroblasts of the 3T3 line, and the results of an *in vivo* experiment on *Danio rerio* fish embryos showed low acute toxicity of PVP-Cur NPs for living organisms.

Thus, curcumin-loaded amphiphilic poly(N-vinylpyrrolidone) nanoparticles obtain antitumor activity without exhibiting a toxic effect for normal cells and living organisms.

*This work was financially supported by the Russian Science Foundation, grant No. 23-15-00468.*



# INFLUENCE OF THE CHEMICAL STRUCTURE OF END GROUPS ON THE PROPERTIES OF POLYPHENYLENE SULPHONE FOR ULTRAFILTRATION MEMBRANES

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Polyphenylene sulfone (PPSU) is a promising material for creating membranes for ultrafiltration, nanofiltration, gas separation, and fuel cells with excellent physical and chemical properties due to its high heat resistance, long-term thermal stability, high mechanical strength, and increased resistance to hydrolysis. However, the hydrophobicity and high susceptibility to contamination of PPSU limits its use in membrane technologies. To solve this problem, various modification methods are used, such as sulfonation, mixing with a more hydrophilic membrane-forming polymer, introducing nanoparticles into the molding solution, grafting hydrophilic functional groups such as carboxyl, epoxy and hydroxyl groups, introducing hydrophilic and oligomeric additives into the molding solution.

The work investigated the possibility of increasing the hydrophilicity of PPSU membranes by regulating the chemical structure of the end groups in the process of high-temperature polycondensation by varying the ratio of 4,4'-dihydroxydiphenyl and 4,4'-dichlorodiphenylsulfone monomers. The kinetics of the synthesis process of PPSU with different end groups was studied using the sampling method. The presence of end groups of a certain type was confirmed by NMR analysis.

Flat membranes were obtained based on the synthesized PPSU. The water permeability of the hydroxyl-terminated membrane is 66.1 l/m<sup>2</sup> h, which is 1.5 times higher than the permeability of the chlorine-terminated membrane. At the same time, both membranes demonstrate high separation characteristics: the retention coefficient for Blue Dextran (Mw = 70,000 g mol<sup>-1</sup>) is 99.9%.

*The work was carried out with the financial support of the Russian Science Foundation, project 22-19-00711.*

# DEVELOPMENT AND STUDY OF COMPOSITES CHITOSAN/CARBON NANOPARTICLES FOR PERSPECTIVE MEMBRANE MATERIALS

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In recent years, mixed matrix membranes (MMMs), which use a polymer as the membrane material and an inorganic and/or organic filler as the modifier, have become the most widely used membranes in most membrane processes. The selection of conditions for the combination of polymer matrix and modifier is the main task in the preparation of MMMs. Among the various fillers used to create MMMs, carbon nanoparticles play a separate and important role due to their unique chemical structure and physicochemical properties.

In the present work, novel mixed matrix membranes based on chitosan modified with different carbon nanoparticles (single-walled carbon nanotubes (SWCNTs), multi-walled carbon nanotubes (MWCNTs), fullerene ( $C_{60}$ ), fullerenol ( $C_{60}OH_{22-24}$ ), graphene oxide (GO) and etc.) were developed. Optimal conditions for the preparation of composites and membranes were selected (solution viscosity, solvent evaporation temperature, modifier concentration, dispersion methods, etc.). The structure, morphology and physicochemical properties of the developed composites and membranes were studied using various physicochemical analytical methods.

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# INFLUENCE OF REACTION CONDITIONS ON CATALYTIC PROPERTIES OF $rac\text{-Et(2-MeInd)}_2\text{ZrMe}_2/(2,6\text{-}^t\text{Bu}_2\text{PhO-})\text{Al}^i\text{Bu}_2$ IN ETHYLENE-PROPYLENE COPOLYMERIZATION

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Metallocene and post-metallocene catalysts are a new generation of catalysts used to produce ethylene-propylene (EPM) and ethylene-propylene-diene copolymers (EPDM) with specific compositions and properties. The thermal and physical-mechanical properties of these copolymers depend on the catalyst used, activation method, and copolymerization conditions.

Effective catalytic systems based on bis-indenyl metallocene complexes and isobutyl aluminum aryl oxides as co-catalysts instead of expensive polymethylalumoxane have been developed in the past <sup>1,2</sup>.

Here we present the results of the copolymerization of ethylene and propylene using the catalytic system  $rac\text{-Et(2-Me Ind)}_2\text{ZrMe}_2$  and  $(2,6\text{-}^t\text{Bu}_2\text{PhO-})\text{Al}^i\text{Bu}_2$  as cocatalyst, which showed the highest activating ability among all tested isobutyl aluminum aryl oxides. The copolymerization was carried out under different reaction conditions, and thermal and physico mechanical properties of resulting copolymers were studied.

The results showed that reducing the reaction pressure from 11 atm to 3 atm resulted in a 63% increase in specific activity, from 3030 to 4840 kg of copolymer/(mol Zr-h). This increase was accompanied by an increase in Mn value from 38 to 89 kg/mol, and an increase in ethylene content from 87 to 92 mol.%. However, increasing the ethylene/propylene molar ratio from 0.7 to 2 did not have a significant effect on activity, but led to increase of ethylene content in copolymers and crystallinity.

Changes in macromolecular chain composition determine the thermal and mechanical properties of copolymers, while changes in the Al/Zr molar ratio greatly influence catalytic activity. The lowest activity (80 kg copolymer/mol Zr hr atm) was observed at an Al/Zr ratio of 100, while the highest activity (8550 kg) was observed at Al/Zr a ratio of 150. It has been demonstrated that metallocene catalytic systems with aryloxyd isobutylaluminium activators are effective in aliphatic solvents such as heptane.

An increase in the resistance of polymer samples to thermal oxidative degradation in the presence of 2,6-ditert-butylphenol, formed from the activator during the decomposition of the catalytic system and washing copolymers, has been demonstrated. The presence of this compound leads to a decrease in tensile strength and an increase in elongation at break of the copolymers.

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# CYSTEINE PROTEASES STABILIZED WITH SULFANILAMIDE CHITOSAN AS NEW PROMISING ANTIBACTERIAL COMPOSITIONS

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Complexes of bromelain (EC 3.4.22.32), papain (EC 3.4.22.2), and ficin (EC 3.4.22.3) with 2-(4-acetamido-2-sulfanilamide) chitosan with molecular weights (MW) of 200, 350, and 600 kDa were obtained via adsorption immobilization in a borate buffer with a pH of 9.0. They were characterized by protein content determined using the Lowry method, as well as by the values of total and specific proteolytic activity in azocasein hydrolysis reactions. The amount of protein in the complexes was optimized using the Langmuir adsorption isotherm equation. The conformational state of enzymes in the complexes was assessed using FTIR and the molecular docking method. The study revealed that complexation increases the specific proteolytic activity of papain when interacting with modified chitosan with a MW of 350 kDa, while for other enzymes, its decrease is observed. At the same time, all the obtained complexes have antibacterial activity at concentrations that allow them to be considered promising antibacterial agents.

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# RELAXATION PHENOMENA IN A COMPOSITE FILM OBTAINED FROM POLYVINYL ALCOHOL AND SILVER NITRATE UNDER UV IRRADIATION

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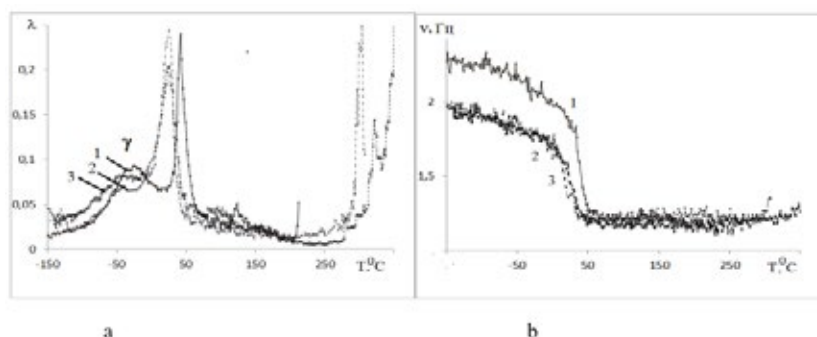
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Hybrid films were obtained from an aqueous solution of polyvinyl alcohol (PVA) and nitrate silver. Silver nanoparticles are formed in the PVS matrix as a result of UV irradiation. Initially, silver ions are coordinated with polymer OH groups to form a chelate structure.

Relaxation processes in such systems were described by analyzing the spectra of internal friction (Fig.1a) and changing the frequency of the damped oscillatory process under external deforming action over a wide temperature range (Fig.1b). It was found that in the chelated system, the relaxation transition, designated as the  $\gamma$ -peak and responsible for the mobility of OH groups, becomes smaller in magnitude. It is OH groups that are associated with silver ions.

Considering the temperature-frequency dependences, we can conclude that there is a significant decrease in the shear modulus (proportional to the square of the frequency  $\nu$ ). Such a decrease in modulus is associated with the change and destruction of hydrogen bonds between the PVA chains, the formation of Ag nanoparticles.

In the temperature range above 200°C, a site of highly elastic thermal stability for a composite material is found.



**Fig.1.** Temperature dependences of the logarithmic decrement  $\lambda$  (a) and the frequency ( $\nu$ ) of freely damped oscillations. 1- pure PVA, 2- PVA+AgNO<sub>3</sub>, chelated form, 3-PVA with silver nanoparticles.

*(The work was completed within the framework of the State assignment).*

# SUPRAMOLECULAR SYSTEMS BASED ON PILLAR[5] ARENES: SYNTHESIS OF MONO- AND DECA-SUBSTITUTED PILLAR[5]ARENE DERIVATIVES CONTAINING AMIDE GROUPS AND THEIR SELF-ASSEMBLY WITH POLYVINITETRAZOLE-CONTAINING COMPOUNDS

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Today, one of the actively studied types of macrocyclic compounds are pillar[n]arenes [1]. Since the discovery [2] of the first representative of this class of macrocycles, pillar[n]arenes have shown their effectiveness in molecular recognition of various substrates, as ion channels, in catalysis, and also as drug carriers [1–3].

In the presented work, approaches to the preparation of the new mono- and decasubstituted pillar[5]arene derivatives containing amide groups (2-hydroxyethylamide or 3-hydroxypropylamide fragments) have been developed. It was shown that pillar[5]arene containing ten 2-hydroxyethylamide fragments forms monodisperse nanosized aggregates with an average hydrodynamic diameter of 117 nm in an aqueous solution in the presence of polyvinyltetrazole. Decasubstituted pillar[5]arenes containing tosylate and phthalimide groups were obtained by direct macrocyclization of the corresponding 1,4-disubstituted benzenes with formaldehyde. Using tosylate and phthalimide protections, pillar[5]arenes containing primary and tertiary amino groups capable of reacting with tetrazole-containing polymers were obtained in high yields. The boundary conditions for the formation and destruction of associates of the three-component system pillar[5]arene/fluorescein/polymer were studied.

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# POLYANILINE-BASED NONWOVEN CONDUCTIVE MATERIALS FOR USE IN ORGANIC ELECTRONICS

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Nowadays, electrically conductive polymeric materials have been applied in organic electronics, being a promising substitute for metal conductors. Such materials are characterized by simplicity and cheapness of production, possibility to regulate electrical conductivity, low density and non-toxicity. One of the methods of their production is the application of a layer of conductive polymer on the surface of fibers of nonwoven matrixes obtained by electrospinning.

In this work, nonwoven hybrid electrically conductive polymeric materials were obtained, using nonwoven materials of polyamide-6, polyacrylonitrile, polypropylene, polylactide, polystyrene, and polyvinylidene fluoride with an average fiber diameter of 0.2-12  $\mu\text{m}$  as a base, and polyaniline (PANI) was used as a conductive component. The morphology of the fibers before and after synthesis of PANI was studied by scanning electron microscopy, and the composition and supramolecular structure was studied by IR spectroscopy and WAXD methods. As a result, hybrid materials characterized by specific conductivity values up to  $6 \cdot 10^{-2}$  S/cm were obtained.

It was found that the main factor determining the conductivity of the resulting sample is the wettability of the initial matrix. Fibers, well wetted with water, allow polymerization in the entire volume of nonwoven material, which leads to composites with high conductivity, weakly dependent on the thickness of the matrix. On materials that are not wetted by water, polymerization occurs only on the surface, so the conductivity of such composites is lower and depends on the thickness of the matrix. The obtained materials were used to create an organic memristive element and an electrode of a biofuel cell.

*The work was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation (Agreement 075-15-2023-324) using the equipment of resource centers of NRC "Kurchatov Institute".*

# SELF-ASSEMBLY OF AMPHIPHILIC BIOCOMPATIBLE ETHYLENE OXIDE AND CAPROLACTONE BLOCK COPOLYMERS AT THE AIR/WATER INTERFACE

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The process of the structure formation in Langmuir films at the air/water interface was studied on the series of di and triblock copolymers of ethylene oxide and  $\epsilon$ -caprolactone. It was found that under compression of Langmuir layers of block copolymers, a plateau is observed on the surface pressure isotherms, which correlates with the phase transition of the layer due to crystallization of polycaprolactone blocks. It is shown that, with an increase in the temperature of the subphase, along with the solid crystalline phase, domains of the liquid-condensed phase are formed, which leads to a change in the shape of the surface pressure isotherms of the copolymers. The occurrence of two-dimensional crystallization under compression of Langmuir layers of block copolymers of ethylene oxide and  $\epsilon$ -caprolactone was confirmed by the data of Brewster microscopy and X-ray diffraction in a grazing angle of incidence (using the synchrotron radiation source KISI-Kurchatov). The GIWAXS patterns recorded on air-water interface for triblock copolymers of ethylene oxide and  $\epsilon$ -caprolactone compressed monolayers show 110 and 200 reflections of polycaprolactone lattice. Moreover, the maximum intensity of these reflections is shifted to higher QZ values indicating an inclination angle of crystal lattice to the surface. The measured angles were 15° and 24°, correspondingly. This complies to 001, 110 and 1-10 lattice direction lying on water level.

*The work was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation (Agreement 075-15-2023-324) using the equipment of resource centers of NRC "Kurchatov Institute".*

# NITRATE-SELECTIVE METAL-POLYMER MEMBRANES BASED ON CARDO POLY(BENZIMIDAZOLE)

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Agricultural activities can result in an increase in nitrate-ion content in wastewater, leading to its accumulation in groundwater<sup>1</sup>. Elevated nitrate levels in drinking water can be extremely harmful to human health<sup>2</sup>. Electrodialysis has been found to be an effective method for removing nitrates from wastewater<sup>3</sup>. However, current anion-exchange membranes are more selective towards the transport of multi-charged ions. One solution to this issue is to use homogeneous ion-exchange membranes that have size-limited ion-channels, such as metal polymer membranes<sup>4</sup>.

A series of new metal-polymer anion-exchange membranes with different molar ratios of metal/benzimidazole rings have been prepared based on cardo poly(benzimidazole). The addition of metal ions has been shown to lead to crosslinking of polymer molecules, which is most pronounced in the case of copper ions. The addition of metal ions can confer anion-conducting properties to the original polymer. Increasing the molar ratio of metal/benzimidazole ring results in higher conductivity and lower nitrate-ion transport numbers for membranes containing copper and chromium ions. The membrane composed of Cu:benzimidazole ring in a 1:2 ratio has demonstrated exceptional selectivity coefficients in chloride-sulfate pair - 370 and nitrate-sulfate pair - 2600, surpassing previously published values.

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# ISSUES OF THERMOGRAVIMETRIC ANALYSIS IN STUDIES OF POLYMERS AND COMPOSITES

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Thermogravimetric analysis (TGA) of non-isothermal kinetics of chemical reactions is widely used in the study of polymers and polymeric materials. Despite the high accuracy of modern measurements, the accuracy of determining the activation energy from TGA data remains low; the results can differ several times. The reason for the ambiguity of the TGA results is considered to be the insufficient accuracy of estimates of the Doyle temperature integral. The second reason is that several parallel thermal degradation processes can occur in polymers, which cannot be described by a simple model with one reaction.

Recent works<sup>1</sup> have proposed series for calculating the temperature integral with high accuracy (relative error within  $10^{-8}$ ). However, the need for massive calculations hinders the use of series for working with experimental data.

In this work, it is proposed to use the expression of the temperature integral through the exponential integrals  $E_1(x)$  and  $E_2(x)$ . From this expression, three simple approximations of the integral are obtained: the first with a relative error of less than  $5 \cdot 10^{-3}$ , the second with an error of less than  $5 \cdot 10^{-5}$ , and the third approximation with an error of less than  $5 \cdot 10^{-8}$ .

The obtained approximations can be used to deconvolute TG curves and determine the parameters of parallel reactions in polymer mixtures. The possibilities of high-precision deconvolution are demonstrated on the example of the Ozawa model of two parallel reactions with different activation energies. Conventional TGA methods in this case give wrong reaction parameters, while deconvolution reveals not only the true parameters, but also the fraction of each reaction.

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# ENCAPSULATION OF THERAPEUTIC COPPER COORDINATION COMPOUND IN POLYMER MATRICES FOR MELANOMA TREATMENT

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Melanoma, the most aggressive type of skin cancer, incidence has increased significantly recently. The rapid spread of tumor cells in the dermis and the increased risk of metastasis, especially in the case of the late disease diagnosis, cause a high mortality rate among patients. In addition, disruption of the immune system in patients is often accompanied by the development of concomitant severe bacterial infections. Therefore, the development of drugs for combined therapy and their targeted transdermal delivery is an important goal.

In this work, we used a new drug, a copper coordination compound based on 2-alkylthioimidazolone ( $\text{Cu}_2\text{Im}$ ), which possess a toxic effect due to the generation of reactive oxygen species and demonstrates anticancer activity and antibacterial properties simultaneously.  $\text{Cu}_2\text{Im}$  was encapsulated in polymer matrices of polylactide (PLA), polycaprolactone (PCL), their blends (PCL/PLA), and blends of PCL and PLA with gelatin (PCL/gelatin and PLA/gelatin). Polymer nanofibers were formed from a suspension of polymers and drug by electrospinning process. According to SEM images, the matrices represent meshes of nanofibers with a thickness not exceeding 500 nm, and EDX confirmed a uniform distribution of copper in the matrix. However, in PCL/PLA systems the formation of 'beads' was observed, which is due to the decrease in polymers solubility. The results of AES and chromatography after 24 hours of  $\text{Cu}_2\text{Im}$  release indicate a higher rate and level of Cu release for PCL-based matrices and polymer blends with gelatin, compared to those for PLA matrices. The ratio of  $\text{Cu}_2\text{Im}$  to total Cu released is also higher in the case of PCL.

The cytotoxicity test of the matrices was conducted on murine melanoma cell line B16. A significant cytotoxic effect was observed in all the samples, presumably differing in mechanism of action in the case of PCL and PLA matrices: toxicity of copper ions in PLA matrices and of the  $\text{Cu}_2\text{Im}$  drug itself in PCL matrices.

Thus, the electrospinning gives an opportunity to produce  $\text{Cu}_2\text{Im}$ -loaded polymer matrices, which exhibit toxic effect and are promising solid carriers for targeted transdermal drug therapy of melanoma.

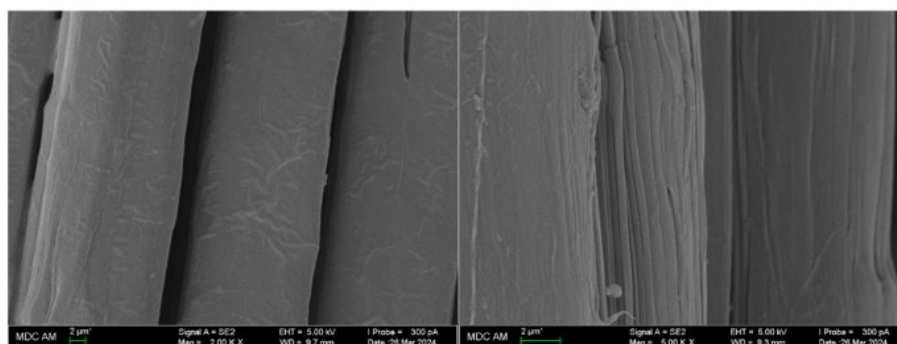
# PLASMA AND CHEMICAL METHODS FOR MODIFYING UHMWPE FIBERS

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One of the most promising polymers in terms of specific strength characteristics is ultra-high molecular weight polyethylene (UHMWPE). The main disadvantage of UHMWPE is its low adhesion to impregnating materials, which does not allow its use as a filler for composite materials.

There are two main directions of methods for modifying the surface of UHMWPE - chemical and plasma. The chemical effect is aimed at etching the UHMWPE surface, coating it with a "binder" film and attaching special functional groups. Plasma exposure is focused on etching the surface or attaching functional groups. Figure 1 shows micrographs of the UHMWPE surface after chemical (a) and plasma exposure. After chemical exposure, a "binding" film is formed, which is responsible for increasing wettability. After plasma exposure, namely a low-pressure high-frequency capacitive (HF) discharge, the film formed after chemical exposure is removed, revealing the fibrillar structure of the fibers. This makes it possible to increase the wettability of the fibers and the contact area between the matrix and the filler (UHMWPE) in the composite material. At the same time, the strength characteristics of the fibers do not deteriorate.



**Figure 1.** A – Chemically treated fiber, B – plasma treated fiber.

Thus, the method of low-pressure HF discharge plasma treatment can be used to significantly increase the wettability of UHMWPE fibers.

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# STRUCTURE AND PROPERTIES OF REDOX-ACTIVE NANOGELS FOR REDOX FLOW BATTERY APPLICATIONS

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Flow batteries are considered one of the promising solutions for stationary energy storage. However, the use of small-molecule electroactive compounds in these systems necessitates expensive ion-exchange membranes to prevent crossover. One approach to reduce these requirements is the use of polymer reagents with "grafted" redox active groups.<sup>1</sup>

For this purpose, weakly crosslinked polymer nanogels based on poly-N-isopropylacrylamide (PNIPA) modified with 4-(3-carboxypropanamido)-TEMPO redox-active groups were prepared and characterized for the first time in this work.

Through cyclic voltammetry, it was discovered that only about half of the nanogel's redox-active groups participate in the electrochemical reactions. We also revealed the effect of nanogel adsorption on the electrode surface.<sup>2</sup>

Using computer simulations of the electron paramagnetic resonance spectra of the nanogels, their structure and mobility of the grafted paramagnetic redox centers were studied.

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# FUNCTIONALIZATION OF PVC WITH LAWSONE RESIDUES AS O-NUCLEOPHILES BY MEANS OF MECHANOSYNTHESIS

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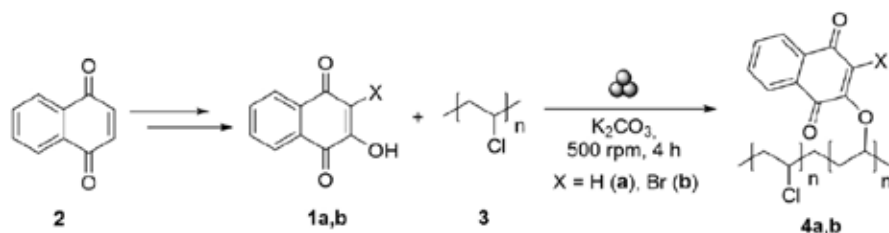
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The accumulation of PVC waste in the environment is a pressing environmental problem. One of the ways to solve this is the processing of PVC, including through chemical modification by using nucleophilic substitution reactions in solutions.<sup>1</sup> At the same time, mechanosynthesis is an illustrative example of the so-called “green methods”, because allows chemical transformations to be carried out without the use of solvents, toxic catalysts, etc., thereby being low-waste and environmentally friendly.<sup>2</sup> The purpose of this work is to test the method of post-modification of PVC by introducing residues of some *O*-nucleophiles by a mechanochemical method.

As such, commercially available lawsones **1a** and its bromo derivative **1b**, obtained from naphthoquinone **2** according to the described procedure,<sup>3</sup> was studied. The further interaction of **1a,b** with PVC **3** under ball-milling in solvent-free conditions led to the formation of polymers **4a,b** (Scheme 1).



Scheme 1

The structure of **4a,b** was confirmed by <sup>1</sup>H NMR and IR-spectroscopy, as well as elemental analysis. In particular, the degree of introduction of lawsones **1a,b** into PVC was calculated to be up to 10%.

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# THERMAL INSULATION MATERIAL USING RECYCLED POLYETHYLENE TEREPHTHALATE

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Recycling of polymer materials is one of the most modern and popular methods of waste recycling. Polyethylene terephthalate (PET) is the fifth largest segment of the polymer market. In 2022, global PET production amounted to 7848 thousand tons <sup>1</sup>. One of the most large-scale methods for recycling PET is physical processing into granules followed by molding of products. However, this method places high demands on the feedstock.

The paper presents a method for producing polyurethane foams for thermal insulation using recycled PET. Glycolysis of PET was carried out with an excess of diethylene glycol for the most complete depolymerization of PET while maintaining the low viscosity of the intermediate product (no more than 500 mPa\*s) <sup>2</sup>. The next step is the synthesis of the polyester by esterification of the resulting intermediate with phthalic anhydride until a hydroxyl number of no more than 300 mg KOH/g is achieved.

Based on the synthesized polyester, polyurethane foams for thermal insulation by spraying were obtained. The physical and mechanical properties of the resulting foams were studied. Comparative tests were carried out with foams obtained from traditional polyesters, based on diethylene glycol and phthalic anhydride.

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# NEW NON-FULLERENE ACCEPTOR MATERIALS FOR ORGANIC SOLAR CELLS

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The development of organic photovoltaics and, in particular, organic solar cells (OSCs) as a means of obtaining clean and renewable energy is of great interest worldwide. The power conversion efficiency (PCE) of OSCs has exceeded 19% for devices based on fused nonfullerene acceptor materials (NFAs), which are complex polyaromatic compounds of donor-acceptor type. The efficiency has also exceeded 17% for simple NFAs of non-fused structure with bulk side substituents in the donor-acceptor structure. Despite the aforementioned successes, the most significant challenge to the commercialization of OSCs based on fused NFAs is the labor-intensive and multistep nature of their synthesis, which renders these materials prohibitively expensive. In contrast, the issues of stability, complementarity of donor materials for them and a number of fundamental questions affecting the structure-property-performance relationships of the device remain unresolved for the realization of non-fused NFAs. Consequently, research in this field is both important and relevant.

In this work, new potential NFAs were designed and synthesized. The structures and purity of the compounds were validated through a complex of physicochemical methods of analysis. The compounds exhibited efficient absorption of sunlight in the red and near-infrared ranges, both in solutions and in thin films. They also demonstrated suitable HOMO and LUMO level energies for use as acceptor materials and exhibited sufficiently high thermal stability suitable for device operating temperatures. The test results of NFAs in blends with commercially available donor material PM6 and acceptor material Y6 demonstrated efficiencies of more than 18% in prototype ternary OSCs, which is comparable to the record values in this field.

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# PHYSICOCHEMISTRY OF ALGAL NANOCELLULOSE HYDROGEL FORMATION

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Cellulose is one of the most demanded and widespread biopolymers around the world. Due to its easy processability, biocompatibility, biodegradability, and non-toxicity, cellulose-based materials find applications in various fields, including technical (electronics, optics, etc.) and biomedical (regenerative medicine). There is currently a growing demand for alternative sources of cellulose, including seaweed biomass.

This study presents a scheme for the production of nanocrystalline cellulose (NCC) using waste generated during the industrial processing of brown algae.<sup>1</sup> The resulting nanocellulose exhibits a needle-like morphology with average dimensions of  $394 \pm 182$  nm and  $33 \pm 6$  nm (length and width, respectively). It possesses a degree of crystallinity of 69%, a specific surface area of  $7.1 \text{ m}^2/\text{g}$ , and a proportion of I $\alpha$  cellulose of 97%.

One of the key and priority properties of nanocellulose is its ability to form stable hydrogels. The interactions in the NCC-water system were studied using IR spectroscopy, relaxometry, and calorimetry. It was observed that the thermal effect was exothermic, with the release of  $29.2 \text{ J/g a.s.c}$  ( $167.9 \text{ J/mol}$ ) energy. The nuclear magnetic relaxometry results showed that algal nanocellulose has a high content of free water, which is likely due to its developed mesoporous surface and small particle size. The formation of the NCC hydrogel with a dry matter content of 2.6% appears to be influenced by the structural organization of metastable I $\alpha$  cellulose and the capillary-porous macrostructure. It is worth noting that this hydrogel has been observed to remain stable for a period of 6 months.

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# INFLUENCE OF BULK AND SURFACE MODIFICATIONS ON PROPERTIES OF NONPOROUS POLYMERIC MEMBRANES FROM BIOPOLYMERS

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Membrane processes are promising methods for the separation of liquid mixtures containing components of different molecular weights. Each separation task requires a specific membrane process, membrane type (non-porous, porous) and membrane material. However, highly efficient separation requires new/advanced membrane materials with desired and improved properties. The improvement of the properties of porous and nonporous membranes can be achieved as by modifying the polymer matrix with an inorganic and/or organic filler (creation of mixed-matrix membranes) as by membrane surface modification.

In the present work novel mixed matrix nonporous membranes based on well-known biopolymers (chitosan and carboxymethyl cellulose) were developed. To improve transport and physicochemical characteristics the bulk modification (by introduction of graphene oxide) and surface modification (by polyelectrolyte layer-by-layer assembly) were carried out. The developed membranes were studied by scanning electron microscopy, atomic force microscopy, Fourier-transform infrared spectroscopy, nuclear magnetic resonance, thermogravimetric analysis, contact angle measurement and swelling experiments. Transport properties of the membranes were evaluated in pervaporation dehydration. It was found that applied modifications significantly changes both the physicochemical and transport properties of the developed nonporous membranes.

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# 3D-SPATIAL CROSSLINKED ORGANOSILICON POLYMERS BASED ON THE REACTION OF SULFENYL CHLORIDE 2,4-PENTANEDIONATES OF CHROMIUM(III) AND ALUMINUM WITH VINYLSILOXANES

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The reaction of sulfenyl chlorides of acetylacetonates of chromium(III)<sup>1</sup> and aluminum with polyvinylsiloxane (polymers I and II) and dimethyldichlorosilane copolymer with vinyltrichlorosilane (polymers III and IV) produced 3D-spatial crosslinked polymetallorganylsiloxanes.

Based on the XRD data, the volumes of coherent scattering were determined and the fractal structure of the isolated polymers was shown. The volumes of fractals increase from I, III to II, IV, which is explained by the introduction of dimethylsiloxy groups into polymers II and IV. In the initial aluminum sulfenyl chloride complex, the value of CSR is lower due to a greater number of violations.

The positron annihilation spectroscopy method made it possible to calculate the elementary volumes of positronium traps and the number of positronium annihilations in 1 cm<sup>3</sup>. It was shown that the number of traps in a fractal corresponds to the number of oxygen atoms in the fractal. According to the results of the calculated values of the annihilation centers, it was noted that the molecular volume of the elementary link turns out to be greater than the volume of CSR due to the fact that the number of bonds formed in the fractal is sufficient for the formation of gel<sup>2</sup>.

According to thermogravimetric research, thermal lability for aluminum complexes turns out to be more characteristic than for similar chromium(III) compounds. However, the complexity of the structure leads to an increase in thermal stability, apparently associated with the formation of a spatial grid.

The morphology of the isolated metallochelate polymers, studied with the help of SEM, has the form inherent in typical xero-gels formed due to the syneresis process during a chemical reaction.

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# DEVELOPMENT OF THERMOSENSITIVE DRUG DELIVERY SYSTEM BASED ON CHITOSAN/ $\beta$ -GLYCEROPHOSPHATE COMPOSITION

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Chitosan (Cht) is a promising polymer for creation of thermosensitive in situ delivery systems. However, in order to impart thermoreversible properties to the solution it is necessary to introduce  $\beta$ -glycerophosphate ( $\beta$ -GP), a cross-linking agent that stabilises the chitosan hydrogel and imparts thermosensitive properties to the composition.<sup>1-4</sup>

The aim of the present study was to create an optimal composition of in situ hydrogel of Xt/-GP with the possibility of parenteral administration and ability to thermoreversible transition at physiological temperature (37-38 °C), as well as to study the dependence of the gelation rate of the obtained solution on the percentage ratio of Xt: $\beta$ -GP in the composition.

Samples of aqueous solutions with concentrations of chitosan (70-80 kDa) from 0.5% to 2.0% in 1.0% lactic acid and sodium  $\beta$ -glycerophosphate pentahydrate in purified water from 2.0% to 4.0% were obtained for the study.

The obtained samples are evaluated in terms of solution pH, solution-gel (sol-gel) transition temperature, dynamic viscosity at temperature change from 10 °C to 50 °C, stability of the obtained hydrogels and cytotoxicity by HET-CAM test.

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# SYNTHESIS OF A COMPOSITE MEMBRANE BASED ON ELECTROACTIVE $\beta$ -PHASE POLYVINYLIDENE FLUORIDE WITH THE ADDITION OF BIFE03 NANOPARTICLES

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Membrane materials effectively address the problem of water pollution by dyes due to their advantages such as reduced area, easy management, cleanliness, and high permeability<sup>1</sup>. Composite materials based on polymers, used in the form of films, have non-toxicity, biocompatibility, and chemical inertness, providing significant benefits. The semi-crystalline ferroelectric PVDF is widely used due to its unique combination of properties such as chemical and thermal inertness, high piezoelectric response, and electrochemical stability<sup>2</sup>. The use of hybrid composites with organic ferroelectrics as a matrix substrate for doped nanoparticles can help combat water pollution by dyes<sup>3</sup>.

In the conducted study, composites based on PVDF were synthesized using the thermally induced phase inversion from a non-solvent method with the Dr. Blade technology (TIPS-NIPS)<sup>4</sup>, with multiferic type BiFeO<sub>3</sub> nanoparticles of different mass loading used as fillers. The catalytic activity of the obtained composite was investigated, and the influence of the dopant addition on the growth of the electroactive phase was evaluated.

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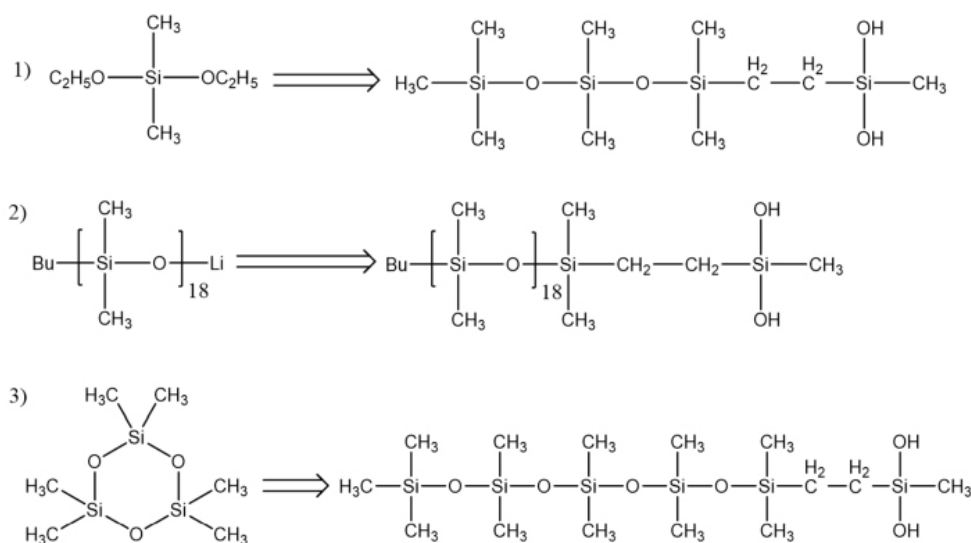
# SYNTHESIS OF SILOXANE MACROMONOMERS FOR THE INTERPHASE POLYCONDENSATION REACTION

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As it is known, the polycondensation process is one of the most common methods of polymer synthesis<sup>1</sup>. Nowadays, the process of interfacial polycondensation is attracting more and more attention of scientists being a new promising approach of organic synthesis. Interfacial polycondensation can be considered as one of the ways to synthesize siloxane molecular brushes by the "grafting through" method. Polycondensation has been previously used to synthesize siloxane molecular brushes. The resulting compounds, however, were closer to star-shaped structures due to the low molecular weight of the main chains. In this article we present the synthesis of new siloxane macromonomers and the synthesis of purely siloxane molecular brushes that will be obtained by interfacial polycondensation method.



**Figure 1.** Main types of siloxane macromonomers

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# BIOSENSOR COATINGS BASED ON POLY(N,N-DIMETHYLAMINOETHYL METACRYLATE) AND GLUCOSE OXIDASE: FORMATION AND APPLICATION FOR GLUCOSE ANALYSIS

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Poly(N,N-dimethylaminoethyl methacrylate) (PDMAEMA) is a pH- and thermosensitive polymer, whose hydrophilic-hydrophobic balance can be changed by varying the conditions of the surrounding medium (pH and temperature). Due to this feature, PDMAEMA easily adapts to surfaces of different nature and can form on them functional coatings (films). In particular, the presence of tertiary amino groups in PDMAEMA imparts to these coatings the ability of binding (electrostatic immobilization) considerable amounts of biomolecules, including enzymes.

In this work, the formation and properties of the polymer-enzyme coatings based on PDMAEMA and glucose oxidase were examined by means of quartz crystal microbalance with dissipation monitoring and atomic force microscopy. At pH 10, PDMAEMA was found to form almost continuous and stable films on the conductive surfaces (gold, graphite). At pH 7, the films were shown to gain positive charge, which makes binding of considerable amounts of glucose oxidase (pI 4.3) possible.

To construct electrochemical enzymatic biosensors for glucose analysis, the surface of screen-printed electrodes was subsequently modified by a peroxide-sensitive mediator (manganese dioxide nanoparticles), PDMAEMA (adsorption at pH 10, 25 °C or 40 °C) and glucose oxidase (adsorption at pH 7, 25 °C). By means of amperometry, the assembled biosensors were demonstrated to exhibit good analytical characteristics, such as the high sensitivity (25 °C:  $4 \cdot 10^{-2} \text{ A} \cdot \text{M}^{-1} \cdot \text{cm}^{-2}$ , 40 °C:  $7 \cdot 10^{-2} \text{ A} \cdot \text{M}^{-1} \cdot \text{cm}^{-2}$ ), the low limit of detection (25 °C: 0.2  $\mu\text{M}$ , 40 °C: 0.1  $\mu\text{M}$ ), the wide linear range (0.1  $\mu\text{M}$  – 0.3 mM), and the high operational stability (-0.1 %).

*The experimental results (Quartz Crystal Microbalance with Dissipation Monitoring and Atomic Force Microscopy) were obtained with the use of the equipment purchased within the M.V. Lomonosov Moscow State University Program of Development.*

# SYNTHESIS AND INVESTIGATION OF PROPERTIES OF A NEW CLASS OF AMPHIPHILIC CARBOSILANE JANUS-DENDRIMERS USING NATURAL COMPOUNDS

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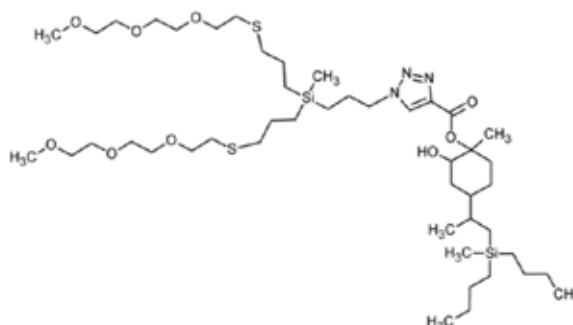
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Janus dendrimers are molecules obtained by coupling two dendrons of different sizes or possessing different chemical properties.

The aim of the work is to obtain a library of amphiphilic carbosilane dendrimers and study the process of their self-organization.

A natural terpene, limonene, was chosen as a base substance for the preparation of Janus dendrimers. In work<sup>1</sup> the possibility of selective hydrosilylation reaction of limonene was shown. In work<sup>2</sup> the possibility of further functionalization of limonene monodendrons by introduction of various functional groups was shown.

This work presents a method for the synthesis of Janus-dendrimers via azide-alkyne cycloaddition reaction.



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# STUDY OF ALCOHOLYSIS OF POLYCARBONATE AND SYNTHESIS OF POLYURETHANE COATINGS BASED ON THE DEGRADATION PRODUCT

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Increasing the production of polycarbonate (PC) results in the accumulation of production and consumption waste. To recycle these wastes, chemical degradation by alcoholysis is an effective method that replenishes the raw material base of hydroxyl-containing compounds.

The purpose of this work is to study the kinetics of the PC alcoholysis process under the action of diethylene glycol (DEG) and the possibility of using the degradation product in the synthesis of PU coatings. The ratio of [unit of PC] to [DEG] is 1:2. The alcoholysis process was monitored by dynamic viscosity from the moment of system homogenization. It was observed that the chemical degradation of PC occurs sequentially through several stages. Initially, a short plateau with a relatively high viscosity value is observed, which is likely associated with the formation of oligomeric products. These products are then rapidly degraded into smaller fragments with lower viscosity. During the second stage, the system reaches an equilibrium state, and the resulting product of alcoholysis is primarily a mixture of bisphenol A and bis[2-(2-hydroxyethoxy)ethyl] carbonate, as confirmed by IR spectroscopy and GC-MS. In the third stage, the decrease in viscosity is attributed to the thermal degradation of the alcoholysis products from the second stage, resulting in the formation of phenol, isopropenylphenol, and DEG.

The degradation product [unit of PC]/[DEG] = 1:2 was tested in the synthesis of PU waterproofing coatings. Tests revealed that the composition, which included above-mentioned product, an isocyanate component, and target additives, lost flowability quickly due to the high content of OH-groups in the destructate. To address this issue, alcoholysis of PC was carried out using polytetrahydrofuran with a molecular weight of 650 (PolyTHF650). The product [unit of PC]/[PolyTHF650] = 1:2 was used to obtain a PU composition with a high viability. The resulting coating based on this composition had superior physical and mechanical parameters compared to the industrial analog, which included PolyTHF650.

*The work was financially supported by a grant in the form of subsidies from the academic leadership program 'Priority 2030'.*

# HETEROCENE CATALYSIS IN THE COPOLYMERISATION OF POLAR VINYL MONOMERS

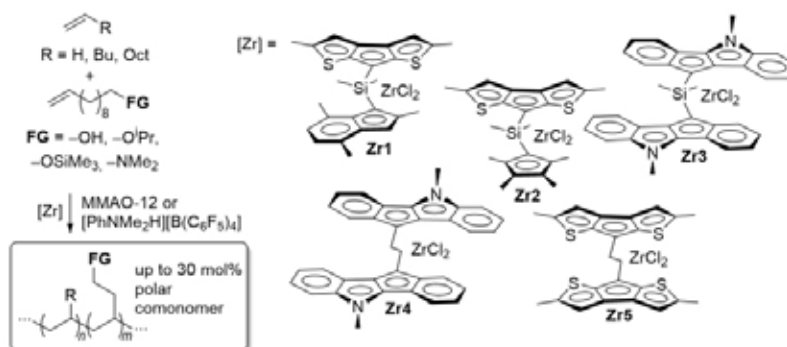
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Polyolefins are the most widely used synthetic polymers (more than 60% of the world plastics market, annual production of more than 200 Mt). Copolymerisation of  $\alpha$ -olefins with  $\omega$ -alkenyl alcohols, esters, carboxylic acid derivatives allows to introduce polar groups into the structure of polyolefins. The source of polar vinyl monomers can be renewable vegetable raw materials. The search for efficient catalytic solutions for the copolymerisation of  $\alpha$ -olefins with polar monomers is an urgent and non-trivial scientific problem. We have succeeded in solving this problem using heterocene catalysts (Fig. 1).



**Figure 1.** Preparation of polyolefins with polar functional groups.

The obtained copolymers of ethylene, hexene-1 and decene-1 with polar monomers were characterised by NMR spectroscopy (microstructure) and GPC (molecular weight characteristics). The rheological and adhesion properties of copolymers of  $\alpha$ -olefins with polar comonomers  $CH_2=CH(CH_2)_8-FG$  were studied for the first time.

# INFLUENCE OF $\text{TiO}_2$ NANOPARTICLES ON THE PROPERTIES OF POLYSACCHARIDE-BASED FILM MATERIALS

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Single-use polymer packaging contributes significantly to the environmental deterioration worldwide. One of the possible ways to reduce the burden on the environment is to create biodegradable packaging materials based on natural polysaccharides - starch (ST) and chitosan (CTS), which are extracted from renewable sources of raw materials, are biocompatible and biodegradable. However, polysaccharides' application is constrained by their low physical-mechanical characteristics. One of the promising ways to improve the tensile strength of ST and CTS is their modification with  $\text{TiO}_2$  nanoparticles (NPs).

In this work, transparent film materials based on CTS and ST modified with  $\text{TiO}_2$  NPs were obtained, their physical-mechanical, antibacterial, barrier properties and biodegradation ability were studied. The modification of ST was carried out by graft polymerization with acrylamide (AA), and CTS - with enanthine aldehyde. The conditions for combining the modified CTS with ST in aqueous acid solutions were worked out.  $\text{TiO}_2$  NPs with average sizes ranging from 20 to 920 nm were prepared from  $\text{Ti}(\text{OPr})_4$  by sol-gel technology.  $\text{TiO}_2$  with concentrations from 0.5 to 10 wt.% was introduced into the polysaccharide films. It was found that the  $\text{TiO}_2$  NPs presence in the CTS films significantly increased its tensile strength, reaching 122.4 MPa at 11.7 % strain at  $\text{TiO}_2$  concentrations up to 3 wt.% versus 24 MPa and

3.4 % for the initial CTS. Moreover, a similar tendency was found for films based on blends of modified CTS with copolymer ST:AA containing glycerol as a plasticizer - their strength reached 30 MPa at 12 % strain, which exceeds the corresponding values of films based on modified ST presented in the literature - 15 MPa, and synthetic packaging materials - 22 MPa. The films are biodegradable and degrade 50 wt.% within 28 days under the action of the fungus *Aspergillus Niger*. Antibacterial activity of the materials against *Staphylococcus Aureus* and *Escherichia Coli* was revealed. The barrier properties of the obtained films exceed those of synthetic films used in packaging.

*The work was financially supported by the Russian Science Foundation, project No. 23-13-00342.*

# POLYMER COMPOSITE MATERIALS BASED ON POLYPHENYLENE SULFIDE: PROPERTIES AND APPLICATION EXPERIENCE IN SPECIAL EQUIPMENT EXPLOITED UNDER EXTREME CONDITIONS

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The physico-mechanical properties of the Russian materials based on polyphenylene sulfide<sup>1</sup> were studied in comparison with the previously used materials. The applicability of materials for production of small-sized critical parts having complicated geometrical shape and integrated into electronic-mechanical devices of special equipment exploited under extreme conditions<sup>2-4</sup> including chemical aggressive media and high dynamic load (figure 1) was tested under the industrial conditions.

The materials based on polyphenylene sulfide were shown to have advantages for the development of efficient manufacturing processes of high-tech products possessing the improved performance properties.



**Figure 1.** a – The appearance of small-sized parts; b – comparison of imperfection degree of the part made of pressing moulding material AG-4V (1) and injection moulding material TERMORAN PPS GF-40 (2) using the color capillary defectoscopy method; c – the appearance of the power source for electronic-mechanical devices.

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# STUDY OF THE REACTION OF HYDROLYTIC POLYCONDENSATION OF MONOSODIUM OXYMETHYL(DIETOXY)SILANE

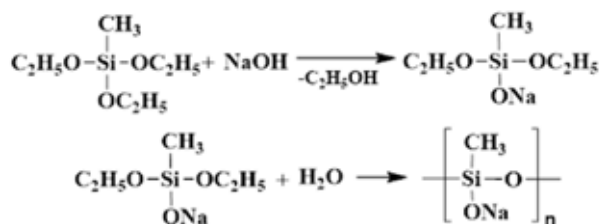
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Molecular brushes are unique polymer systems due to their specific structure, referring to macromolecules-particles<sup>1</sup>. Despite a huge number of publications, rather little information on the synthesis of purely siloxane molecular brushes can be found in literature. This is primarily due to the specific behavior of the siloxane bond to many approaches used in the synthesis of molecular brushes of organic nature. According to the literature analysis<sup>2</sup>, the "grafting-to" method can be considered as the most suitable method for the synthesis of purely siloxane molecular brushes.

In this work we present the synthesis of siloxane polyfunctional polymer matrix by hydrolytic polycondensation (HPC) of monosodiumoxymethyl(diethoxy)silane in organic solvents such as methanol, ethanol, propan-2-ol and butanol. The effect of the concentration of GPC monomer on the molecular weight characteristics and chemical structure of the resulting polymers will also be considered in this work.



**Figure 1.** Scheme for the synthesis of poly(sodiumoxy)methylsiloxane, which is based on the hydrolytic polycondensation reaction of mono(sodiumoxy)methyldiethoxysilane

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# CLIMATIC TESTS OF POLYMER COMPOSITE MATERIALS IN THE SHARPLY CONTINENTAL CLIMATE OF THE NORTH

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The development of polymer materials for Arctic purposes [1], intended for use in the conditions of underdeveloped transport and industrial infrastructure of the northern territories, requires a special approach to ensuring their reliability and operating efficiency. The complex impact on the material of significant temperature changes throughout the year, including extremely low temperatures down to  $-60^{\circ}\text{C}$ , high solar radiation and other factors, can cause premature loss of performance of polymer parts and products during operation.

The presented work will present the results of a long-term comprehensive study of the influence of destructive factors of the North on the degradation of properties and changes in the structure of polymer and polymer composite materials, carried out on the territory of the climatic test site of the Institute of Oil and Gas Problems of the Siberian Branch of the Russian Academy of Sciences in Yakutsk [2-4].

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*The work was carried out within the framework of the state assignment of the Ministry of Science and Higher Education of the Russian Federation (registration No. 122011100162-9) using the scientific equipment of the Center for Collective Use of the Federal Research Center YSC SB RAS.*



# SYNTHESIS AND INVESTIGATION OF THE PROPERTIES OF POLYPHEYLSILSESQUIOXANES OBTAINED FROM PRECURSORS OF VARIOUS STRUCTURES

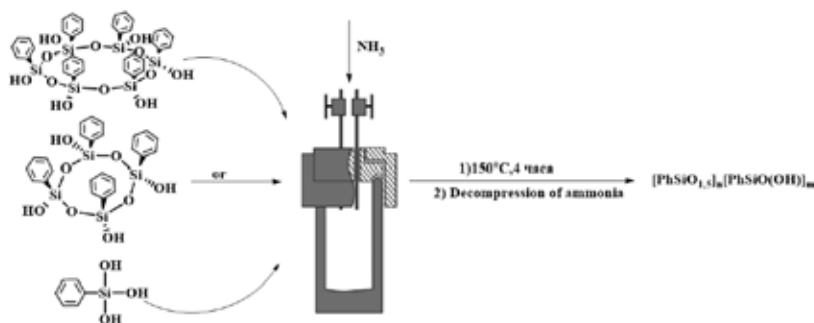
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Ladder polyphenylsilsesquioxanes are a class of silicon organic compounds with a number of physico-chemical properties. The classic method of obtaining l-PPSQ is laborious. <sup>1</sup> Thus, the search for new methods for obtaining polymers of this class is an urgent task. Earlier, INEOS RAS developed and optimized a method for the synthesis of l-PPSQ was first developed and optimized by condensation of *cis*-[PhSi(O)OH]<sub>4</sub> in an ammonia medium, which acts as a solvent and catalyzer. <sup>2</sup> Purpose of the work: synthesis and study the properties of l-PPSQ obtained from precursors of various structures. We selected *cis*-[Ph(O)OH]<sub>6</sub> and PhSi(OH)<sub>3</sub> as the initial monomers (Fig.1). As a result, soluble high-molecular-weight l-PPSQ capable of forming transparent films were obtained. The structure and properties of polymers were investigated by a complex of physico-chemical analysis methods.



**Figure 1.** General scheme of l-PPSQ synthesis in ammonia medium.

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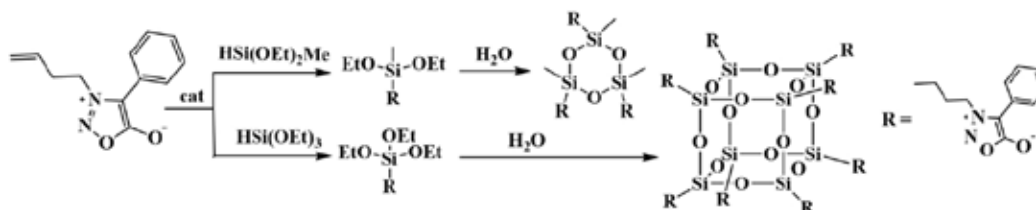
The work was carried out with the financial support of the RSF (grant No. 21-73-20225)

# SYNTHESIS OF SILANES AND SILOXANES CONTAINING MESOIONIC SUBSTITUENTS

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In modern chemistry of organosilicon polymers the field of the synthesis of new polysiloxanes with various functional groups in their structure is actively developing, which would improve strength characteristics of materials based on them due to various types of intermolecular interactions. Mesoionic compounds have a unique electronic structure, uncommon physicochemical properties, as well as a wide range of biological activity. Their introduction into the structure of polyorganosiloxanes can not only improve intermolecular interaction, but also give properties unusual for traditional polymers. One of the main methods of POSs synthesis is hydrolytic polycondensation (HPC) of alkoxyasilanes containing functional groups. A convenient way to introduce various functional groups into an organic substituent at a silicon atom is the hydrosilylation reaction. Hydrosilylation processes are widely used both in the synthesis of new functionalized silane monomers and in the chemical modifications of organosilicon polymers. In this work we studied the hydrosilylation reactions of olefin derivatives of sydnones with alkoxyasilanes followed by the HPC of new silane monomers (Fig.1).



**Fig.1** The scheme of hydrosilylation reactions of olefin derivatives of sydnones followed by HPC.

The optimization of the conditions of hydrosilylation process (temperature, time, catalyst loading) made it possible to obtain alkoxyasilanes containing sydnonyl substituents with high yields. The HPC of the obtained silanes leads to the formation of siloxanes of a predominantly cyclic structure, which was confirmed by the data of GPC and NMR-Si spectroscopy.

# MORPHOLOGICAL FEATURES OF EPOXY COMPOSITIONS MODIFIED WITH THERMOPLASTIC POLYURETHANE

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Polymer binders based on epoxy resins, due to a wide range of properties of materials based on them, are in high demand in leading industries. Modification of thermosetting binders to create bipolymer matrices, in particular, by dissolving thermoplastics in epoxy oligomers, is of interest. When they are introduced into the formulation, there is a significant increase in viscosity, which affects processability and limits the use of high concentrations. We have developed an approach based on combining different amounts of thermoplastic polyurethane (TPU) with triethylenetetramine (TETA) with subsequent curing of ED-20 epoxy resin (RF patent 2813712). The physical and mechanical characteristics of the obtained materials reach 110.6 MPa. The abrasion resistance index increases by 0.95-2.31 units for the modified samples.

The aim of the work is to study morphological features of materials based on epoxy polymer resin ED-20 cured with triethylenetetramine modified with thermoplastic polyurethane Ecopur-T (LLC PF "Axios-Jet"). Mechanically pulverized PU was dissolved in THTA at 80 °C with periodic stirring for 24 hours. The obtained solutions with PU concentration from 20 to 30 wt.% were used as epoxy hardener. Microscopy of the TPU-based compositions modified with TETA after curing at 60°C showed the presence of a large number of coacervate droplets ranging in size from 10 to 40 µm. At 20°C, the droplets coalesced into larger droplets up to 400 µm in size. At the same time, microheterogeneous structure is observed in the cured samples. It is suggested that TPU, due to the presence of hydrogen atom in the nitrogen of the urethane group, is able to form chemical bonds with the epoxy cycle during the curing process. The preparation conditions of the modified hardener will influence the structure of the polymer.

*This work was financially supported by the Ministry of Science and Higher Education of the Russian Federation under the state assignment (FZUS-2024-0001).*

# ELECTRO CONDUCTIVE POLYMER COMPOSITES FOR BIOMEDICINE

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Electrically conductive polymer composite materials (EPCMs) have a wide range of applications due to combinations of properties of various polymers and fillers. Currently, there is interest in the development of composites containing carbon fillers, for example, carbon black (CB), graphene and functionalized graphene, carbon nanotubes, and thermally expanded graphite (TEG).<sup>1</sup>

In the 1960s, the influence of electrical stimulation on the growth, migration and differentiation of various types of cells was proven, which means that EPCM can find their use in medicine as scaffolds for the regeneration of nervous, muscle, cardiac and bone tissue.<sup>2</sup> For such applications, both high conductivity and developed porous structure of the material, which makes the creation of such materials an actual task.

In this work, approaches to the production of EPCM based on cellulose acetate (CA) with the addition of CB, TEG and aminated graphene (AmG) have been developed. The properties of the resulting materials were studied by scanning electron microscopy, dielectric spectroscopy, Brunauer, Emmett and Teller (BET) methods, and mechanical compression tests were carried out. The percolation threshold in these materials was also determined and the elastic modulus was calculated (Table 1).

Composite	CA/CB	CA/TEG	CA/AmG
Maximum SSA, m <sup>2</sup> /g	45,4	10,4	10,4
Elastic modulus, MPa	4,8 ± 0,5 5,8 ± 0,4	2,3 ± 0,1	2,5 ± 0,3 2,5 ± 0,1
Percolation, wt.%	15	25	22

**Table 1.** Material characteristics

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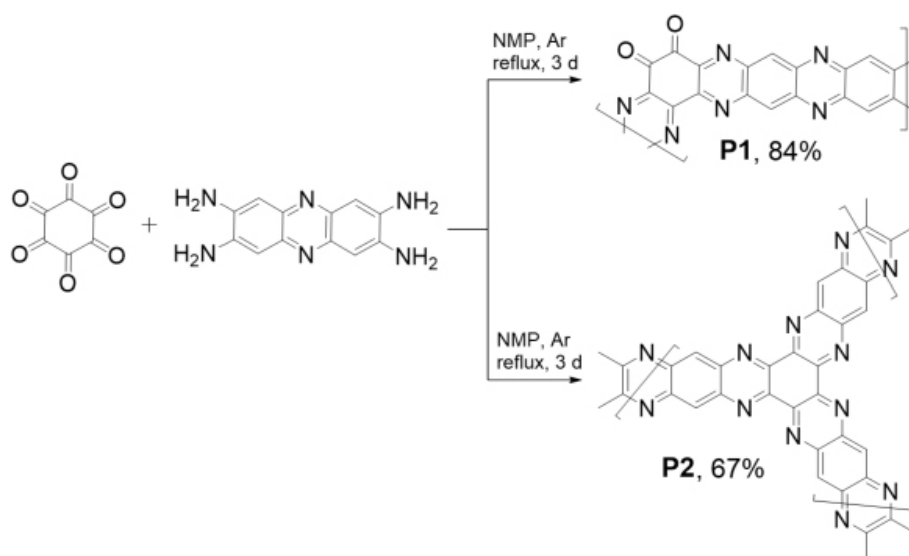
# PROMISING ORGANIC CATHODE MATERIALS FOR POTASSIUM BATTERIES

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The interest to the development of metal-ion batteries with electrode materials based on organic small molecules and polymers has significantly grown over the past two decades. Organic materials have such advantages as their great structural diversity, low cost, availability of raw materials, potential for recyclability, and relatively low toxicity. Furthermore, organic materials are characterized by facilitated ion diffusion, which allows redox conversions to occur faster and with less polarization — some organic-based batteries have achieved full charge within minutes or even seconds rather than hours. Therefore, batteries based on organic electrode materials are particularly attractive for high-power applications.

This work reports the synthesis and investigation of polymers **P1** and **P2** obtained by polycondensation reaction of triquinoyl and tetraaminophenazine (Scheme 1). In particular, the electrochemical characteristics of the obtained materials were studied in potassium batteries. Polymers **P1** and **P2** demonstrated record-high energy density ( $>800$  Wh  $\text{kg}^{-1}$ ), which corresponds to the best values for known organic and inorganic cathodes for potassium-ion batteries. Furthermore, the batteries showed efficient operation at low temperatures (down to  $-55^{\circ}\text{C}$ ), which allows their use in Arctic area or for aerospace applications.



**Scheme 1.** Synthesis of polymers **P1** and **P2**

*This work was supported by the Ministry of Science and Higher Education of Russian Federation (project № 075-15-2024-532)*

# SYNTHESIS AND INVESTIGATION OF SURFACE ACTIVITY AND SELF-ORGANIZATION OF AMPHIPHILIC STEREOREGULAR CYCLOSILOXANES

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Amphiphilic substances of various nature and structure are used in almost every field of human activity, so the task of creating, studying and searching for new applications has always been and will always be urgent. Among other things, siloxane surfactants are widely used due to their unique surface-active properties. In the course of this work, a representative number of amphiphilic stereoregular organocyclosiloxanes with phenyl substituents at the silicon atom were synthesized on the basis of previously obtained and developed methods of template synthesis of stereoregular metallocyclosiloxanes [1] at INEOS RAS. The study of monolayers of these compounds using a Langmuir bath and their visualization using Brewster-angle microscopy revealed a number of dependences of the self-organization of stereoregular cyclosiloxanes on their size and their stereoregularity (fully stereoregular or tris-cis/ tris-trans). The dependence of the tendency to form intermolecular bonds in the monolayer on the cycle size was revealed by the method of multiple compression of monolayers. The study of the equilibrium spreading pressure of amphiphilic stereoregular cyclosiloxanes confirmed the dependence of the thermodynamically stable state of the monolayer on the presence of a spacer between the siloxane ring and the hydrophilic group and on the stereoregularity of the cycle (fully stereoregular or tris-cis/ tris-trans).

## Acknowledgments

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# NMR STUDY OF IONIC AND MOLECULAR MOBILITY IN POLYSTYRENE SULFONIC ACID AND ITS SALTS

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The results of studies of low molecular weight aqueous solutions of metal chlorides have contributed to the interpretation of data on ion exchange membranes<sup>1</sup>. Aqueous solutions of electrolytes are uncrosslinked polymeric analogs of membranes. The study of such systems will provide insight into the mechanisms of ion transport and the formation of transport channels in membranes.

NMR has been successfully used to obtain unique information on the structural and dynamic characteristics of complex molecular systems<sup>2</sup>.

Films of polystyrene sulfonic acid and its Li, Na-, Cs-sols, which we believe are models of the ionogenic part of sulfocation exchange membranes, were studied<sup>3</sup>. Good agreement was obtained between the self-diffusion coefficients of water molecules and lithium cations measured by pulsed field gradient NMR and the self-diffusion coefficients calculated from spin-lattice relaxation data. These results are similar to the behavior of water and cations in sulfocation exchange membranes and resins.

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*NMR measurements were performed using equipment of the Multi-User Analytical Center of the Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS and Multi-User Center of Osipyan Institute of Solid State Physics RAS in Chernogolovka. This work was supported by Ministry of Science and Higher Education of the Russian Federation, state registration number 124013000743-3 (FFSG-2024-0008).*

# SYNTHESIS OF SILOXANE COMB-SHAPED POLYMERS WITH PERFLUORINATED SUBSTITUENTS

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Comb-shaped polymers are high-molecular compounds whose macromolecules contain side branches.

Silicone comb polymers and molecular brushes have been used to produce polymers that are used in areas such as gene therapy and 3D bioprinting, and they also play a huge role in the chemical and medical industries<sup>1</sup>.

It was decided to introduce a perfluoroalkyl substituent as a substituent in our comb-shaped polymers, since the introduction of perfluoroalkyl components into siloxanes changes their properties. They are oil and heat resistant and have an extended operating temperature range.

In our study, we selected hexafluoropropylene dimer and F3 as one of the most commercially available and easily modified organofluorine compounds. It is worth emphasizing that perfluoroalkyl derivatives based on hexafluoropropylene dimer and F3 are not included in the Stockholm Convention on per- and polyfluoroalkyl substances (PFAS), which cause serious harm to the environment. Thus, their use is justified from the point of view of environmental safety<sup>2</sup>.

Thus, the goal of the work is to obtain siloxane comb-shaped polymers with perfluoroalkyl substituents

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# COMPOSITE SUPERABSORBENT POLYMER MATERIALS FOR THE TRANSITION TO RATIONAL AGRICULTURAL TECHNOLOGIES

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Food security is one of the key factors in maintaining the sovereignty and sustainable economic development of the Russian Federation. Therefore, the development of modern agricultural technologies, independent of imported goods, is critically important for maintaining the economic security of the Russian Federation.

Modern agricultural technologies require the use of a significant number of specialized preparations, such as plant protection products, growth stimulants, etc. Most of these substances are hydrophobic, so it forces the introduction of them more often and in larger quantities leading to the accumulation of toxic substances in products. A potential solution to the problem may be the creation of a new generation of superabsorbents capable of prolonged release of the active substances directly in the root zone, as well as to accumulate and, if necessary, give moisture and minerals to the plant.

A series of composite superabsorbents was synthesized. Indolyl-3-acetic acid, a widely used plant growth stimulant, was chosen as a model drug for the study. During the experiment, explants of the fluffy birch (*Betula pubescens*) were transplanted into a natural soil containing a swollen superabsorbent. The effect of superabsorbents with and without growth stimulant on plant growth has been studied. According to the results of the study, it was found that the introduction of a composite superabsorbent containing a growth stimulant into the soil leads to a statistically significant increase in the average number of leaves on the plant, compared with the control. At the same time, no such effect was observed for a non-biodegradable superabsorbent containing a growth stimulant.

Thus, composite superabsorbents may have the potential to be used as carriers for the prolonged release of biologically active substances in crop production.

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# MODIFICATION OF COATINGS BASED ON POLYUREA

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Currently, to protect against abrasive wear of equipment operating in extreme conditions (wide temperature range, contact with aggressive environments, constant high abrasive loads), lining materials based on rubber and polyurethanes with a service life of less than 7 years are used. Therefore, coatings based on polyureas (PU), which have high resistance to abrasive loads, have recently become widespread. A major obstacle to the distribution of this type of material is considered to be the need to use complex and expensive equipment and skilled workers, which is associated with the kinetic characteristics of the reaction during their production: the reaction rate of isocyanate and amine groups in the production of PM is almost 100 times higher than the reaction rate between isocyanate and hydroxyl groups groups, making it difficult to regulate the ongoing reactions.

The goal of the work was to develop a polyurea composition with a lifetime of at least 8 minutes for application of the system without special equipment and performance characteristics at the level of sprayed systems and increased chemical resistance

For the first time, a hand-applied polyurea composition based on aspartates has been developed for insulating small areas with a lifetime of 12 minutes. The optimal quantity of aspartates in a component of the polyurea system was determined. The resulting coating fully matches the performance characteristics of coatings applied using special equipment.

Chemical resistance was increased by introducing epoxy oligomers into the system. It was shown that the introduction of epoxide is possible only by obtaining an intermediate product based on isocyanate. It has been established that the resistance of polyurea coatings to acids increases by 35% and to alkalis by 42%

The modified coatings were produced and tested at the scientific site of Elast-PU LLC. An interim analysis after 12 months of operation of the coating showed that there was no critical surface damage in the structure, and the elasticity index decreased by less than 5%.

# FIRST STEPS TOWARDS OBTAINING A MODEL FOR FORMING FILMS FROM SOLUTIONS OF POLYSACCHARIDES IN MIXED SOLVENTS

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The paper presents the results of studies [1, 2] devoted to establishing the rate of solvent evaporation and assessing the surface roughness of film materials obtained from chitosan-based solutions using mixed solvents [3] containing ethyl alcohol. Solvent evaporation rates were calculated based on the spin-coating model of thin films. For chitosan solutions, the evaporation rate of the water-acetic acid-ethyl alcohol solvent is three orders of magnitude higher than for water-acetic solutions.

Comparative studies of the surface topology of films formed from aqueous and aqueous-alcohol solutions of chitosan polysaccharides were carried out. It was found that in the presence of alcohol, surface roughness decreases for films obtained at room temperature and increases upon annealing.

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# STUDY OF INTERACTION OF EPOXY RESIN ED-20 WITH 1,2,3-BENZOTRIAZOLE BY NMR SPECTROSCOPY

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The interaction of ED-20 epoxy resin with 1,2,3- benzotriazole used as a modifier has been studied by NMR spectroscopy using a Bruker Avance DPX 300 spectrometer with an operating frequency of 500.13 MHz for  $^1\text{H}$  nuclei and 125.76 MHz for  $^{13}\text{C}$  nuclei. Introduction of 1,2,3-benzotriazole into ED-20 epoxy resin is a promising direction of modification, which allows to improve the operational characteristics of the material: thermal and moisture resistance, resistance to aggressive media, increase strength characteristics, which is important in the creation of stressed structures and adhesive joints operating in extreme temperature and humidity conditions.

By comparing the  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the original and modified epoxy resin, some differences are observed. An additional signal at 2.0 ppm appears in the  $^1\text{H}$  spectrum of the modified resin, which is absent in the spectrum of the original ED-20. This signal can be attributed to the protons of the benzene ring of the modifier 1,2,3-benzotriazole. In addition, the  $^1\text{H}$  spectrum of the modified resin shows broadening and complication of the shape of some signals compared to the original ED-20, such as in the 2.5-2.7 ppm region. This may indicate a change in the chemical environment of protons due to the interaction of components. The most probable type of interaction is the formation of hydrogen bonds between the polar groups of the epoxy resin and the heterocyclic ring of benzotriazole. This interaction leads to changes in the electron density and, as a consequence, chemical shifts of the signals in the NMR spectra.

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*The study was carried out on the equipment of the Collective Facilities Center «The Far Eastern Center for Structural Molecular Research (NMR/MS) PIBOC FEB RAS.*



# THE EFFECTS OF LOW-TEMPERATURE THERMAL OXIDATION OF ISOTACTIC POLYPROPYLENE, POLYAMIDE 6/66-4 AND BLENDS BASED ON THEM

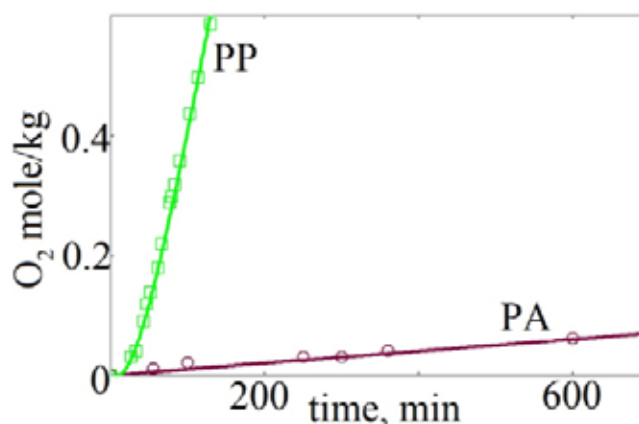
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The effects of non-inhibited low-temperature thermal oxidation of blends based on isotactic polypropylene (PP) and aliphatic polyamide 6/66-4 (PA) at 130 °C. The samples were obtained in a brabender mixer at 190 °C in an argon atmosphere with 5, 10, 20, 30, 40 and 50 wt % PA.

It was found that oxygen uptake by PP/PA mixtures at 130 °C proceeds with a long oxidation induction time, which increases with an increase in the PA content in the mixture. After leaving the induction period, a constant oxidation rate is established, characteristic of the auto-oxidation mechanism. Typical oxygen absorption curves for individual PP and PA are shown in Figure 1.



**Figure 1.** Kinetics of oxidation of PP and PA at 130 °C.

The kinetic curves calculated with the parameters are shown in Fig. 1. The values of the oxidation parameters  $B$ , and  $\tau$  for pure polypropylene are consistent with the literature data. It is noted that the values of  $B$  and  $a$  in mixtures of PP/PA at 5-20 wt.% PA are close to the values in pure PP.

The discovered effects of thermal oxidation of composites open up prospects for directional control of the oxidation rates of PP and PA, which is important for their stabilization or decomposition in vivo.

# POLYMER SORBENTS FOR RARE EARTH METALS EXTRACTION

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Synthesis of new domestic nitrogen- and phosphorus-containing complexing ionites for specific sorption of rare earth elements is a relevant and long-term task.

Copolymers of N,N-diallyl-N'-acetyl-(neopentanoyl-, benzoyl-)hydrazine with acrylonitrile (DAAH-AN; DANPH-AN; DABEH-AN) and diallylaminophosphonium salts with acrylonitrile (DAAP-BF<sub>4</sub>-AN and DAAP-Cl-AN) were obtained by free radical polymerization in bulk in the presence of radical initiator azobisisobutyronitrile.

The obtained copolymers are stable up to 160–260°C, which allows their use at high temperatures. The influence of solution anionic composition on complexation and sorption of La<sup>III</sup>, Ce<sup>III</sup>, Pr<sup>III</sup>, Nd<sup>III</sup>, Sm<sup>III</sup>, Gd<sup>III</sup> from sulfuric acid, hydrochloric acid, nitric acid, mixed (H<sub>2</sub>SO<sub>4</sub> + H<sub>3</sub>PO<sub>4</sub>) media with the above copolymers was studied. The study of the proceeding processes kinetics allowed to determine the optimal time for the equilibrium adsorption establishment: the maximum degree of the sorbent surface filling is achieved within 20 min.

In acidic and weak acid media (pH 2–5) sorbents have no activity towards the investigated ions. With increasing of sulphuric acid concentration (pH 0.3) the capacity of sorbents increases. In mixed media sorption reaches 30%. During the study of La<sup>III</sup>, Ce<sup>III</sup>, Pr<sup>III</sup>, Nd<sup>III</sup>, Sm<sup>III</sup>, Gd<sup>III</sup> ions sorption, in their combined presence in solution, by DAAP-BF<sub>4</sub>-AN and DAAP-Cl-AN reagents it was found that in acidic media La<sup>III</sup>, Pr<sup>III</sup>, Sm<sup>III</sup>, Gd<sup>III</sup> can be separated from Ce<sup>III</sup>, Nd<sup>III</sup>. Through the sorption of these six metals in mixed media, La<sup>III</sup> and Nd<sup>III</sup> are not recovered.

High sorption activity associated with the formation of hydroxocomplexes is observed in the medium with pH > 6.5. DABEH-AN-AN and DAAP-BF<sub>4</sub>-AN are the most interesting as sorbents. Taking into account their higher values of sorption exchange capacity for hydroxide ions and relative stability of these polymers in alkaline medium, it is possible to suggest them as sorbents from solutions with pH > 6.5.

*This work was financially supported by the Russian Science Foundation, project 24-23-00072.*

# METAL-ORGANIC COORDINATION POLYMERS BASED ON IODO-SUBSTITUTED CARBOXYLATES: SYNTHESIS, STRUCTURE AND PROPERTIES

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Metal-organic frameworks (MOFs) are an actively developing scientific topic with tens of thousands of published scientific papers over the past two decades. MOFs attracts such attention due to a wide range of possible applications, including gas storage and separation, targeted drug delivery, and sensor use. Further development of the topic involves searching for new "building blocks", which can be modified to determine both the physical and chemical properties of MOFs and their potential applications.

One of the possible options for new "building blocks" could be iodo-substituted carboxylates for a number of reasons. First, the presence of an iodine atom can lead to the formation of specific non-covalent interactions through the formation of a halogen bond (HB). This will, for example, improve the selectivity of sorption and/or increase the luminescent response to halogen-containing substrates. Second, methods for obtaining substituted carboxylic acids tend to be relatively simple and are well-known in the literature.

The combination of these factors makes iodo-substituted carboxylates promising "building blocks" for the creation of new metal-organic frameworks. In this work, we will discuss the synthesis, characterization, and study of the sorption and luminescent properties of several metal-organic frameworks based on iodo-substituted acids such as 2-iodoterephthalate, 2,5-diiodoterephthalate, and 5-iodozophthalate, among others.

*The work was carried out with financial support from the RSCF project 21-73-20019.*

# THERMOPLASTIC COMPOSITIONS BASED ON CHITOSAN-POLYLACTIDE-POLYCAPROLACTONE BLENDS

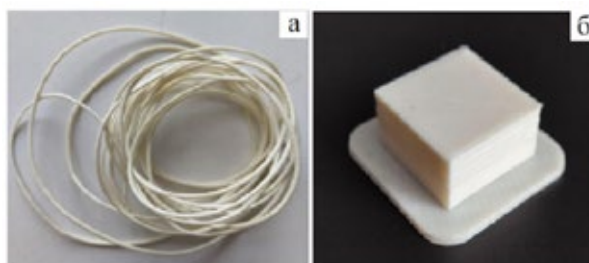
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The relevance of the research topic is related to create polymer materials for biomedical purposes and suitable for use as matrices for regenerative medicine.

Current methods for obtaining blends based on chitosan and polyesters requires using a third polymer as a compatibilizer, mainly polyvinyl alcohol, using emulsifiers or mechanochemical activation reactions in an extruder. Addition of third substances is undesirable, since they can negatively affect the properties of the composition, and mechanochemical synthesis allows to compatibilize polymers on the limited surface area.

Homogeneous thermoplastic compositions based on chitosan and biodegradable polyesters (polylactide, polycaprolactone) were obtained in common solution. The samples were characterized by high mechanical properties (tensile strength up to 70 MPa, elongation at break about 25-30%) and biocompatibility. Powder of the chitosan-polylactide-polycaprolactone composition (1:1:1) was loaded into a laboratory extruder and a 1.75 mm thick filament was obtained at a temperature of 120°C (Fig.1a) Using direct 3D printing at a printing temperature of 150°C, a sample was obtained from the filament (Fig.1b) Thus, for the first time, it was possible to obtain a thermoplastic material containing up to 33 wt.% chitosan in the composition with polyesters.



**Figure 1.** Photos of a sample of chitosan-polylactide-polycaprolactone (1:1) filaments:  
1) (a) and the bulk sample obtained from it (b)

*This work was supported by the Russian Science Foundation (project No 23-13-00342).*

# OXYTHERMOGRAPHY AS A NEW ANALYTICAL METHOD FOR STUDYING THE THERMAL OXIDATIVE DEGRADATION OF POLYMER MATERIALS

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Products made of polymer materials are very widely used in everyday life and industry. Moreover, these products are often subject to temperature influences, which can lead to shape changes and their destruction. Thermal degradation (thermodestruction) occurs – a set of destructive chemical processes in plastic that occur at elevated temperatures. To study the properties of polymer materials associated with their heating, two methods are traditionally used – thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). A fundamentally new analytical method for studying the thermal degradation of organic substances is proposed. The method is based on programmed temperature oxidation of the sample in an air stream or a binary oxygen-inert gas mixture. By registering the oxygen and carbon dioxide content from the heating temperature of the sample in the gas stream at the reactor outlet, it is possible to obtain a thermooxidation spectrum – an oxythermogram and study the kinetics of thermal degradation of the polymer. The method was used to study the thermal degradation of polypropylene samples with and without the addition of titanium dioxide. Samples of a composite material containing from 1% to 5% (by weight) of  $\text{TiO}_2$  were obtained by introducing a filler into the polymer melt. Extruded samples of the original polypropylene or filled composite material in the form of cylinders with a diameter of 3 mm were cut into discs with a thickness of 50 microns. The mathematical processing of the thermal oxidation spectrum obtained by linear heating of samples at a rate of 10 degrees per minute allows us to determine the initial temperature of destruction. It has been shown that the addition of 5%  $\text{TiO}_2$  reduces the temperature of the onset of thermooxylative degradation of the polymer. The method allows to examine samples weighing from 0.1 mg.

## ***References***

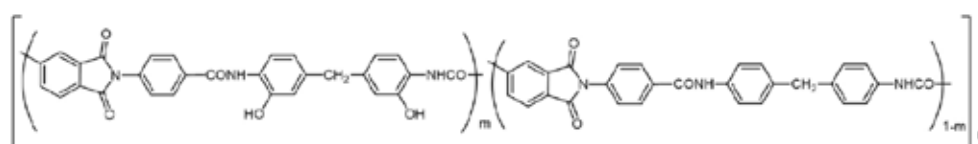
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# STRUCTURE AND PROPERTIES OF NOVEL (CO) POLYAMIDE-IMIDES FOR MEMBRANES TECHNOLOGY

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Novel pervaporation membranes from (co)polyamide-imides (coPAI's) based on diacid chloride of 2-(4-carboxyphenyl)-1,3-dioxoisindoline-5-carboxylic acid and diamines: 5,5'-methylene-bis (2-aminophenol) and 4,4'-methylenebis(benzeneamine), taken in molar ratios of 7:3, 1:1 and 3:7, were obtained by low-temperature polycondensation reaction in N-methyl-2-pyrrolidone (N-MP) solution<sup>1</sup>. Structural formula of coPAI's is shown below.



The change in the composition of copolymers is accompanied by some changes in their molecular weight and hydrodynamic characteristics. In solutions of hydroxyl-containing copolymers coPAI's in N-MP ( $m = 0.5$  and  $m = 0.7$ ), in addition to individual macromolecules with hydrodynamic radius  $R_{h-f}$ , associates formed due to the interaction of chain fragments of different macromolecules of the copolymer with each other were present in very small amounts. The hydrodynamic radii  $R_{h-s}$  of the associates exceeded the sizes of macromolecules by more than 3-7 orders of magnitude.

A set of methods as TGA, DSC, X-ray diffraction and IR spectroscopy were used to study the influence of residual solvent on the process of membrane formation, as well as changes in their properties after removal of the solvent. It has been shown that the presence of the residual solvent N-MP in the films not only has a plasticizing effect on the characteristics of film membranes, but also promotes the preferential transmembrane transport of polar liquids. The results obtained are very important not only for academic interest, but also in practice in the formation of membranes with predictable properties.

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# TURBIDIMETRIC TITRATION METHOD FOR PREPARATION OF PHASE-INVERSION MEMBRANES

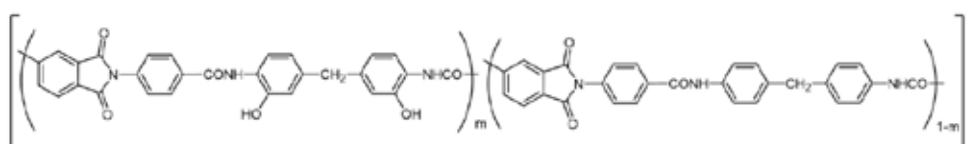
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The development of new polymeric membranes of complex morphology and obtaining the desired physical and chemical characteristics as a result of their formation remains an urgent task. Nowadays polymeric membrane separation methods are the basis of many technological processes. In order to predict membrane characteristics such as permeability, selectivity and durability, a deeper understanding of membrane formation by film casting and/or phase inversion is required.

The standard method for thermodynamic characterisation of a polymer solution is the determination of the cloud point.

In the present work, solutions of hydroxyl-containing (co)PAI polymers:



synthesised by low-temperature polycondensation were investigated by turbidimetric titration for further use of the results in establishing the correlation «the structure (morphology) of membranes and their properties»<sup>1</sup>.

In this work, the dependences of the scattered light intensity, optical transmittance, hydrodynamic radii of scattering objects and their fraction in solution on the volume concentration of the added precipitant in the system of hydroxyl-containing (co)PAIs in N-methyl-2-pyrrolidone were studied by light scattering and turbidimetry methods. The influence of addition of precipitants of different nature (hard precipitant: water, or soft precipitant: ethyl alcohol) on the character of these dependences was established.

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# SYNTHESIS AND PROPERTIES OF NANOGELS BASED ON POLY-N-ISOPROPYLACRYLAMIDE FOR APPLICATION IN REDOX FLOW BATTERIES

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Redox flow batteries are devices that use charge-storing reagents in dissolved or dispersed form. They are promising due to the independence of power and capacity, scalability and the ability to smooth out peaks in production and consumption.<sup>1</sup> Nanogels are submicron sized three-dimensional cross-linked polymer networks.<sup>2</sup> The utilization of nanogels aqueous colloids as an electrolyte contributes to the environmental friendliness, cheapness and safety of batteries. In this paper, nanogels that can play the role of a catholyte are considered.

Nanogels based on N-isopropylacrylamide (NIPA) and N-(3-aminopropyl)methacrylamide hydrochloride (APMA) copolymers were synthesized via free-radical thermo-initiated precipitation polymerization. To make the nanogels redox-active, 4-(3-carboxypropanamido)-TEMPO radicals were grafted to APMA units.<sup>3</sup>

Using the dynamic light scattering (DLS) technique, the parameters of the medium under which nanogels in salt solutions maintain the stability of the colloid were studied since salt solutions are the working environment for redox flow batteries.

Based on the electrochemical activity of the samples studied by cyclic voltammetry and EPR spectroscopic data, the number of TEMPO groups in the nanogel that are effectively involved in charge transfer is calculated. The data confirm the stable redox behavior and, consequently, the possibility of using nanogels of this composition for redox flow batteries.

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# PROSPECTS IN THE FIELD OF IMPROVING THE PHYSICAL AND MECHANICAL CHARACTERISTICS OF CURED POLYMER COMPOSITE MATERIALS

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The constant expansion of the areas of application of polymer composite materials (PCM), including in strategically important industries such as rocketry and aircraft shipbuilding, leads to the search for new methods. aimed at achieving a given set of properties. Methods for modifying PCM are usually divided into 2 groups – chemical and physical. Chemical modification is most often carried out with the direct participation of modifying agents in the curing reaction. Physical modification represents a targeted change in the physical structure of PCM and can be used at all stages of the technological cycle, which explains their high prevalence at enterprises of the machine-building complex<sup>1</sup>.

Currently, there is an active study of the processes and results of PCM modification by physical methods, which include, among other things, electrophysical methods. They involve the use of electrical energy, which determines the availability of their implementation, and make it possible to change the properties of the material, such as strength, heat resistance, dielectric and other characteristics<sup>2</sup>.

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*Analytical studies were carried out using the scientific equipment of the Research Chemical Analytical Center of the National Research Center Kurchatov Institute.*

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*“Substantiation of the methodology for complex modification of composite materials for extreme operating conditions based on the study of phase-structural transformations under the influence of electrophysical influences of various frequency ranges.”*

# TO THE PROBLEM OF DETERMINATION OF MOLECULAR WEIGHT CHARACTERISTICS OF CHITOSAN

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Chitosan (deacetylated chitin) is an aminopolysaccharide that has a wide range of potential applications in various fields, including medicine and pharmaceuticals, cosmetology and cosmeceuticals, food industry and agriculture. Chitosan has a unique complex of physicochemical and biological properties, and the presence of reactive hydroxyl and amino groups allows the preparation of various chitosan derivatives with desired properties. The molecular weight (MW) of chitosan is an important parameter that determines its physicochemical and biological properties. The polydisperse nature of chitosan and its tendency to aggregate in aqueous solutions lead to conflicting results regarding the MW even within a single method. Therefore, it is difficult to compare the results of studies from different research groups and to standardize chitosan-based products for the pharmaceutical industry.

This study compares the main methods currently used to determine the MW of chitosan. Methods for determining the MW of chitosan include various analytical techniques such as capillary viscometry, static light scattering, size exclusion chromatography with different detectors (e.g., refractometer and multi-angle light scattering detector), and NMR relaxation. Methods for determining the MW of chitosan have their advantages and limitations, and the selection of the optimal method depends on the specific conditions and requirements of the study. Based on the analysis of literature data and our own experimental material, recommendations for the selection and use of different methods for the determination of the MW of chitosan are given.

*This work was financially supported by the Russian Science Foundation, project 19-73-20157-P.*

# SYNTHESIS AND RESEARCH OF PROPERTIES OF STARSHAPED POLYMERS OBTAINED BY «GRAFTING-ONTO» AND «CORE FIRST METHODS»

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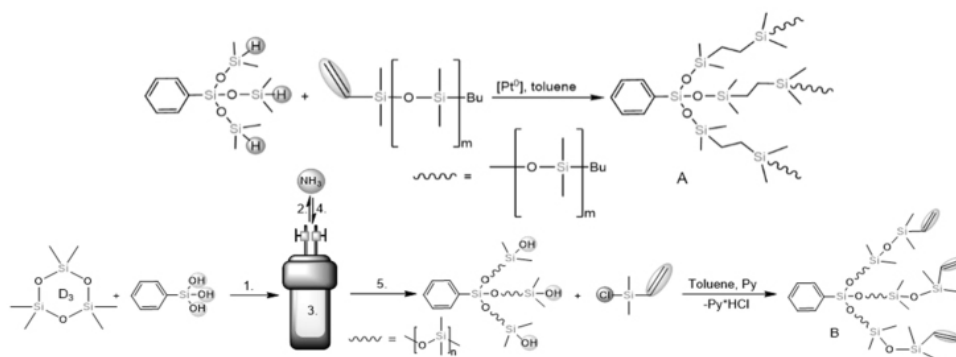
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Polydimethylsiloxanes are widely used polyorganosiloxanes with a unique set of physico-chemical properties. INEOS RAS has recently developed a new method for the production of highly dispersed PDMS<sup>1</sup>, which allows to obtain polymers without additional purification stages at high monomer conversion. It is also interesting to obtain star-shaped polymers based on PDMS.

In this work, two models of a star-shaped polymers (A, B) were used, which are called the "grafting-onto" and "core first methods".



**Figure 1.** The scheme of obtaining of model star-shaped polymers A («core first»), B («grafting- onto»)

The purity and structure of the obtained compounds were confirmed by a complex of methods of physico-chemical analysis, their thermal and rheological properties were investigated.

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*The work was performed with the financial support of the RSF, project 21-73-20225.*



An abstract, vibrant image featuring a complex, multi-colored structure resembling a molecular model or a nebula. The structure is composed of numerous small, glowing particles in shades of red, orange, yellow, green, and blue, arranged in a swirling, organic pattern against a dark background. The overall effect is one of dynamic energy and scientific wonder.

SECTION 9

# CHEMICAL EDUCATION



# THE BEST EDUCATION TECHNOLOGIES AVAILABLE FOR SUSTAINABLE DEVELOPMENT: NEW TRAINING OPPORTUNITIES FOR CHEMICAL ENGINEER

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The current system of organizing higher education in the Russian Federation is entering a new stage of reform in accordance with the requirements of the time<sup>1</sup>.

The training of chemical engineer within the framework of higher educational institutions currently solves the problem of forming specialists who can systematically think and make decisions not only within the framework of the technological process. A modern chemical engineer should consider chemical technology as an element of human and environmental co-evolution on a planetary scale.

G. A. Yagodin became an absolute innovator in the qualitative reform of the educational system of Russia at the end of the 20th century. In many ways, modern education for sustainable development was formed precisely under his leadership within the walls of Mendeleev University<sup>2</sup>.

The situation in Russia and in the world requires the training of specialists aimed at obtaining products with competitive characteristics. Here it is impossible to do just an assessment of the quality of the product and its cost. A competitive product must be "green" at its core.

The uniqueness of the present moment lies in the return to the historical experience of the Russian and Soviet systems of higher education, supplemented by achievements in educational technologies of recent years. This can be seen as the implementation of the best available technologies (BAT) in the educational environment. The concept of education for sustainable development and its implementation at the Mendeleev University is one example of such BAT<sup>3</sup>.

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# CHEMICAL OLYMPIADS OF SCHOOLCHILDREN: PROBLEMS AND PROSPECTS. THE VIEW OF A UNIVERSITY TEACHER

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The history of chemical olympiads in Russia dates back to the 1930s, when the first competitions for schoolchildren were held in Moscow and Leningrad. In 1964, the first all-Russian olympiad was held in Moscow, and in 1967, it became the all-Union olympiad. This means that in 2024, we will celebrate the 60th anniversary of this movement at the national level.

The purpose of chemical olympiads is to identify and foster students' creative abilities, as well as their interest in scientific research activities. They also aim to promote scientific knowledge among young people. Over the last ten to fifteen years, a variety of new olympiads have been created in Russia, including design olympiads and chemical tournaments, as well as traditional all-Russian olympiads for schoolchildren and university olympiads focused on selecting the most qualified candidates. The main goal of these olympiads is not only to interest students in chemistry but also to encourage them to pursue a career in this field. One significant difference between chemical olympiads and olympiads in other subjects is that they often include an experimental component, where participants can demonstrate their skills in conducting a chemical experiment. This allows students to apply their knowledge in a practical setting and gain valuable experience.

The positive aspects of student participation in olympiads are clear: the identification and support of talented students, benefits when applying to universities, which makes it easier for those who can solve non-standard problems, and the skill of competing among participants. However, there are also possible disadvantages, such as loss of confidence and interest in the subject due to more challenging tasks.

Russian schoolchildren have traditionally demonstrated significant success in international olympiads, with the International Chemistry Olympiad and International Mendeleev Olympiad being the most notable.

This report will analyze different types of Olympiads and the experience of teaching winners and medalists of Olympiads at different levels at the Chemistry Department of Moscow State University.

# CREATIVE COMMONWEALTH “SCHOOL-UNIVERSITY”

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The report examines the experience of organizing research activities of schoolchildren using the example of chemical project shifts of the Institute of Chemistry of St. Petersburg State University in the Sirius Educational Center, the Intellect Center (Leningrad Region), the creative union of the Institute of Chemistry of St. Petersburg State University and the university school of natural sciences – the Academic Gymnasium – with prolonged supervision of students from his first visit to a university research laboratory in 10th grade to undertaking his own serious research.

It is much easier to formulate a problem than to solve it. The Federal State Educational Standard for Basic General Education of the Russian Federation (FSES) pays special attention to the project activities of schoolchildren. At the same time, it is important to maintain a balance between reasonable conservatism and innovation in educational programs and pedagogical technologies, i.e. ensure a spirit of proportion, harmony and clarity. Project or research activities of schoolchildren are in no way an alternative to fundamental education, but if a number of conditions are met, they can be a powerful help to it. This is another facet of the unified educational process, contributing to the formation of significant motives for learning and readiness for constant self-education. experience of independent creative activity. The sense of matter has practically disappeared among current generations of schoolchildren, and for the majority it has never appeared. But the truth of the famous saying – “I heard – I forgot, I saw – I remembered, I did – I understood” – no one has canceled it. Students of senior classes (grades 10–11) of specialized schools have a special responsibility: during this period they decide on their future profession. Having chosen a chemical specialization class, it is important that the motivation for this science not only was not lost, but also received noticeable support. An indispensable aid in organizing the productive activities of a specialized school is the creative collaboration between school and university.

The innovative educational project of the Institute of Chemistry of St. Petersburg State University is to create and develop a mentoring system within the framework of continuous multi-level education, in the formation of significant motives for learning. School, unlike a university, requires much greater effort and deeper penetration in terms of individual trajectory: you need to see everyone, be able to say and explain a lot during your school years. Established traditions, graduates who followed this path and then returned to school as scientific supervisors, and, of course, a special intellectual environment formed over time, all contribute to effectiveness.

The main change in recent years is the introduction of a competency-based approach. After all, education is not only a goal, but also progress towards this goal with the acquisition of new knowledge. In this regard, the mission of the teacher and supervisor is special: to be a catalyst for the self-development of their students, to facilitate the mastery of a “learning strategy.” All this brings emotional comfort and a sense of belonging to the educational process.

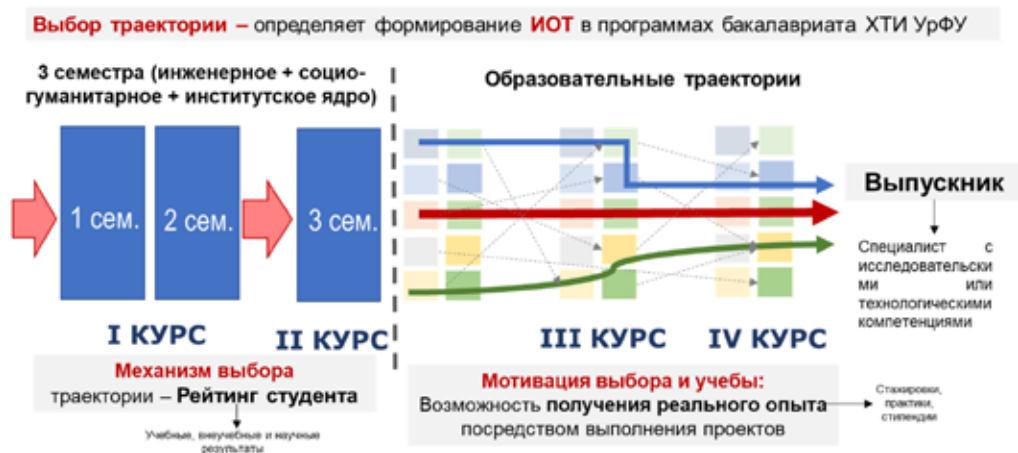
# MODERN UNIVERSITY CHEMISTRY EDUCATION: TRENDS, APPROACHES AND PROSPECTS

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One of the key elements of sustainable scientific and technological development is known to be a harmonious system of university education for the scientific and industrial staff. To provide highly qualified personnel to be capable to realize research projects and to develop high-tech products, universities actively use versatile methods and approaches to organize the training process:

## Модель организации базового высшего образования в ХТИ УрФУ



## Перспективная модель организации специализированного высшего образования в ХТИ УрФУ



This communication reports promising models for chemical personnel training at basic and specialized university levels being realized at the Chemical Engineering Institute of Ural Federal University (ChemTech UrFU).

# SCIENTIFIC AND METHODOLOGICAL APPROACHES TO THE DEVELOPMENT OF CONTROL MEASURING MATERIALS STATE FINAL EXAMINATION IN CHEMISTRY

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1. The regulatory framework for the development of CMM SFC in chemistry: The Federal State Educational Standard of OGE (BSE – Basic State Exam) and EGE (USE – Unified State Exam) as a system of requirements for the educational preparation of students. Features of the content of the Federal State Educational Standard of basic and advanced levels.
2. The purpose of the OGE and the EGE in chemistry: different levels of education – different approaches to the selection of the content and the level of complexity of the included tasks.
  - OGE is the choice of a path for continuing education, selection to colleges and specialized classes of the school.
  - EGE is the differentiation of graduates by level of training in order to be selected for study at a university.
3. Criteria for the selection of content for the preparation of tasks for examination options: an invariant part of the current chemistry programs; the actuality for material for continuing education in high school and university; activity orientation of tasks; focus on the practical component of the course.
4. Features of task models for final certification: the focus of tasks on the control of knowledge and skills of students with different levels of training; checking not factual knowledge, but the ability to reason, establish cause-and-effect relationships, etc., i.e. demonstrate mastery of both subject knowledge and meta-subject skills; the complex nature of the knowledge and skills being tested; variability of solutions to tasks in part 2.
5. Prospects for the development of models of CMM SFC examination tasks in chemistry: levels of controlled material; competence – based approach; virtual and real experiment; artificial intelligence, etc .



# SOCIAL PARTNERSHIP, REGIONAL GOVERNMENT-UNIVERSITY-INDUSTRIAL ENTERPRISE, AS A TOOL TO IMPROVE THE QUALITY OF NATURAL SCIENCE EDUCATION. THE EXPERIENCE OF THE KAZAN NATIONAL RESEARCH TECHNOLOGICAL UNIVERSITY

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Petrochemical assets of the leading Russian partner companies of KNRTU play a significant role in the processes of industrial development in Russia: Sibur Holding, Gazprom, Ammonium, which form an order for the training of engineering personnel of a new formation. The answer is the integration of the teaching staff of KNRTU into the innovative processes of companies in terms of knowledge about the industrial application of world achievements in chemical technologies, which makes it possible to prepare a new type of specialists for the petrochemical industry, taking into account the best achievements in educational technologies and the trend of digital transformation.

We solve the problem of qualitative transformation of personnel and the effectiveness of scientific research in the petrochemical and gas processing industry through participation in federal projects “Priority 2030” and advanced engineering schools (PISH). Moreover, the transformation affects all levels of education – schools, colleges, higher education, scientific personnel. Educational programs at the University are implemented in new scientific and educational spaces and laboratories specially created for these purposes.

The main focus of Promkhimtech is on products and technologies of low-tonnage chemistry (MTX) used in the technological chains of our partners – Sibur Holding, Gazprom, Ammonium, as well as the transition of the chemical industry to a new way of life through the use of digital technologies with the support of the project from IT companies – RTSim LLC and System Solutions LLC.

*The work was carried out within the framework of the project “Advanced Engineering School «Promkhimtech”.*



# SCHOOL CHEMISTRY TEACHER: REALITY AND PERSPECTIVES

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The education system is traditionally one of the priorities of the state policy of our country. However, the shortage of chemistry teachers, especially those with sufficient qualifications to work in specialized classes, is currently acute. At the beginning of 2024, 590 vacant positions of chemistry teachers were recorded in Russia. At the same time, training in bachelor's, specialist and master's programs in the UGSN 04.00.00 "Chemistry" is provided by only 7 pedagogical universities, with a total number of students in all courses of less than 500 people.

In addition, the following problems can be distinguished related to the training of qualified teaching staff for teaching chemistry in school.

1) For several years, there has been a decrease in the average Unified State Exam score of applicants to pedagogical universities in natural sciences, while not all universities require the presentation of USE results in chemistry. Thus, adaptation modules and additional classes for freshmen with weak subject and general education training are needed.

2) For admission to pedagogical universities, the results of the USE in social studies are mandatory, which limits the contingent of applicants. Applicants for medical or fundamental scientific specialties do not have the opportunity to consider pedagogical universities as a second option for admission.

3) In pedagogical universities, there is a tendency to reduce full-time teaching hours allocated for the study of specialized disciplines. Some courses of chemical disciplines are excluded from the curriculum, as is the course of mathematics, which is necessary for mastering the material of any of the natural sciences.

There are other challenges that have been addressed by measures aimed at improving the quality of training of chemistry teachers, developing mentoring in schools, improving the system of advanced training and the exchange of best teaching experiences.<sup>1</sup> An important role in improving the current situation belongs to the All-Russian public organization of chemistry teachers and lecturers.

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# MULTIDISCIPLINARITY IN GREEN CHEMISTRY EDUCATION

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Since the formulation of green chemistry as a novel approach in chemistry, green chemistry education has received increasing attention, resulting in a variety of approaches for its incorporation into chemistry teaching at all levels of instruction.<sup>1,2</sup> Just as the development of green chemistry – being a novel perspective of doing chemistry – entailed the exploration and design of new routes for the production and management of substances, green chemistry education entailed the exploration and design of novel instruction approaches. Since green chemistry interfaces with all the other areas of chemistry, it appears natural to infer that green chemistry education needs to adequately highlight such interfaces as components of the teaching of all the chemistry areas. Since green chemistry is also part of the sustainability discourse,<sup>3</sup> it shares the multidisciplinary character of sustainability, and green chemistry education needs to reflect such multidisciplinary character. The presentation highlights pathways for the integration of cross-area and multidisciplinary routes into green chemistry education, providing criteria and examples to make the proposed routes concrete for different levels of instruction.

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# ONLY SPECIALIZED TRAINING CAN BE THE HOPE

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Due to chemistry's low standing in the educational system, the role of specialized education is increasing, allowing both students to gain deeper knowledge and teachers to reach their academic and methodological potential.

However, the creation of such classes causes certain difficulties. In addition to the necessity of having a competent and enthusiastic teacher, a separate room for a chemical workshop is desirable, a qualified laboratory assistant is required, and equipment and reagents need to be purchased and constantly replenished. School principals generally wish to avoid these problems.

There has been a long practice of having classes that major in chemistry and biology in our country's schools, classes which major in chemistry and physics emerged later. We have both specializations at the gymnasium. How do they differ? It is first and foremost the degree of mathematical training; "biologists" have less of it. Naturally, this has a negative impact on chemical education. We believe that students pursuing a degree in chemistry and biology are more interested in careers in medicine, whereas those specializing in chemistry and physics are more interested in scientific research in their fields and engineering. Both specializations have the right to exist. However, the Federal document provides a curriculum for only a chemical and biological learning profile.<sup>1</sup>

How does studying in specialized classes benefit students? Our observations show that in most cases it mobilizes students and helps them reach their potential. There are striking examples confirming this. It is confusing that in recent years, students have been required to be selected for the 10th grade only based on their student portfolio and the outcomes of the OGE exam.

Usually, grades 10 and 11 make up the profile classes. Our experience indicates that four-year profiling works better.<sup>2</sup>

In light of the fact that our nation is in dire need of skilled engineers and that university professors feel that school graduates know very little about natural science, we think that "specialized chemical classes" will play a significant role in helping to solve these state tasks going forward.

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# PHYSICAL AND CHEMICAL EDUCATION: INTERDISCIPLINARY RELATIONS WITHIN THE ERA OF TECHNOLOGICAL CHANGE

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The term “technological mode” (TM) (way of life) is usually used to define the general state of a set of related industries in selected time periods, having a single technical level, developing synchronously, shaping the environment and living conditions of humans. Changes of TM occur, as a rule, as a result of technological revolutions and predetermine the uneven progress. Despite all the subjectivity in determining such time periods, six technological modes are usually distinguished, where the transition to the last one occurs nowadays (2010–20s) and implies the revolutionary development of nano- and biotechnologies, DNA technologies and genetics, quantum technologies, computer technologies and artificial intelligence, telecommunications, innovative material science (including manipulation of individual atoms/molecules and engineering of living tissues), robotics, active use of green energy.

An obvious consequence of such a change of technical modes is the convergence of sciences, which requires a reconfiguration of the education system at all levels. The interdisciplinary nature of the problems being solved is especially evident at the intersection of physics, chemistry, and life sciences. New technologies (hybrid, neuromorphic, cyber-organic...) and fields of knowledge (medical physics, agrophotonics, sociophysics...) are emerging.

In this lecture, interdisciplinary relations in education and science will be discussed on the example of fundamental and applied photonics, a branch responsible for the instrumentation and research of the interaction of electromagnetic radiation (photons) with matter, including issues of generation, conversion and detection of radiation.

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# ON THE PROBLEMS OF TRAINING AND RETRAINING OF TEACHING STAFF

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The training of teachers in pedagogical universities has been significantly influenced by the transformations carried out in secondary schools. These changes have reduced the prestige of the teaching profession and made the working conditions of teachers extremely unattractive.

Major changes in the system of general secondary education occurred as a result of the introduction of universal compulsory secondary education in the USSR, enshrined in the Constitution (article 45), adopted in 1977. The adoption of the law did not take into account the opportunities and desire of students to receive secondary education. As a result, teachers have lost the right to objectively assess students' academic achievements. Schools have lost the opportunity to leave underachieving students in the second year of study.

The prestige of the teaching profession declined even more in the 80s and 90s, when the sphere of education and the activity of a teacher from "service" has been legally transformed into a low-paid "service". The cooperation of teachers and parents, which is extremely necessary for the education of schoolchildren, has stopped. Parents have the right to demand high-quality educational services from teachers, regardless of their children's educational opportunities and desires.

The subsequent introduction of per capita financing in schools and universities has led to the creation of comfortable conditions for students who do not want to study. The disenfranchisement of teachers has received an economic basis. Paradoxically, university students have the right not to attend classes.

The situation in secondary school has affected the desire of young people to enroll in pedagogical universities, or specialists without pedagogical education to undergo retraining.

The state of teacher education was influenced by the accession of our country to the Bologna Process in 2003, which was accompanied by a decrease in the knowledge requirements of applicants and students.

The listed consequences of the reforms require early adjustment, since modern geopolitical challenges imply a decisive improvement of natural science and pedagogical education. The urgent need for trained teachers for both secondary and higher education is obvious.



# DEVELOPMENT AND IMPLEMENTATION OF ONLINE COURSES AT THE DEPARTMENT OF GENERAL AND INORGANIC CHEMISTRY OF ST. PETERSBURG STATE UNIVERSITY

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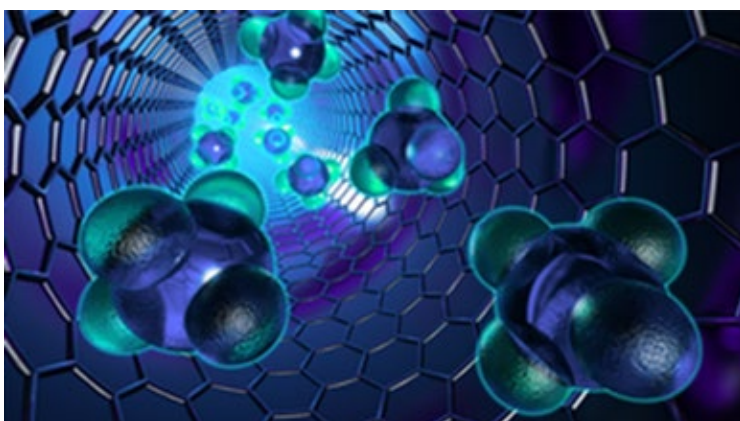
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The history of the creation and implementation of the online courses “Inorganic chemistry: Introduction to chemistry of the elements”<sup>1</sup> and “Structure of matter: atoms, molecules, nanomaterials” (in two parts) will be presented. The courses are implemented on the National platform “Open Education”, the Stepik platform, and were also implemented on the Coursera platform. The courses are accompanied by original demonstration experiments.<sup>2</sup>

The ideology and structure of courses, content creation, forms of control (self-examination questions, control tests, final exam), features of the implementation of courses on different platforms will be discussed, statistical data (regional coverage and student success in mastering the course) will be presented.



2016–2024



2020–2024

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# TRAINING OF CHEMISTRY TEACHERS AT A CLASSICAL UNIVERSITY

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The paper deals with the strategy of pedagogical education development at the Faculty of Chemistry of a classical university.

More than 10 years ago the Faculty of Chemistry of MSU began to train specialists according to the educational standard “Basic and Applied Chemistry” with the qualification “Chemist. Chemistry teacher”. In order to build the foundations of the graduates’ pedagogical literacy, the lecture course “Teaching Methods and Innovative Educational Technologies in Chemistry” was developed (total capacity of 144 academic hours), the obligatory pedagogical practice was introduced in the final year (total capacity of 72 academic hours)<sup>1</sup>.

As a result of the analysis of students’ requirements, the specialization “Theory and Methodology of Chemistry Teaching” will be introduced at the Faculty of Chemistry of MSU in 2022. The volume of disciplines of the specialization is more than 2000 academic hours. Such capacity allows students to form a professional level of pedagogical literacy. For the implementation of the program the staff of the Faculty of Chemistry is involved, who in practice implement such directions of chemical education as: educational and career guidance activities, extracurricular and extra-curricular work, etc. The staff of the Faculty of Pedagogy of MSU and the teachers of the University Gymnasium – a department of MSU are also involved in the educational process. Special attention is paid to modern educational trends, for example, the course “Communication in a Multicultural Environment” contributes to work with pupils whose native language is not Russian.

Since 2024 the issues of the methodology of education in chemistry have been included in the program of the Lomonosov Conference.

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# POSITIVE EXPERIENCE OF DISTANCE LEARNING OF STUDENTS

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The unexpected involuntary switch to distance learning in early 2020 due to the coronavirus pandemic became a difficult test for university teachers, especially those teaching disciplines with laboratory sessions. Distance learning required the development of new or adaptation of well-known educational tools, including videos demonstrating the experiments, the use of Internet platforms for giving lectures and conducting online seminars, the development of regulations for conducting tests and exams, in which teachers could control the independence of preparation and oral responses of students etc. The main of the many problems that arose during the transition to distant learning was the impossibility of developing real experimental work skills in students without contact with the instructor. All aspects of the said changes were analyzed in detail at a symposium on the teaching of analytical chemistry that was held as part of the IV Congress of Russian Analysts in 2022.

At the same time, during the discussion, some positive aspects of distance learning were also noted. Thus, the computer literacy of teachers has significantly increased, they have mastered new platforms and Internet resources and prepared new clear and informative presentations of lectures and seminars. The use of distance learning systems in many universities (DLS at Moscow State University) has become useful, allowing, in particular, to send out materials for students to prepare for classes, check and discuss homework. The mastered techniques of remote work with students have already been successfully used to attract leading Russian and foreign scientists to give lectures on various sections of the discipline. It became possible for sick or lagging students to additionally view materials from lectures, seminars, and laboratory works; checking and discussing homework, etc. Thus, the experience gained has shown that some of the created distance learning tools can be useful and appropriate for increasing the efficiency of the educational process in normal working conditions.

# CRITERIA FOR CHEMICAL OLYMPIAD TASKS

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Researchers have noted a shortage of qualified personnel in the chemical industry<sup>1</sup>. We can attract talented youth to the field of chemistry through schoolchildren's chemistry Olympiads. The content of high-level Olympiad tasks goes beyond the scope of the school curriculum, so many students with good academic preparation get close to zero results which demotivates them to study chemistry.

One way to solve this problem is by improving the quality of Olympiad tasks. G.V. Lisichkin suggests building tasks based on the knowledge and skills that students acquire in the classroom<sup>2</sup>. V.V. Eremin emphasizes that more than 80% of participants should score at least 20 points for a task, while 80 points should be scored by less than 20% of the participants, corresponding to the Gaussian distribution<sup>3</sup>.

Let's highlight three criteria for the Olympiad tasks:

1. The criterion of entertainment
2. Educational potential
3. Normal (Gaussian) distribution.

A normal distribution can be achieved if:

- the Olympiad task includes questions of three levels: reproductive, heuristic, and creative, in an approximate ratio of 1:1:1.
- avoid the "inverted funnel" structure, which is most difficult for students to guess which chemical element is being tested and then reveal the answer.
- organize a competition among compilers to ensure the correct distribution of results.

The educational potential of the task can be enhanced by including real scientific searches, rather than fictional ones, including those of Russian and Soviet chemists<sup>4</sup>.

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# APPLICATION OF AR | VR TECHNOLOGIES IN THE PHARMACISTS-ANALYSTS TRAININGS: THE EXPERIENCE OF THE PHARMACY AND BIOTECHNOLOGY COMPETENCE CENTRE OF SECHENOV UNIVERSITY

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The A.P. Nelyubin Institute of Pharmacy has experience in developing and implementing AR | VR technologies in pharmacists' educational process. Based on the established Centre of Competence in Pharmacy and Biotechnology at Sechenov University two original educational products are being developed and implemented in 2024 – VR module “Titration” and PC program “High-performance liquid chromatography”.

The Virtual Reality module “Titration” is designed for career guidance of students and finals of academic olympics, as well as for industrial practice in the discipline of “Pharmaceutical Chemistry” for foreign students. The module is available in demonstration and exam modes, also suitable for students certification.

The PC programme “High-performance liquid chromatography” is intended for advanced students who wish to acquire a basic knowledge of the operation of chromatographs, as well as for analytical chemists – for skills training and assessment of competence. The programme offers two levels of complexity – beginner and expert; real professional cases are considered for solving according to the chosen level.

From November 1<sup>st</sup> till December 1<sup>st</sup> 2024 at the A.P. Nelyubin Institute of Pharmacy the developed digital educational products will be tested on 400 students of specialist, residency and magistrates programmes within the further professional education. If successful, the programmes will be made available to outsiders and students of other industrial universities.

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# CHEMICAL EDUCATION: INTEGRATION THROUGH STEAM TECHNOLOGY

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The development of natural science competencies is becoming relevant in the modern educational space: we are seeing more and more achievements in the field of chemistry.

STEAM education is aimed at integrating knowledge from different academic subjects, meaningfully, more deeply approaching the understanding of educational material and solving real problems.

In a dynamically changing environment, STEAM education is a tool for the development of critical thinking, research competencies, as skills of the 21st century.

One of the basic principles of STEAM education is broad interdisciplinary integration, built in different directions. Demonstration of the integrity, material unity of the surrounding world – acquaintance with the basic laws and methods of cognition – this is the main goal of integration in education.

Five areas of integration can be identified, which make it possible to demonstrate the interconnections of all elements of the surrounding world:

**1. Emphasis on modern research in various fields of human activity, especially those that are carried out at the intersection of sciences.**

Initially, it is necessary to teach students to distinguish between related areas of knowledge that are involved in solving a problem, which subject areas are aimed at solving it, what terms can be attributed to a particular area.

**2. Demonstration of the commonality of methods that are used in various fields of cognition.** Find the most convincing explanation for why subject areas should be integrated.

**3. Comprehensive study of objects and phenomena, theories, principles that reflect the integrativity of the objective world.**

**4. Demonstration of the use of processes built on the basis of interdisciplinary integration to solve problems of various scales.**

Algorithm for considering a real life situation:

- Choosing a situation.
- Development of a solution to a situation for a number of tasks that correspond to the logic of finding a solution (tasks are set together with students in the course of a collective discussion).
  - Collective determination of the final goal (what will be the solution to this situation).
  - Search for a solution. Students are divided into teams that will solve specific problems, look for answers to specific questions. Next, each team presents the results of the study. Under the guidance of the teacher, the final answer is extracted from the entire product.
  - Collective discussion of the results obtained and putting forward a hypothesis.
  - Collective development of an alternative solution.

**5. Comprehensive study of the achievements of scientific and technological progress.**

An interdisciplinary analysis of the proposed achievements on a number of issues, as a result of which students come to the conclusion that the creation of an invention requires the integration of various fields of knowledge

Chemistry is one of the most important branches of science, it serves as the basis for research in the field of biology, geology, astronomy, etc. Methodological criteria for the selection of content for the subject chemistry, the content of which would satisfy the basic principles of STEAM education: scientific, accessible, systematic.

An important process of integrating STEAM education in chemistry teaching is the introduction of project-based learning, which focuses on schoolchildren, and includes an approach in which students acquire deeper knowledge through the active study of problems in practice. Applying this approach encourages students to understand every component of STEAM: science, technology, engineering, arts, and math in the study of chemistry.

The introduction of elements of the STEAM approach can be implemented as a homework. Especially interesting for students are tasks that require the creation of something new, the development of a start-up project or the visualization of an idea. For example, soap making with an interesting design and marketing development. After such classes, all

children agree that STEM is practical and educational. After all, STEM is about experiments, scientific experiments, studying the structure of the world and the universe, creating your own games and your own projects.

Having studied the scientific and methodological foundations and applied aspects of the study of STEM approaches in the educational process in chemistry lessons, the following conclusions are made: STEM training is a universal practice-oriented approach that allows students to cope with tasks of any complexity. This approach creates a learning environment for future professionals who require comprehensive training and knowledge from various educational areas of natural sciences, engineering and technology. STEAM-education is a link between the educational process and future employment and professional career development. Successful specialists will need competencies related to various areas of natural and mathematical sciences, engineering and technology. The difference between the STEAM approaches is an integrated educational environment and interdisciplinary organization of the educational process. This method allows students to get a holistic picture of the world under study and demonstrates the conventionality of dividing science into separate disciplines. The STEAM method focuses the attention of students on the real application of knowledge to solve existing problems. This approach will allow you to build a training system in which the maximum quality of education is achieved. The STEM method acquires a special value and importance in the bilingual educational space.

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# WORKSHOPS ON 3D MODELING AND 3D PRINTING WITHIN OF CHEMISTRY COURSES

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Despite the limited use of 3D printing technology in modern Russian laboratories, the potential of using additive technologies to solve technological and especially research tasks is beyond doubt<sup>1</sup>. Similarly, there is no doubt about the potential of 3D printing in the field of teaching chemical sciences, in particular crystal chemistry and organic chemistry, while there are no sections in the chemistry course programs in which students could gain 3D modeling and 3D printing skills.

We have developed and conducted a workshop on 3D modeling and assembly of crystalline structures of inorganic compounds, in which students get acquainted with databases of crystalline structures, choose representatives from them who meet certain requirements, build the bond systems, transfer the constructed models to 3D format, correct them and prepare them for printing, then independently they are printed using the FDM method and assembled, then made conclusions about the chemical properties and capabilities of the chemical application (if necessary, the latter can be organized in the format of round table). Thus, within the framework of the workshop, the student gets acquainted with the main stages of the search of new materials with specified properties. Over the years of the workshop, we have developed a scheme that allows us to expand one or more of the listed modules, say, devote more time to 3D modeling and 3D printing, or, conversely, to search for structures in the database. In the latter case, it is possible to use highly specialized software packages such as ToposPro.

The workshop showed that students are actively and with interest mastering the methods of 3D modeling and 3D printing, considering them promising for their career.

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# INVOLVING UNIVERSITY STUDENTS IN MENTORING SCHOOL STUDENTS: ON THE EXAMPLE OF PREPARING SCHOOLCHILDREN FOR CHEMISTRY OLYMPIADS

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One of the most important conditions for effective work with gifted students is the presence of competent teachers in the position of mentors. According to research<sup>1</sup>, mentoring from students who themselves, as schoolchildren, had successful experience of participating in Olympiads, is an effective practice in preparing schoolchildren for Olympiads. The work explores the phenomenon of mentoring development using the example of the Regional Public Organization “Association of Mentors of the Olympiad Movement” (ANOD) in the Republic of Bashkortostan<sup>2</sup>. Based on 25 semi-structured interviews with members of the association, features of motivation and involvement in mentoring and reasons for leaving were identified. The most productive way of becoming a mentor in the Olympiad movement has been identified as a transition from the Olympiad participant’s own experience through the position of an assistant mentor to the independent position of a mentor. Moreover, starting from high school. Olympians do not experience methodological difficulties when starting teaching: they themselves have undergone successful training and are willing to share it. Despite the proactive position of mentors and their willingness to work even for free and overtime, they encounter difficulties that may cause them not to achieve their goals, and at the same time, leaving mentoring. The results of the conducted research will be useful for educational managers to involve students in the implementation of mentoring and the development of the Olympiad movement in schools.

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# A MODEL OF INTERACTION BETWEEN A TEACHER-MENTOR AND A STUDENT DURING EDUCATIONAL AND RESEARCH ACTIVITIES IN THE CONTEXT OF THE ACADEMIC SUBJECT OF “CHEMISTRY”

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The development of students’ research skills, which include the ability to identify the essence of a problem, formulate hypotheses, set goals and objectives, conduct experiments, observe, analyze results, draw conclusions, is one of the main objectives of the Federal State Educational Standards for Basic General and General Secondary Education in the Russian Federation<sup>1,2</sup>. This process is most often carried out through educational and research activities organized by a teacher-mentor.

We have developed and tested, within the framework of the academic subject “Chemistry”, the technology of organizing educational and research activities for students in grades 9–11 of general education organizations. This technology includes four stages: analytical and diagnostic, preparatory, implementation, and reflexive-ascertaining.

During the implementation stage, student interaction with the teacher-mentor occurs. The use of this technology and the analysis of the results from its approbation have shown that it is essential for the student and teacher-mentor to cooperate on an equal footing during the implementation phase. The traditional approach of teacher-student interaction should be excluded, and we have therefore developed a model for interaction between the student and teacher-mentor that is based on the principles of educational and research activities<sup>3</sup>.

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# CHEMISTRY OLYMPIADS IN RUSSIA – A SOCIAL LIFT AND A MATTER OF NATIONAL PRIDE

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Chemistry Olympiads for high school students are not only a scientific, but also a social phenomenon, reflecting society's attitude towards the natural sciences and chemistry in particular. In our country, they started in 1938, when the state, in the face of many challenges, realized the need to attract children to science and select the most gifted of them.

Since then, the national Olympiad (in Soviet times, the All-Union, and after 1991, the All-Russian) has grown into a well-developed multi-level structure, which was not broken even by the collapse of the country in 1991. After this, the All-Union Olympiad was transformed into the Mendeleev Olympiad, and the All-Russian Olympiad inherited the best features of the All-Union Olympiad and managed to maintain its role in the education system even during the transition to capitalism.

The goals of the All-Russian Chemistry Olympiad have remained unchanged throughout its history: it is the promotion of science, the search for gifted children and creating the conditions for the development of their abilities. The latter means that the Olympiad serves as a social lift. This role has noticeably increased in the last decade, when the need to support the gifted children was formulated in the Education Law, and the bonuses for winners and prize-winners increased manifold. Some experts even believe that the role of the Olympiads in the ratings of participants, school teachers and schools is overestimated.

The modern features of the Olympiad system are considered - the formation of a list of Olympiads that complement the All-Russian Olympiad, and the development of remote competitions. The All-Russian Olympiad in its early stages covers all schools in Russia (for comparison, in the UK - not more than 10%), and the traditionally high scientific and creative level of tasks forms a highly competitive environment among the participants, which allows only the strongest children to reach the very top of the Olympiad pyramid. For this reason, the Russian national team in chemistry is always a favorite at all the international competitions, and its successes in recent years have been widely covered in the mass-media and have become one of the matters of national pride in our society.

# ROLE OF PROFESSIONAL DEVELOPMENT PROGRAMS IN CHEMICAL ENGINEERING EDUCATION

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The last decade has seen a significantly increased growth in the number and quality of professional development programs, both upskilling and reskilling, in Russian higher education, including engineering universities. Federal academic leadership development programs “Priority-2030” and “Leading Engineering Schools” set new challenges for professional development programs highlighting the new framework of lifelong learning and enhancing its role as an important activity of universities alongside with undergraduate, graduate and post-graduate programs.

The enhanced role of professional development programs and vocational education results from the changes in the Russian labor market where the demand is shifting from basic higher education programs to upskilling and reskilling programs due to their flexibility and a quick response to the requests of the industrial companies. In particular, many chemical, petrochemical and gas processing enterprises address universities to fill the gaps in professional competencies of their employees in chemical engineering, including those who are willing to find new career opportunities.

One of the strategies in developing such upskilling and reskilling programs is to integrate professional development and research. Successful universities run professional development programs in the areas where professors are good in their research. Practice shows that professional development programs in research universities are much more attractive for industrial enterprises as well as other students. Under these circumstances, however, universities face low motivation of professors to combine research and teaching in professional development programs. Finding the ways to solve this problem is one of the challenges for engineering universities.

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# CHEMISTRY OLYMPIAD “YOUNG TALENTS”

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The Faculty of Chemistry of Perm State University has been holding school olympiads for many years. Since 2009, the faculty has been holding the Multi-subject Olympiad “Young Talents” in chemistry together with universities in Krasnoyarsk, Samara and Saransk. The Olympiad has been repeatedly included in the List of Olympiads for schoolchildren of the Russian Ministry of Education and Science as a 1st level Olympiad. To date, it has already been held 17 times.

The Olympiad tasks are developed for four age groups (11, 10, 9, 8 and more junior schoolchildren)<sup>1</sup>. One of the advantages of the Olympiad is presence of experimental round. It should be noted that, thanks to a fortunate coincidence, the final stage of the Olympiad was always held in person, even during the pandemic. Every year, about 2,500 schoolchildren from more than 75 constituent entities of the Russian Federation take part in the Olympiad. Schoolchildren from more than 25 constituent entities of the Russian Federation become winners and prize-winners. In 2023/24, the final stage of the Olympiad was held in 19 regions.

Holding an Olympiad for regional universities has its pros and cons<sup>2</sup>. As an absolute plus, I would like to note the identification of talented schoolchildren who are interested in the subject, for whom participation in the Olympiad does not pass without a trace. These students, as a rule, are successful in their future activities. But often they are also passionate about the Olympiad movement, and, despite their busy lives, participate in organizing Olympiads and writing assignments<sup>3</sup>.

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# INTRODUCTION OF STEAM METHODOLOGY IN SCHOOL CHEMISTRY EDUCATION

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The modern labor market needs specialists capable of working with complex multifaceted tasks involving several fields of scientific knowledge, engineering and technology. Working with big data and implementing AI requires a strong mathematical foundation. Application of STEAM methodology in the educational process makes it possible to solve the issue of inter- and meta-subject learning at different levels – from kindergarten to university. World practice proves the effectiveness of STEAM implementation at school<sup>1</sup>, however, the application of the STEAM approach in Russian schools is still fragmented in nature<sup>2</sup>.

In 2023, a school STEAM center was established in the MBEI Gymnasium of the Leningradskaya stanitsa of Krasnodar region, which is implementing a program to integrate this approach to the mastery of disciplines in the natural sciences. The teachers of the gymnasium and experts involved develop and successfully implement<sup>3</sup> classroom and extracurricular programs for studying chemistry in grades 8–9 and building cross-curricular competences. It should be noted that creating a STEAM lesson is a time-consuming process and the result depends on the skill of the teacher, so there is a need for experience sharing and professional development programs for STEAM teachers.

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# THE OLYMPIAD MOVEMENT IN THE PROFESSIONAL DEVELOPMENT OF A CHEMISTRY TEACHER

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The Olympiad movement for schoolchildren as a socio-educational phenomenon occupies an important place in the modern education system. By enhancing the leadership and competitive abilities of students, the olympiads promote their intensive intellectual growth and socialization.

The involvement of teachers in the olympiad movement within the domestic educational system involves participation in the organization and management of the olympiads and pedagogical support for students in their preparation for these competitions. Experimental studies have shown that the organization of a specialized olympiad-oriented educational process within the system of additional professional training is a powerful tool for enhancing the professional skills of chemistry teachers<sup>1</sup>.

However, there is still room for improvement when it comes to involving teachers in actual olympiad competitions, or the organization of teacher olympiads. Some previous attempts at organizing such events have not been particularly successful in terms of either the seriousness of approach or depth (for example, see <https://education.apkpro.ru/courses/1049/>).

It seems relevant to organize and conduct chemistry teacher olympiads on the basis of leading universities in Russia, with the assistance of the Ministry of Education. It is expected that stimulating the professional development of teachers, as well as their personal qualities, through communication with scientific and pedagogical staff in the Olympiad environment, will improve the quality of chemistry education in Russia.

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# ADDITIONAL EDUCATION AS A FACTOR IN CHEMISTRY STUDENTS ACADEMIC MOBILITY FORMATION

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Students' academic mobility is a tool aimed at keeping the labor market in balance, as well as a vector of knowledge exchange and personal enrichment. Academic mobility is a prerequisite for scientific excellence, which involves international collaboration between scientists and researchers and integration into scientific communities. In addition, it improves university education quality and ensures the competitiveness of higher education institutions, scientific and research laboratories.

There are two main types of academic mobility: internal (training and internships at Russian universities and organizations) and international (training and internships abroad). KNSTU Supplementary Education Faculty offers training for academic mobility to students in chemistry and other subjects. Educational programs, customized educational pathways, and conducive environments for academic mobility have all been developed and put into place to facilitate this.

Students need to enhance their language skills and communication competence for studying and internships abroad. One of the solutions to the problem seems to be in Professional Translation additional program where students learn to use a professionally oriented foreign language. The experience in training chemists in these additional programs facilitates understanding how well this program is being mastered by students. The results are visible.

Academic mobility training helps students adjust to their courses more quickly and encourages them to study and complete internships at Russian and international universities. Thanks to such training, chemistry students win scholarships and study at Russian and foreign universities, then return to Tatarstan and find employment in their field, making use of their knowledge, skills, and experience.

# ANALYSIS AND EVOLUTION OF CHEMISTRY OLYMPIADS: ALL-RUSSIAN AND OLYMPIADS OF THE LIST

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Every year, about half a million schoolchildren take part in the stages of the All-Russian Olympiad for Schoolchildren in Chemistry. About three hundred of them are eventually selected and participate in the Final stage of the All-Russian Olympiad. There is also a huge number of participants in the list of Olympiads in chemistry, conducted mainly by universities – olympiads on the list of the Russian Council of Olympiads for schoolchildren, the list of which is established annually by the Ministry of Education<sup>1</sup>. The rapid development of chemistry olympiads has led to the formation of a special culture of preparing schoolchildren for them. At the same time, the diversity of the Olympiads and the existing history of development in recent years provides fruitful material for analyzing the evolution of the Olympiad tasks themselves.

In this work, such an analysis was carried out, the result of which is a brief description of the main level I Olympiads and their comparison with the All-Russian Olympiad in Chemistry (regional and final stage). The main problems of both the Olympiads in general and the current state of their development have been identified. Conclusions are drawn about the possible development trajectories of individual Olympiads and the movement as a whole.

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# INTEGRATION AND ADAPTIVE PROCESSES IN UPDATING OF CONTENT OF CHEMICAL EDUCATION

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At the present stage of development of society, the importance of chemical education in solving global problems of society and implementing the concept of national security is becoming more and more obvious<sup>1</sup>. Today, in the teaching of chemistry, there continue to be acute and challenging issues related to low motivation of students, insufficient conditions for creative thinking, difficulty in understanding the subject by students in humanities classes and students under various restrictions<sup>2</sup>.

The system-activity approach, which is mentioned in the modern Federal State Educational Standard, is aimed at achieving competencies of the 21<sup>st</sup> century, among which are subject, meta-subject and personal competencies. However, the implementation of an approach aimed at training and educating a creatively thinking individual faces a number of difficulties, primarily with the insufficient involvement of integration and adaptive processes, the effectiveness of which directly determines the success of teaching chemistry. Currently, the challenges of society call for updating the content of chemical education at the levels of basic and secondary general education. First of all, consideration of such processes as 1) interdisciplinary integration requires attention; 2) scientific and practical integration; 3) vertical interactions of different levels of education; 4) adaptation of chemistry teaching to students of non-chemical profiles; 5) adaptation to special categories of students and the digital environment.

In practice, the implementation of these processes comes into contact with a number of problematic issues, including the insufficient development of content, methodological, material, technical and personnel support. At the same time, the greatest emphasis, from our point of view, currently needs to be placed on creating a system of integrative forms and methods in teaching chemistry and natural sciences.

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# DISTANCE LEARNING AND CHEMICAL EDUCATION: PROBLEM OF COMPATIBILITY

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Among the numerous problems associated with the COVID-19 pandemic, the problem of implementing the educational process in conditions of factual isolation from each other of its two key constituent subjects – the educational (teacher) and the educable (student) – has become particularly relevant. The Ministry of Science and Higher Education of Russian Federation responded quickly enough to the current situation and strongly recommended that all Russian higher education institutions switch to the so-called a distance format for conducting the educational process, which to one degree or another remains in them to this day. Moreover, the opinion has begun to be seriously promoted that this format should become more and more dominant, and in the future, completely displace the traditional (contact) format of education from practice.

In this connection, the given report examines and discusses the problems associated with the possible widespread introduction of distance learning into the practice of Russian higher education in general and chemical education in particular. The advantages and disadvantages of distance learning are presented and analyzed in detail in comparison with contact learning, which involves contact communication between the teacher and the student(s), and it is stated that, regardless of the specifics of the discipline being taught, the disadvantages of the distance learning form generally prevail over its advantages. Particular attention is paid to the fact that in a number of disciplines, namely those where, for their full development, along with the acquisition of KNOWLEDGE, it is absolutely necessary to acquire SKILLS to perform specific experimental work (which includes chemistry), the distance learning format can only be partially used. Because if it is fully implemented, students will definitely not be able to acquire those skills that are formed only as a result of them performing relevant laboratory work, which requires working with their hands. It is concluded that distance education in chemistry can become dominant only in completely unique situations in which “live” (contact) communication between people in general and teachers and students in particular, for one reason or another, should be minimized or even eliminated altogether.



# QUALITY OF TEACHING CHEMICAL DISCIPLINES IN HIGHER SCHOOL THROUGH THE INTEGRATION OF EDUCATIONAL PROGRAMS WITH PRODUCTION IN HIGHER SCHOOL (BASED ON THE EXAMPLE OF METALLURGICAL SPECIALTIES OF THE VYKSUNSKY BRANCH OF NUST MISIS)

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The main task of higher education is to train highly qualified specialists in various fields of human activity. The reality is that a modern highly qualified specialist has to work in complex, rapidly changing conditions of scientific and technological progress; it is important to rebuild the educational process. The most important component in the training of a specialist in the metallurgical industry is the block of natural science disciplines; one of the main areas of this block is chemical disciplines. To implement such a policy, integration between the university and the employer is necessary. The main objective of such a partnership is the formation of a unified fundamental and practical knowledge in the technical field for bachelors, the so-called "University-Employer" system. To successfully implement such integration, young specialists need knowledge in the natural sciences, in particular within the chemical disciplines. To form fundamental and practical knowledge, you need knowledge in the field of chemistry. To solve this problem, the following areas of interaction were chosen: introduction to the educational process – visiting the plant and conducting practices, seminars and laboratory and scientific work on their territory. Carrying out joint projects in chemistry not only within the course and beyond.

All ideas and ideas about the organization of teaching chemistry in higher education, using the example of metallurgical specialties, are aimed at improving the quality of chemical education and its further development and improvement.

# MATRIX LAB COURSE – AN INNOVATIVE APPROACH TO LABORATORY PRACTICUM ON THE EXAMPLE OF SPECIALIZED CHEMICAL DISCIPLINES

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One of the main tasks of higher education is developing in students critical (scientific) thinking, the ability to analyze information and experience in writing scientific texts. These skills are mostly developed in laboratory and practical classes than in lecture-type classes. Traditional laboratory practice, where students reproduce single experiments using known methods, does not fully allow develop above mentioned skills. Reproduction of standard procedures does not allow identifying patterns and conducting a full analysis of an array of experimental data. Traditional laboratory classes are usually does not involve the possibility for creativity of students. In foreign literature, the need to provide reports on laboratory work in the format of a scientific article is actively discussed<sup>1</sup>, which is difficult to implement within of a traditional laboratory practice. Thus, new approaches to organizing laboratory classes are required.

At the department of chemical technology of organic dyes and phototropic compounds of the St. Petersburg State Technological Institute (Technical University), a new approach to conducting laboratory classes was developed. This approach, called matrix lab course, is successfully used to train students in master's programs. During the laboratory course, in addition to theoretical and practical material and experimental techniques, students obtain enough experimental data for analysis and for reporting in the format of a scientific article. At the end of the semester, students also prepare an oral presentation.

Reported herein are the details of lab classes with detailed description of the methodology, with examples of laboratory work, and the results of a statistical study demonstrating the positive response of students to the new methodology, as well as its impact on their critical thinking and scientific writing skills.

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# EXPERIENCE IN DEVELOPING EDUCATIONAL PROGRAMS ON THE APPLICATION OF DIGITAL TECHNOLOGIES IN THE PRODUCTION AND OPERATION OF REFRACTORY MATERIALS AND PRODUCTS FOR METALLURGICAL PROCESSES

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Intensification of resource saving (saving raw materials, increasing the lifespan of trouble-free operation of metallurgical units, recycling waste, using secondary energy resources) and increasing the requirements for environmental safety of production leads to the need to train qualified specialists<sup>1</sup>. The developed educational programs allow, based on the use of digital technologies (intelligent decision support systems, virtual simulators), to conduct project-oriented training of engineering teams (materials scientists, technologists, operators, etc.) in the field of resource-saving operation of linings of metallurgical units, understanding the complex relationships between process parameters; determination of technological modes to increase the yield and quality of steel; converter slag processing; reducing emissions of pollutants<sup>2</sup>. Educational programs are focused on the formation of individual training trajectories for specialists, which makes it possible to implement the training of individual groups of personnel.

Educational programs comply with the requirements of Federal State Educational Standards for Higher Education 4 projects and are aimed at training specialists with basic education to deepen their knowledge and skills in professions that meet the specific requirements of enterprises. Educational programs have been tested in the educational process of Saint-Petersburg State Institute of Technology and during advanced training of employees of NLMK PJSC, Severstal PJSC.

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# EARLY PROFESSIONAL ORIENTATION OF STUDENTS IN THE FIELD OF NATURAL SCIENCES IN THE SYSTEM OF ADDITIONAL EDUCATION

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The acquisition of important ideas about the importance of science in the modern world by students from an early school age, as well as the formation of interest in natural sciences in general, is possible through extracurricular activities. Extracurricular activities should be supported by students' project activities in chemistry and other related sciences. Thus, the relevance of this study is due to the need to modernize the existing model of school chemical education.

On the basis of the educational center for additional education "Mendeleev" in Arzamas, in cooperation with the AF of UNN, early professional orientation of students in the field of natural science education is being implemented, which is aimed at preparing well-oriented students with solid basic knowledge for the school course of knowledge in core disciplines of students; at developing personality qualities that allow in the future quite quickly, according to the profile, to master new equipment and technology, and, if necessary, a new profession, as well as apply theoretical knowledge in practical activities.

The center's teachers have developed sets of educational and cognitive programs and master classes for students in grades 1–11, as well as mass events aimed at popularizing science, expanding horizons and increasing interest in natural sciences.

Priority programs are: "Chemistry of Joy" (grades 1–4), in which students learn the basics of chemistry in a playful way, conduct entertaining experiments and experiments; "Chemistry of Life" (grades 5–8), where students study the basics of chemistry, conduct experiments to consolidate theoretical knowledge, laws and facts in practice, get acquainted with the basis of research and project activities in chemistry and "Chemistry without Borders" (grades 9–11), in which students study the basics of theoretical and experimental chemistry, biochemistry, pharmacology, get acquainted with chemistry as part of choosing a future profession.

# CHEMICAL ENGINEERING EDUCATION AT TECHNICAL UNIVERSITY

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Qualified engineering specialists are in great demand in the labor market today. And therefore, the issues of their preparation, and therefore the issues of implementing chemical education at a technical university, are of paramount importance.

The report presents the results of work on the development of chemical engineering education at the Kalashnikov Izhevsk State Technical University on the basis of the department of “Chemistry and Chemical Technology”.<sup>1</sup> Currently, specialists are trained in the following educational programs:

- master’s program “Nanotechnologies in electrochemical production”;
- Specialist program 04.05.01 “Fundamental and applied chemistry”;
- Bachelor’s program 04.03.01 “Chemistry”;
- advanced training program “Fundamentals of physical and colloidal chemistry”.

Training within the framework of educational programs is focused on meeting the needs for highly qualified personnel in the labor market of the Udmurt Republic, the Volga Federal District and the Russian Federation as a whole.

The work is being carried out jointly with the Competence Center for the Technology of New and Mobile Energy Sources at the Institute of Problems of Chemical Physics of the RAS, the Udmurt Federal Research Center UB RAS and enterprises of the region: Joint-stock company (JSC) ‘Sarapul Electric Generator Plant’, JSC ‘Elecond’, JSC ‘Izhevsk Radio Plant’ JSC ‘Izhevsk Electromechanical Plant ‘Kupol’.

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# KEY ASPECTS OF THE DE-WESTERNIZATION OF THE MODERN CHEMICAL EDUCATION SYSTEM FOR SCHOOLCHILDREN

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The results what obtained in the process of a comprehensive historical and pedagogical analysis of the development of chemical education of schoolchildren in the Soviet period and reflected in the works<sup>1,2</sup>, allowed us to identify and explain the key aspects of improving the modern system of chemical education of schoolchildren, taking into account the growing trends of modernization:

1. To resume the priority of natural science education with the preservation of the principle of humanitarization of school education.
2. To ensure the accessibility of high-quality chemical education for every student through the development of a wide network of institutions of additional chemical education and the implementation of measures to popularize it.
3. To bring the content of chemical education of schoolchildren in line with scientific and technological progress and the pace of social development.
4. To ensure a practice-oriented orientation of chemical education of schoolchildren and to improve the process of teaching chemistry through the implementation of the principle of intersubject.
5. To resume the practice of polytechnic elective courses in chemistry, which will provide conditions for the formation of engineering thinking and functional literacy.
6. To improve the assessment systems of chemical knowledge, skills and abilities of schoolchildren due to the predominance of practice-oriented forms of control.
7. To provide schools with scientifically reliable and accessible information on paper and electronic media for students to receive additional chemical education.

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# SPECIALIZED CHEMISTRY EDUCATIONAL SESSIONS BASED ON THE SIRIUS MODEL IN THE SYSTEM OF ADDITIONAL EDUCATION OF THE STAVROPOL TERRITORY

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Annually, Sirius's experience reaches different areas. Local centers make a great contribution to development of young talents. New opportunities are emerging to address the territory's strategic challenges. The local center Sirius 26 of the Stavropol Territory organized educational specialized sessions in chemistry, astronomy, biology, information technology, mathematics, physics and project activities for students who demonstrate success in STEM disciplines.

Specialized sessions consist of theoretical and practical tasks including training on solving Olympiad tasks and in-depth study of individual topics of school curriculum. School contest movement is one of the current trends of today<sup>1</sup>. These days, the goal of the family is to see the child's potential in time, while the purpose of local centers of additional education for children is to support the child and develop his abilities preparing the ground for these abilities to be realized. After all, the school age is fundamental for growth of a thoughtful, independent and creative personality<sup>2</sup>. Participation in specialized sessions and school contest movement is very important, since it: contributes to their self-realization, expands and deepens their knowledge in a certain subject area, and allows them to make a choice of a future profession<sup>3</sup>. Students who successfully perform at the Olympiads have advantages when entering prestigious universities of the country and their own region – and this, in return, raises the entire school contest movement's status.

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# ONLINE TEACHING: A COURSE ON METROLOGY OF CHEMICAL ANALYSIS

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Although the pandemic has ended for many and most universities are returning to in-person teaching, online learning still has certain advantages. Recent experience has shown that it can be justified in a number of disciplines, including chemistry.

One of the disciplines offered in the master's program in Chemistry at St. Petersburg State University is 'Metrology of Chemical Analysis', which is an elective course. This course is unique in that it only consists of lectures and seminars, unlike most practical chemical courses. As a result, transitioning to online teaching is relatively straightforward without compromising the knowledge gained by students.

This discipline, from the pandemic to the present, has been implemented online. All classes are held on the MS Teams platform, while the remaining work is completed on the LMS Blackboard of St. Petersburg State University. Lectures are supplemented by traditional presentations and reinforced with tests immediately after class and remotely during the week, as well as electronic homework and class recordings for students to review the material on their own.

The seminars cover practical skills for applying different approaches to metrological processing of chemical analysis results. They also include debates on the concept of uncertainty and its application in analytical laboratories. The course employs a point system to grade students on their completion of current assignments and exams. Students can take a test or a classical oral exam if they do not agree with the 'automatic' grading. Based on the results of an anonymous survey, students have provided a positive assessment of the proposed teaching model.

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# OVERDUE REFORMS OF HIGHER CHEMICAL EDUCATION

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Let's compile together the problems of higher chemical education (subjective and objective), with which most chemists can agree:

- The need for teachers to combine research and teaching. Consequence 1) since a teacher's salary depends on the quantity and quality of papers, and not at all on the quality of lectures, both science and teaching suffer.
- Methodologically verified basic courses, a once-determined sequence of presentation and contents, fixed for at least 2–3 years by the academic council – the lecturer must adhere to all of this. Consequence 2) new scientific methods fall into the topics of basic courses several years after their appearance. Lack of motivation for development on the part of the lecturer.
- Interdisciplinary disunity – mathematicians teach everyone pure mathematics, physicists – physics. Applied topics are rather an exception. The idea of N.S. Zefirov of the early 90s (mathematics for chemists, a ready-made set of programs) is firmly forgotten. Without this, the most important courses fall into the pass-and-forget category.
- Workshops in which the student masters methodically verified syntheses, the results of which go to waste. Consequences 3,4) lack of motivation in the student; Huge funds for maintaining the workshop go down the drain.
- Scientific work of students, as usually, during 1–2 years is decorative. And this is an important age for his motivational development as a scientist.
- And finally, the result of higher chemical education is graduates. Can any university say, a year after graduation, where all the graduates work – in their specialty or not?

For the last 30 years, there has been a solution to all of these problems – the *administrative* participation of RAS Institutes (both organizations and employees) in the higher education system. Not decorative, in the form of a “net form of education” or scientific work of students at the Russian Academy of Sciences against the backdrop of 40 classroom hours per week, but real – with the involvement of lecturers “from the plow” to teaching basic courses and conducting practical work in their laboratories, with a list of necessary skills instead of a methodically verified workshop. The possibilities of RAS institutes for scientific work of students are still higher than those of universities. Creation of courses “mathematics for chemists”, “computer science for chemists” (not for programmers), urgent introduction into the programs of courses “AI in chemistry”, all kinds of practical courses on working with modern equipment. There are teachers and resources at the institutes; we need the administrative will of both sides to unify science and education in a *non-imitative* manner.

# DISCIPLINES OF THE BLOCK 1 SET AND VARIABLE PART FORMING THE PROFILE OF CHEMISTRY PROGRAMS FOR BACHELOR AND MASTER DEGREE

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Within the framework of the Law of the Russian Federation “On Education”, since 1992 Russian universities have been able to implement programs of level training: bachelor and master degrees.

According to the current Federal State Educational Standards (FSES), the bachelor and master degree program consists of several blocks, including academic disciplines (set, variable and elective), practices and State Final Certification<sup>1,2</sup>.

FSES of Higher Education 3++ according to the program 04.03.01 and 04.04.01 “Chemistry”, which were approved in 2017, take into account the professional standards<sup>1,2</sup>. On the one hand, FSES allowed the bachelor degree profiles to be regulated giving the universities the opportunity to independently choose disciplines, types of practices, vary the number of weeks of study, etc. On the other hand, this led to a significant difference in curricula, and, as a result, difficulties in transferring to another educational institution.

Currently, in the process of developing the next generation of Federal State Educational Standards, and taking into account the Russia’s exit from the Bologna system, it is necessary to systematize, preserve and develop those positive qualities of the higher education system that have appeared over the past three decades, and, if possible, avoid accumulated shortcomings.

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# MODERNIZING THE CONTENT OF EDUCATIONAL PROGRAMS THROUGH BUILDING AN INTERNSHIP SYSTEM AT INDUSTRIAL ENTERPRISES

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Integration with industrial enterprises of the petrochemical complex has necessitated the need to dynamically update the content of training courses taught at graduating chemical departments. The development of modern petrochemical complexes in Siberia and the Far East requires training of personnel capable of solving complex technological problems and working on state-of-the-art equipment. For this purpose, in 2023, at KNRTU, a decision was made by the Academic Council of the university on mandatory annual internships for 20% of the teaching staff of departments at industrial enterprises and leading scientific centers in Russia. To increase the effectiveness of internships, together with the SIBUR company, KPIs were created for teaching staff sent for internships, a system for supporting teachers at the enterprise and a list of responsible persons on the part of the industrial enterprise were created too. In 2023, 152 teachers were sent for internships, including 90 to industrial enterprises located outside the Republic of Tatarstan. This initiative made it possible to strengthen the interaction of graduating departments with major employers, formulate topics for joint R&D, determine a list of advanced training programs necessary for enterprises, and significantly update production and pre-graduate internship programs for students.

At the end of the internship, the teacher must identify 3 KPIs from the list and coordinate their implementation with the internship supervisor, a representative of an industrial enterprise. At the same time, KPIs related to updating the content of courses taught are mandatory, the other two indicators are differentiated in complexity depending on the position of the faculty. The period for fulfilling the obligations assumed is 4–6 months; upon achieving the KPI of the teaching staff, a rating payment is expected.

# EXPERIMENTAL MODEL OF LABORATORY INFRASTRUCTURE OF SIRIUS UNIVERSITY

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Modern scientific researches determine new requirements for the formation, provision and organization of scientific laboratory infrastructure<sup>1,2</sup>. To increase the efficiency of laboratory infrastructure usage, shared access formats are being introduced in academic organizations and service units are being created to provide services; administrative units for organizing operational activities and administering project activities; resource centers for providing highly specialized research services and supporting scientific and educational activities.

In accordance with this, Sirius University has implemented a structural unit – a laboratory complex, the main task of which is to provide the scientific and educational activities of the University's scientific areas with laboratory infrastructure, high-tech and general laboratory services.

The main goals of the laboratory complex:

- ensuring maximum availability, operability and safety of the laboratory and digital infrastructure of the University in the interests of internal and external customers in the format of shared use centers and design laboratories;
- improving the quality of the University's scientific and educational activities by involving specialists from resource centers in scientific projects and educational programs;
- ensuring compliance of laboratory infrastructure and processes with legal requirements and industry best practices

The development and improvement of the Laboratory complex is an important factor for the successful scientific and educational activities of the University and ensuring its competitiveness.

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# MODULAR SYSTEM IN MEDICAL CHEMISTRY

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Sirius University of Science and Technology is the youngest and fastest growing university in Russia, implementing a qualitatively new approach to education and research activities. It does not have the usual faculties and departments, the core of the university consists of Research centers in priority areas for Russia, which are headed by world-renowned scientists.

The scientific center of Translational Medicine has opened training in the field of Medical Chemistry. The Master's degree program is aimed at training highly qualified specialists who are ready for independent professional research and innovation in the field of drug development both in the pharmaceutical industry and in scientific organizations.

The program is focused on in-depth study of both fundamental and the most demanded disciplines by the industry, such as medical chemistry, pharmaceutical development, pharmanalysis, pharmaceutical substances production technologies. Thanks to the involvement of practical teachers in the educational process, including employees of industrial partners, graduates of the program master modern physical and chemical research methods, learn regulatory requirements for the development of medicines of various nature, gain knowledge about the specifics of conducting preclinical and clinical trials of medicines.

Sirius University implements a modular learning system that makes it possible to overcome the fragmentation of programmed learning through the creation of an integrated visual program and problematic presentation of content in the module. Advantages of the modular form of education: individualization of learning; adaptation of educational material according to individual capabilities and pedagogical goals; uniform distribution of the academic load; assessment of knowledge based on the results of the work done; shortened training periods; full immersion in the subject; the opportunity to study with leading specialists; the possibility of remote learning.

# ALL-RUSSIAN CHEMISTRY TOURNAMENT FOR SCHOOLCHILDREN AS A PROMISING WAY TO INTRODUCE TALENTED YOUTH TO SCIENCE

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The issue of identifying and attracting talented young people to enter chemical fields and subsequently enter science is of extreme importance. In addition to the classical Olympiads and scientific and practical conferences, chemical tournaments have been held for schoolchildren in Russia from the 8th through 11th grades for the past two decades. The chemical tournament is a team-based competition that involves solving tasks and preparing multimedia presentations. The assigned tasks are of a scientific and applied nature and require a creative approach from schoolchildren.

This format of the tournament teaches participants to formulate scientific hypotheses and defend them during discussion. It also develops public speaking skills, teamwork, and creative thinking when solving scientific problems.

The tournament helps to foster cooperation between participants, scientists, and universities. Currently, there are two large chemical tournaments in Moscow (ICT) and in Novosibirsk (RCTS). Being a hybrid form of activity, the tournament allows students to showcase their research and discussion skills, and is much more effective than classical scientific or practical work. The competitive format of the event motivates teams to learn from each other's mistakes and improve their approaches to solving and presenting problems.

An integral part of the program is the development of a scientific mindset, the ability to search for literature, and the creation of beautiful and understandable presentations. The results from several events demonstrate that the involvement of university and research institute staff can lead to significant improvements, even without increasing the resources available in schools' laboratories.

# CHEMICAL START: FROM SCHOOL LESSON TO FUTURE PROFESSION

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An important link in the training system for a modern chemist is the early professional orientation of students in high school (grades 6–7). A special place in this process is occupied by specialized schools or individual classes with a chemical bias. Since 2019, a regional center for identifying, supporting and developing abilities and talents in children and youth has been operating in Samara – “Vega”. “Vega” is a structural unit of the Samara Regional Center for Gifted Children (SRCOD, created in 2016) and operates, like other similar centers in 70 regions of the Russian Federation, according to the “Sirius” OC model. The paper provides a detailed analysis of the results of educational activities and pedagogical approaches in teaching chemistry at SRCOD and its structural unit – the “Vega” center.

Chemistry at SRCOD is taught from the 7 grade with an obligatory additional special course in each parallel with a gradual increase in the weekly number of hours to 8–10 hours at the 11 box office. The educational process involved 4 teachers-chemists (2 full-time chemistry teachers and 2 co-teachers). Of the 200 students at SRCOD, more than 50 children study chemistry in depth, demonstrating remarkable results: For seven years of work, SRCOD received 25 diplomas of winners and 5 diplomas of winners of the final stage of the All-Russian Olympiad for schoolchildren in chemistry (VsOSH), over 300 diplomas of winners and prize-winners at Olympiads of I and II levels from the list of the Ministry of Education and Science, absolute leadership in the region at the municipal and regional stages of VsOSH in chemistry, scientific articles in chemistry in publications included in the WoS and Scopus databases, a large number of victories in all-Russian and international competitions of scientific works. In 2023 and 2024 bronze and silver medals were won at the 57 and 58 International Mendeleev Chemical Olympiad. Over 70 graduates of SRCOD connected their future life with the profession of a chemist, becoming students of Moscow State University, St. Petersburg State University, KFU, RUDN University, RCTU and other scientific and educational chemical centers of the country. Many guys chose medicine as their future profession. SRCOD is rightfully proud of its chemistry students and is considered one of the flagships of school chemical education in the Russian Federation.

# ENVIRONMENTAL EDUCATION IN TEACHING CHEMISTRY AT THE UNIVERSITY

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At the present stage of society's development, environmental education acquires ideological significance and becomes an integrative factor of education, upbringing and personal development<sup>1,2</sup>. D.I. Mendeleev especially persistently pursued the idea of the need to link educational material with life, with its needs. We consider that point of the pedagogical concept to be an integral component of environmental education.

**Table 1.** Forms of environmental education and practical examples

Forms of environmental education		
massive	group events	individual
interuniversity environmental festivals, intellectual games, conferences, Olympiads	thematic excursions, group activities, chemical and environmental workshop	preparation of reports, lectures, projects, individual reports

Currently, students show great interest in environmental issues, environmental chemistry and a healthy lifestyle. In accordance with this, the main directions of classroom and extracurricular work are being formed. The process of environmental education of a future chemistry teacher should be systematic, using interdisciplinary integration, local history material. This process should be carried out using a variety of forms, methods and techniques of organizing students' activities.

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# VULNERABLE POINTS IN THE EDUCATIONAL PROCESS IN HIGHER EDUCATION, TAKING INTO ACCOUNT THE CLIP THINKING OF STUDENTS AND THE DEVELOPMENT OF NEURAL NETWORKS (USING THE EXAMPLE OF TEACHING CHEMISTRY)

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In the modern educational process, we are dealing with a contingent of students whose clip thinking is decisive. It is characterized by fragmentary and discrete assimilation of information, and radically differs from the conceptual and logical. However, many educational programs, including chemistry, do not pay due attention to the development of this type of thinking among students, which slows down the assimilation of the material and can lead to problems for young professionals who try to fulfill their professional duties without detailed study and analysis. The traditional forms of chemistry classes in higher education are lectures, laboratory and practical work. The most difficult thing is to keep your attention on the lecture for a long time and to control the material being presented. It is very important to get interested in the first minutes of a speech, to hold attention with demonstration pauses, practical examples, and to give short group tasks using modern information technologies. When conducting laboratory work, there is a problem with thoughtlessly rewriting material from undergraduates, using search engines to write reaction equations. In solving these pedagogical difficulties, it is important to identify reliable sources of information on the Internet. You can create individual laboratory tasks in which you need to solve a specific problem using theoretical material. Practical classes involve memorizing formulas, ready-made solution algorithms, and involving artificial intelligence in the solution. To maintain interest in the subject, you can create tasks that are close to the topics of your chosen profession. The use of neural networks in chemistry teaching can be an effective tool to improve understanding of complex concepts and increase the interactivity of classes. But this requires the development of special techniques and materials adapted to the use of neural networks to ensure optimal assimilation of information. The introduction of innovative methods and technologies will make learning more interesting, accessible and effective for students in higher education.

# INTEGRATION OF CHEMISTRY CONTENT INTO BIOLOGY CURRICULUM

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Integration means linking content of different school subjects. It allows to form holistic scientific worldview. It is essential to understand biochemistry and ecology as well as project activity.

The goal of the present work is to integrate chemistry content into biology curriculum. For that we elaborated tasks and problems (including hands-on ones) for biology lessons (7–11 grades) that incorporate chemistry content. We also suggested topics for learning projects that require knowledge both in chemistry and biology.

Here are the examples of the tasks of different types.

1. Multiply choice

Anticodon of t-RNA that recognizes methionine codon 5'-AUG-3' has the following sequence:

- a) 5'-AUG-3'
- b) 5'-UAC-3'
- c) 5'-CAU-3'
- d) 5'-GUA-3'

2. Young students collected Invertebrates for biology classroom. They had read that to store biological objects they use 10% formaldehyde solution. The technician of chemistry lab offered his assistance in preparation the necessary solution from 37,5% solution of formaldehyde. Calculate masses of this solution and water to prepare 270 g of 10% solution.

Here is the list of hands-on tasks for biology lessons: isolation of DNA of banana; determination of ascorbic acid in juices; investigation of catalytic activity of ferments; fermentative hydrolysis of starch; dying bacteria by Gram method.



# PROPAEDEUTIC CHEMICAL EDUCATION: EXPERIENCE OF THE PHYSICS AND MATHEMATICS SCHOOL OF THE TYUMEN REGION

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In modern context of searching for responses to the strategic challenges of the economy, the need for early mastering of technical subjects at the school level is acute. Provision of personality-oriented education, with the disclosure of features of thinking, memory, emotions, perception, volition, interests oblige to choose an effective individual educational route; preparation for life in changing socio-economic conditions, which leads to continuous self-education.<sup>1</sup>

The key to effective early chemistry education is the structure of our school's curriculum, due to which a high mathematical load is realized. The classical mathematical view of solving open-answer tasks, approaches in calculations of fractions, proportions, putting coefficients in front of unknowns, gives quick results in mastering primary mathematical techniques in chemistry. The introduction of early learning of chemical skills for mathematically educated children allows concentrating only on chemical laws, as pupils cope with mathematical calculations independently. In addition, in general, at first, novice chemists prefer to use math rather than new knowledge (for example, solving tasks on the arrangement of coefficients in redox reactions with three components). These same children easily overcome the challenges of independently assuming the geometric structure of chemical formulas of acids, with the laws of arrangement of elements in which they are just beginning to familiarize themselves. In addition, surprisingly pupils cope quickly and successfully, putting themselves in the place of researchers of the 18th-19th century, remaining until the last in complete ignorance of their correctness, using only the knowledge of stereometry and geometry obtained before that.

Thus, the attraction to the chemical profile of pupils of 7–8 grades with mathematical level above average allows to pass the basic level program quickly and effectively in the subject “Chemistry” of the 9th grade for three quarters of the school year with high results of trial versions of the general state examination: “5” – 60%; “4” – 33%; “3” – 7%. Having mastered and consolidated the basic knowledge of chemistry proceed to the study of olympiad tasks, opening new horizons of application of mathematics in chemistry.

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# COMMON DIDACTICAL PRINCIPLES FOR CONSTRUCTION OF THE CONTENT OF EDUCATIONAL DISCIPLINES BOTANY AND INORGANIC CHEMISTRY

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Currently, the importance of integrated forms of education and the combination of several training profiles is becoming more and more obvious. The natural sciences of botany and inorganic chemistry, as well as their didactic equivalents, the educational disciplines of botany and inorganic chemistry, are closely interconnected in the field of objects, subject matter, research approaches and methods of cognition<sup>1,2</sup>. These disciplines are united by a number of common didactic principles for constructing their content<sup>3,4</sup>, including the principle of scientific character, accessibility, consistency, and historicism<sup>5</sup>.

The scientific principle reflects the connections between real processes and objects. For these disciplines, this is, for example, respiration and photosynthesis and water, oxygen and carbon dioxide involved in them. The principle of accessibility of content is manifested in logical transitions in interdisciplinary knowledge. The more such transitions are identified, the more versatile the object is revealed, the more accessible it is. An example is nitrogen fixation and physiology of plant of *Fabaceae* family. The principle of systematicity implies the formation of a knowledge system in combination with facts, theories, and mechanisms. Substances and processes are examined from a chemical and biological perspective, which creates an objective view, for example, of the Krebs' cycle, sodium channels in cells, and the regulatory function of microelements. The systematic approach takes into account the laws of the cognition process, the movement from simple to complex, from substance to organism. The principle of historicism presupposes the use in the content of both disciplines of facts from the history of scientific discoveries and biographies of natural scientists, which contributes to the implementation of many parenting tasks.

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# ORGANIZATION OF CHEMISTRY OLYMPIC TRAINING IN CHEMIS ON THE EXAMPLE OF THE CLUB FOR GIFTED CHILDREN “MATRITSA”

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The system of supplementary education offers opportunities to deepen knowledge, develop skills and acquire new competencies outside the main educational program. The club for gifted children “Matritsa” (Krasnodar) demonstrates an example of effective work in the direction of Olympiad training of schoolchildren in chemistry in the system of supplementary education among commercial educational organizations.

The work of the club in the field of Olympiad chemistry began in 2017 with one student, and at the moment there are several dozens of them. The organization of Olympiad work required solving the following problems: 1) creation of material and technical base (it was gradually implemented at the expense of the club); 2) methodological training of teachers and training system taking into account the specifics of training in an institution of additional education (creation of author’s programs); 3) regular participation of students in Olympiads (in this regard, the club “Matritsa” organizes sites of RSOSH Olympiads). The organization of Olympiads in the absence of state support requires significant resources, primarily financial. However, these expenses allow to effectively develop the Olympiad movement not only within the club, but also in the region.

The coordinated work of all departments of the club in the field of Olympiad work during seven years has provided the following results:

1) since 2021 the team of the region is represented by at least 2–3 participants at the final stage of the All-Russian School of Olympiads and always returns with diplomas, whereas before 2020 the usual result was the participation of 1–2 people, often passing only by quota and without prizes in the final stage;

2) the number of diplomas of PSOSH Olympiads has increased from 3 to 68, 50 of which were awarded to students of the “Matritsa” club;

3) only for the previous academic year 24 Olympiads from the list of RSOSH Olympiads were held, including practical rounds in chemistry.

Thanks to the work of the club, the number of participants in chemistry Olympiads in Krasnodar Krai has increased more than 5 times in the last 5 years.

# GREEN CHEMISTRY IN EDUCATIONAL PROGRAMS OF HIGHER EDUCATION INSTITUTIONS

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Modern chemical enterprises are increasingly focused on sustainable production and the application of the principles of green chemistry: the demand for specialists in green technologies in 2022–2023 has already exceeded the number of workers employed in this field, and without proper training this gap will only increase over time<sup>1</sup>. The implementation of green chemistry into educational programs in chemistry and chemical technology increases the competitiveness and demand of university graduates in the labor market. There are a number of examples of such implementation in universities both abroad and in Russia. Thus, at the University of Oregon (USA) the catalytic synthesis of adipic acid is being studied instead of synthesis in the presence of nitric acid<sup>2</sup>; at the University of Winnipeg (Canada) microwave synthesis is used to achieve higher yields with less solvent and energy<sup>3</sup>. In Russia at KFU, RSU named for S. Yesenin, and SUSHPU the discipline “Green Chemistry” is taught, including lectures and/or seminars on the principles of green chemistry, catalysis, safe solvents, energy-saving technologies, green production, etc. Special educational programs are implemented at ASU (“Green Chemistry”) and at the MUCTR (“Green Chemistry for Sustainable Development”), where innovative technologies, life cycle analysis, legal aspects, etc. are additionally studied. An advantageous feature of the last example is the laboratory workshop on green chemistry, which promotes the development of practical skills. In general, Russian examples are more fundamental in nature, while foreign ones are more practice-oriented. The implementation of green chemistry in educational programs is necessary for gaining the skills of a responsible approach to the development of chemical syntheses, while it does not require a complete redesign of programs and can be achieved through the teaching of traditional chemical knowledge in the context of green chemistry.

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# DEVELOPMENT OF AN EDUCATIONAL PLATFORM FOR THE MENTORSHIP IN THE SYSTEM OF TRAINING SCHOOL STUDENTS FOR CHEMISTRY OLYMPIADS

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The school olympiad movement, with more than half a century of history, remains one of the main tools for identifying and developing talent in chemistry in Russia. In recent years, the number of participants and the impact of the Olympiads have been increasing: winners receive the right to enter universities without entrance tests or 100 points of the Unified State Exam, large prizes and grants, and increased scholarships from universities<sup>1</sup>.

The Olympiads are becoming a social lift, but there is educational inequality between schoolchildren in different regions in terms of access to it, which is confirmed by the number of diplomas of the All-Russian Schoolchildren Olympiad per the number of population<sup>2</sup>. The mentoring model of the Association Of Olympic Movement Mentors built in Bashkortostan made it possible to reduce this inequality by involving students – winners of Olympiads – in work with schoolchildren: implementation of regular face-to-face classes, holiday schools and organisation of competitions. This led to a significant increase in the number of participants and winners of Olympiads in chemistry, but did not allow to involve students from remote areas of the republic<sup>3</sup>.

In this work, to solve this problem, an educational platform anodrb.ru was developed, which has functionality for distance learning, a calendar of Olympiad rounds, a bank of tasks with video solutions and automatic checking of different types of answers (test, short text, numerical, structural formulas of compounds). The platform has been successfully used for organising open online classes, hosting free courses in general, inorganic and physical chemistry, organising preliminary stages of a few Olympiads, and as an supportive digital tool for the organisation of face-to-face educational process.

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# THE DEVELOPMENT OF PEDAGOGICAL IDEA OF THE CONTINUOUS EDUCATION BY D.I. MENDELEEV WITHIN THE MODERN EDUCATIONAL SPACE IN THE ACADEMY OF TALENTS ST. PETERSBURG

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In order to develop regional system for working with talented children and youth in St. Petersburg, a Regional center for identifying and supporting gifted children in the field of art, sports, education and science has been operating on the basis of “Academy of Talents” since 2018. Within the framework of natural science area, Academy of Talents implements the following programs of additional education for schoolchildren:

- “Infochemistry”, where attention is focused on research activities in the field of chemistry and chemical engineering, as well as specialized training of students for successful performance at competitions: NTI competitions, “Big Challenges” and the IChemPrize;
- “Laboratory of Chemical +”, which is focused on identifying, supporting and accompanying gifted children interested in studying chemistry both theoretically and practically;
- “Biochemistry and Molecular Biology”, where the combination of theoretical knowledge in chemistry and biology is performed, as well as an approach to solve Olympiad tasks of different level;
- Chemexpert, which includes a significant number of integration elements with other sciences (mathematics, physics, biology), as well as modules on inorganic and organic chemistry and also fundamental physico-chemical issues.

The Academy of Talents conducts intensive specialized educational programs, project programs for high pupils, as well as advanced training courses for St. Petersburg school teachers. Each program provides the participant with access to special high-tech equipment that allows them to carry out this project and educational activity successfully.



# A NEW APPROACH TO CHEMISTRY LESSONS FOR AN IN-DEPTH STUDY OF METALLURGICAL PRODUCTION ON THE EXAMPLE OF THE CITY DISTRICT OF VYKSA CITY OF THE NIZHNY NOVGOROD REGION

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The study of chemistry in primary and secondary school is the study of industries related to the field of chemistry. Such as pharmaceutical, petrochemical, metallurgical and others. It is one of the important approaches to the development of career guidance activities for students. This not only allows you to gain theoretical knowledge, but also connect theory with practice, specify, deepen and consolidate knowledge, but also helps graduates navigate their choice of profession.

The metallurgical industry for Russia is one of the main ones in terms of its scale, number of employees in the industry, share in GDP, exports, and volume of tax revenues.

In g.o.g. Vyksa, Nizhny Novgorod region, teaching chemistry is carried out in close connection with the Vyksa branches of NUST MISIS and one of the main employers of the city (Vyksa OMK plant).

For career guidance of students for the metallurgical industry and teaching chemistry, a program for studying chemistry has been developed on the territory of the branch. The program includes two projects: conducting binary chemistry lessons and "ProGUL (Urban Educational Landscape)"<sup>1</sup>.

The first project includes conducting lessons on the territory of the branch in two formats: a school teacher and a teacher of the branch: in one subject, chemistry or the connection of chemistry through other subjects from literature to physics. These lessons last an hour and a half and are divided into two parts where the school teacher gives knowledge on the Federal State Educational Standard, then this knowledge is superimposed on the practical (laboratory) part with an in-depth understanding of metallurgy, which is taught by a branch employee. The second project ProGUL (Urban Learning Landscape) is to transform Vyksa into a unified educational environment. One of the sites for this project is the branch. Lessons are taught by teachers, assisted by teachers. The lesson lasts 40 minutes according to the Federal State Educational Standard. There are also training days.

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# DIGITAL TECHNOLOGIES IN EDUCATION: POSSIBILITIES AND LIMITATIONS

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The violent development of information technologies in the perspective of storage, processing and transferring of information essentially alters matter of many traditional kinds of professional activities including education, medicine, arts, state administration, manufacturing, services sector and others<sup>1</sup>.

Digital transformation is laid out as one of national goals of evolution of Russian Federation for the period until 2030<sup>2</sup>. At the December of 2020 the regulation of Ministry of Education and Ministry of Digital Transformation “On adoption of experimental implementation of digital educational environment” has come into force.

Opinions of Russian universities faculty members on necessity of full digital transformation of education are widely held. 61% of respondents prefer hybrid form of education (full time with faculty members and remotely). Student can himself learn the theoretical material by means of online technologies with the help of educational software of University, but must have an ability in “physical” form to work in chemical laboratories, on modern equipment, if required to contact faculty members<sup>3</sup>. Other authors consider<sup>4</sup> the necessity of application of artificial intelligence methods for individual curriculum for every student according to his knowledge and talent. It will take the time to accumulate and summarize founded results, and to make conclusions.

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# AN EFFECTIVE INSTRUCTIONAL STRATEGY IN CHEMISTRY FOR HEARING-IMPAIRED STUDENTS – SUBJECTS OF INCLUSIVE PROGRAMS OF A TECHNICAL UNIVERSITY

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At BMSTU hearing- impaired students study chemistry within the framework of inclusive basic professional undergraduate educational programs (IP), in special conditions: a transformable digital environment; specific organizational and pedagogical solutions; comprehensive support of the study process<sup>1</sup>. Instructional strategies used by teachers in the classroom are of particular importance.

The goal of the study is developing and implementing an effective instructional strategy in chemistry for hearing impaired students taking into account their individual cognitive peculiarities and needs. The research methodology is based on a five-stage strategy<sup>2</sup>, which is implemented in a digital transformable environment and is the basis for applying a technological approach in teaching and learning<sup>3</sup>. Each stage of the strategy – orientation, presentation, practice, review and assessment – includes its own set of effective methods and technologies according to Universal Design for Learning Guidelines<sup>4</sup>, to ensure multimodality of information perception in students. The strategy has proven effective in teaching chemistry to both hearing-impaired students and ordinary ones.

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# USE OF MODERN EDUCATIONAL TECHNOLOGIES IN CLASSROOM AND EXTRA-CLASSROOM ACTIVITIES AS A MEANS OF ACHIEVING PLANNED RESULTS

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In my work I would like to see students who show interest in chemistry with high performance in mastering the educational program. My task is to teach children to think, because only the knowledge that is acquired independently, through work, is truly laid down and is the most valuable. Today, every teacher is looking for effective ways to interest students and improve the educational process. Taking into account modern requirements for the quality of education, it is simply not possible without the active use of modern educational technologies in classroom and extracurricular activities.

In my work, I implement and use several modern educational technologies.

The essence of our didactics is to find a way to teachers would teach less, but students would have learned more.

*(Jan Komensky)*

When choosing technology, it is necessary to take into account the capabilities of students and their age. When using modern educational technologies, students' educational motivation, quality of education, and cognitive activity increase both in class and outside of class time.

I use the following technologies: information and communication technology, research technology, gaming technology, health-saving technology, distance learning and reflection

Thus, I believe that by using modern educational technologies in teaching, I discover new interesting opportunities for myself in professional activities, I try to organize and direct the educational activities of students so that they themselves obtain knowledge and can practically use it. As a result, students' activities are activated and motivation to study the subject increases.

# PROBLEMS OF MODERN PROFESSIONAL PEDAGOGICAL EDUCATION

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At the present stage, the problems of professional training of chemistry teachers have sharply worsened, which invariably led to a decrease in the quality of the educational process in schools, both basic and advanced training of students.

1. Applicants to pedagogical universities take only one of the core subjects as an entrance exam, despite the fact that the training of future teachers (bachelors) is more often conducted in two profiles. And this exam, as a rule, is biology. The initial level of knowledge in chemistry of such applicants leaves much to be desired.

2. Focusing on the results of the entrance control, teachers are forced to compensate for the subject knowledge, skills and abilities necessary for the educational process of higher education. This requires considerable time, and sometimes correction of the content of academic disciplines.

3. The solution to this problem is seen in changing the rules of admission to universities at the federal level. If a graduate of a school claims to master vocational training programs in two profiles, then he must present the results in two disciplines corresponding to these profiles.

4. Natural sciences, and chemical sciences in particular, always require not only sufficient general pedagogical and methodological training, but also a powerful scientific base. Only then will the subject-based learning outcomes at school fully correspond to the required level of modern education.

5. At the same time, the content of professional pedagogical chemical education requires a certain correction in order to make it more applied, functionally literate and fully contributing to the formation and realization of opportunities for self-development and the formation of a creative personality of the future teacher.

# QUESTIONNAIRE AT CHEMISTRY UNIVERSITY

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In order to conduct an internal system for assessing the quality of education, the Kazan National Research Technological University conducts a survey of undergraduate and full-time students of enlarged groups of specialties. The questionnaire consists of 4 questions: “evaluate the relevance of the knowledge gained; «evaluate the ability to arouse interest in the subject”; “evaluate the accessibility of the material presented”; “your suggestions / wishes” (open type). Each of the indicators is evaluated on a five–point scale in the appropriate gradation (where 1 is the lowest score, 5 is the highest score). The survey is conducted in an anonymous form.

The comments received from students serve as a kind of determinant of criteria and quality indicators. Thus, through an anonymous survey of students, it is possible to determine the degree of anti-corruption education, the quality of material and technical equipment of classrooms and laboratories, the relevance of educational programs, the functioning of the administrative part of the University, as well as the professional skills of the teaching staff.

Also, the indicator of the anonymous questionnaire “Teacher through the eyes of students” (taking into account the achievement of the minimum established indicator for values) is included in the rating of the teaching staff as one of the elements of the rating assessment of the activities of the University teaching staff.

Over the course of several years of conducting an anonymous survey, the average indicator for the University has increased from 4.3 to 4.5. The experience gained in conducting a sociological study allows us to characterize the quality system of education in key aspects – the quality of the final result of the educational process and the quality management system at the University. The formed quality research system provides an objective “picture” of the educational institution’s activities.

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# CREATOR OF RUSSIA'S TECHNOLOGICAL INDEPENDENCE

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Many Russian scientists have made more than significant contributions to the treasury of world chemistry. Six of them were included in the list of one hundred outstanding chemists of Europe.<sup>1</sup>

Among these names there is at least one more missing – the name of a person who did not receive a special chemical education, but was a member of the Russian Chemical Society since 1890, completed an internship in the Munich laboratory of A. Bayer in 1896/1897, defended his doctoral dissertation in chemistry at St. Petersburg State University in 1908, was the clerk of the 2nd Mendeleev Congress in 1911, became an academician in the chemistry department of the St. Petersburg Academy of Sciences in 1916., member of the Supreme Economic Council in 1918–1930, Chairman of the Main Directorate of Chemistry in 1921–1927, named V.I. Lenin “the head of our chemical industry” in 1921.<sup>2,3</sup>

From 1936 to 1990 his name was banned as a “deserter of socialist labor”.<sup>4</sup> In 1994, he was restored to his rights, and the RAS Prize was established in his honor.

It's time to reveal his name – this is Vladimir Nikolaevich Ipatiev. “Never in the entire history of chemistry has a greater man appeared in it than Ipatiev”, said his contemporary Richard Martin Willstätter (1872–1942), an organic chemist and Nobel Prize laureate in chemistry for 1915.

The Mendeleev Congress is a worthy reason for making a decision to create a separate hall within the All-Russian Museum of Russian Chemistry, dedicated to the greatest chemist of Russia, who did a lot to create and strengthen the technological independence of the country. The Ipatiev family archive is open for this work.

This idea was supported by RAS academicians S.N. Kalmykova and Yu.G. Gorbunova. Perhaps the words of Bishop Anastasy Bratanovsky will come true: “Resurrect, resurrect in your memory those men who were an adornment of the human race”.

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# SIMULTANEOUS TEACHING STUDENTS WITH DIFFERENT BACKGROUND IN CHEMISTRY

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Fundamental and practical knowledge in chemistry is necessary for MISIS students for further specialization in areas such as the development of new materials, mineral processing, etc.

The difficulty of teaching chemistry in non-chemical universities is due to the enormous differences in the student's background.

To solve this problem, we have made changes to the organization of two types of chemistry classes: practical and laboratory (lecture classes remained unchanged).

We conduct practical classes in parallel for several groups of the lecture stream, but these are not academic groups, but groups "A", "B" and "C", which are based on the results of the test in accordance with increasing background in chemistry. The first classes in groups "A" are devoted to studying the basic laws of chemistry, in groups "B", to solving simple problems, in groups "B", to solving complex combined problems. In subsequent classes, the difference in the complexity of the problems solved in different groups gradually decreases, which is associated with the study of material that is new for all students.

During laboratory classes, students remain in their academic groups, and part of the group performs work in accordance with the main program. Students with a high background perform (in the same laboratory) more complex laboratory work from the alternative practical works we have developed. For example, in the laboratory work on the properties of solutions, strong students prepare a series of electrolyte solutions, measure their electrical conductivity, and analyze the dependence of the molar electrical conductivity of electrolyte solutions on the concentration.

This approach allows (within the same number of teaching hours) to make the first lessons in chemistry interesting for strong students by increasing the complexity of theoretical and experimental tasks, and at the same time, enables students who are poorly prepared in chemistry to quickly reach the level required for mastering the university program.

# THE SENSE OF SUBSTANCE

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The author has been observing many people of different ages manipulating with substances. Somebody manipulates unsuccessfully, somebody – successfully, even if they had never studied chemistry.

We believe that some people possess an ability to manipulate with substances without explicit instructions. We call this ability “the sense of substance”. It comprises “chemical eyes” (ability to notice essential features of substances and processes) and “chemical hands” (ability to put substances into optimal conditions).

The sense of substance is necessary but insufficient condition for effective treatment of substances and materials. Thus this sense should be developed during any learning.

In terms of cognitive psychology we believe that the sense of substance is a set of structures in long-term memory that is in good connection with structures that govern hands-on manipulations. It could be regarded as a complex product of implicit learning that is based on experience. In terms of connectionism we can state that implicit learning forms neural networks that don't include verbal components.

The assessment tool for the sense of substance is practical tasks. It could be to boil water in a test-tube\$ prepare mixture of two solid substances; dissolve a substance.

To develop the sense of a substance one should provide opportunity to get experience of working with substances accompanied with immediate feedback “right-wrong”. The best way is to provide this opportunity since birth. For example, a baby of several months begins to manipulate with materials touching them and feeling difference before he can walk. A 4 y.o. child being in appropriate environment would work through the skills that are necessary for posed task. A 6 y.o. child can perform quite complicated manipulations such as weighting substances and making mixtures. Thus we can state that the sense of the substances arises in early childhood and then is developed during the whole life. So one needs to care about development of the sense of substance at least at kindergarten. The 8<sup>th</sup> grade of the secondary school, when students begin to study chemistry, is too late.













Экологические проблемы планеты становятся все более значимыми и тревожащими, поэтому инновации, которые помогали бы эти проблемы решить, не просто привлекают интерес, а приобретают поистине глобальную актуальность. Сохранение окружающей среды и природных ресурсов для будущих поколений – суть новой этики прогресса.

## ПРОГРЕСС, БЕЗОПАСНЫЙ ДЛЯ ПРИРОДЫ

Компания «ФосАгро» – лидер российской химической промышленности выступила с инициативой создания фонда для финансовой и научной поддержки перспективных ученых-химиков, в сферу интересов которых попадают охрана окружающей среды, здравоохранение, продовольствие, повышение энергоэффективности и рациональное использование природных ресурсов.

В 2013 году между ЮНЕСКО, Международным союзом теоретической и прикладной химии (IUPAC) и компанией «ФосАгро» было подписано соглашение о партнерстве в создании программы грантов для ученых, занимающихся так называемой «зеленой химией». Предметом этого направления в науке является создание производственных технологий и материалов, безопасных для природы и человека.

Так родился проект «Зеленая химия для жизни», помогающий талантливой молодежи не только материальными средствами для

продолжения исследовательской работы и реализации проектов, но и плодотворным общением со старшими коллегами – видными современными химиками, и организацией информационного обмена в научной среде. Это первый проект в истории ЮНЕСКО и ООН, реализуемый за счет средств российского бизнеса. ФосАгро выделила более \$2,5 млн на развитие и реализацию проекта.

## ТРИНАДЦАТЬ МУДРЕЦОВ

Отбор заявок на участие в проекте – обязанность компетентного жюри, в которое входят 13 ученых из 11 стран. Проект-победитель должен соответствовать нескольким критериям. Оцениваются его научная новизна, глобальная и локальная значимость, соответствие принципам «зеленой химии», компетентность молодого ученого и его команды, оснащенность института и лабораторий, в которых предполагается вести проект. Качество работ очень высокое, и членам жюри приходится порой вступать в длительные диспуты по той или иной кандидатуре.

## НАУЧНЫЙ ПОИСК БЕЗ ГРАНИЦ

В 2016 году был учрежден специальный грант за исследования в области применения фосфогипса. В 2019 году в штаб-квартире ЮНЕСКО в Париже в рамках открытия Года Периодической таблицы химических элементов было принято решение продлить грантовую программу «Зеленая химия для жизни».

Проблемы экологического характера, к сожалению, есть во всем мире, и во всем мире есть ученые, которые предлагают решения для многих из этих проблем методами и технологиями «зеленой химии». Это наглядно демонстрирует география проекта «Зеленая химия для жизни». За время реализации программы на рассмотрение жюри поступило более 1000 заявок, 55 грантов было присуждено молодым ученым из 33 стран. Самый главный результат грантовой программы – практическое применение разработок молодых исследователей.



## ЖИЗНЬ ПОСЛЕ ГРАНТА

Дважды за первые 10 лет существования проекта победителями конкурса становились ученые из России. Одна из них – Галина Калашникова, заведующая лабораторией синтеза и исследования минералоподобных функциональных материалов Центра наноматериаловедения ФИЦ КНЦ РАН. В 2019 году грант «Зеленая химия для жизни» был присужден проекту «Разработка универсального и экологичного метода гранулирования синтетических титаносиликатных материалов (сорбентов, катализаторов, регенерируемых матриц), полученных на основе отходов региональных горно-обогатительных и металлургических производств».

### Галина Калашникова:

– В рамках проекта удалось опробовать 5 разных методов грануляции для новых материалов с широким функционалом свойств (сорбенты, катализаторы для органического синтеза, керамические матрицы), которые мы синтезируем именно в нашей лаборатории. Мы смогли выбрать наиболее подходящий метод получения гранул для каждого из них, а также приоритетные нетоксичные связующие. Полученные гранулы были опробованы в качестве сорбентов для очистки жидких радиоактивных отходов от радиоизотопов  $^{137}\text{Cs}$  и  $^{90}\text{Sr}$  совместно с лабораторией хроматографии радиоактивных элементов и станцией переработки радиоактивных отходов Института физической химии и электрохимии им. А. Н. Фрумкина РАН.

Работа по проекту продолжается, несмотря на окончание действия гранта. Все полученные средства были потрачены только на выполнение основной задачи, благодаря чему мы приобрели необходимое оборудование, получили хороший опыт в работе с зарубежными коллегами и выстроили приоритетные направления дальнейшей совместной работы со многими научно-исследовательскими организациями.

Хочется пожелать организаторам конкурса еще больше новых проектов, которые были бы направлены на самые острые вопросы взаимосвязи экологии и современной промышленности.





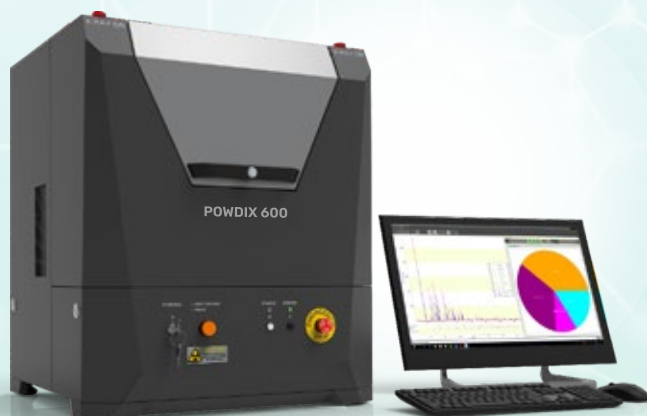
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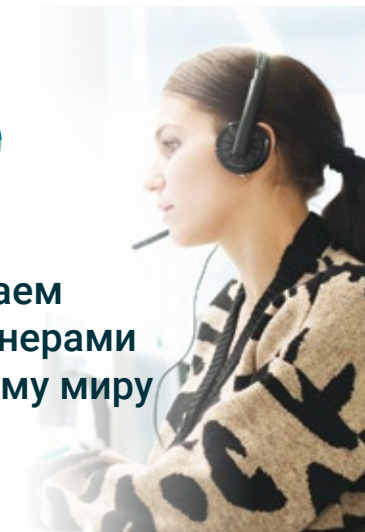
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