

75 YEARS



**Laboratory of Catalysis and Gas Electrochemistry
Physical Chemistry Chair**

Chemistry Department
M.V. Lomonosov Moscow State University

Edited by S.V. Savilov

**Current Achievements
2021/22**

THE LABORATORY HEAD

Dear colleagues and friends,
this year our Laboratory of Catalysis and Gas Electrochemistry is celebrating a memorable date - 75 years since its foundation. Throughout its history outstanding scientists have worked within its walls, which have made a significant contribution not only to Soviet and Russian science, but also to the development of world scientific thought.



Serguei Saviolov

As a tradition, the laboratory staff are actively participating in teaching activities and have nurtured a dozen of talented followers who are continuing the work of their teachers and developing new scientific directions.

Today our state-of-the-art laboratory is the largest at the Chemistry Department and one of the biggest in Europe. Its peculiarity is the combination of deep fundamental research and the development of applied technologies.

This anniversary issue is dedicated to the main scientific areas in which honored professors and doctors, young scientists, as well as talented people from the technical and engineering staff are involved.

CGE is more than a laboratory – it is the world of opportunity!

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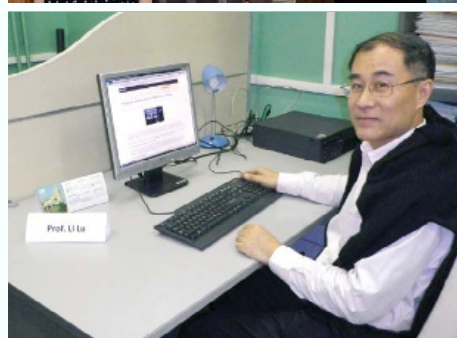
STRUCTURE

The laboratory is currently organized into 7 research groups focused on different areas of chemistry, material science, gas electrochemistry and catalysis.

Research groups, as key units of laboratory, develop research projects and collaborations to drive the frontier of science forward and transfer fundamental knowledge into valuable technologies.

Materials for Multifunctional Applications	Ionistors, Li-ion and Na-ion batteries	Catalysis and Green Chemistry	Ozone Applications and Atmospheric studies
• Synthesis and integration of carbon nanomaterials and polymer-based composites • Development of new carbon-based 2D materials and 3D frameworks • Synthesis and characterisation of hybrid polymer superabsorbents	• New 1D and 2D carbon nanomaterials for electrochemical energy storage • Design and application of new high-voltage ionic liquids • Multiscale characterization of electrode materials and processes	• Applications of functionalized carbon nanomaterials for Fischer-Tropsch synthesis and CO₂ conversion • Catalysts regeneration processes • Composite materials in gas-phase hydrodechlorination • Rice-husk utilization	• Physicochemistry of ozone reactions with halogen-containing compounds • Atmospheric Chemistry • Ozone oxidation activity • Technologies of water purification by ozone • Atmospheric aerosols
Advanced Ceramics	Supercritical Fluids	Biological Applications	Cellulose derivatives
• New generations of ceramic materials • Elaboration of new synthetic approaches • Systematic studies of ceramics • Application of ceramics in functional devices	• Studies of compounds and mixtures in supercritical state • Discoveries of new processes • Development of new laboratory and manufacture practice	• Laser technologies for tissues treatment • Magnetic materials for anticancer therapy • Carbon nanotubes for the biomarker delivery • X-Rays tomography	• Study of biomass delignification by ozone • Extraction of native lignin • Nanocellulose techniques • Cellulose esters for cosmetics and building industry

INTERNATIONAL COOPERATION



PROJECTS IN FOCUS

Achieving Coupling MnO₂ Electrode-Redox Electrolytes via Functional Interface for High-Performance Supercapacitors

Funding: Russian Science Foundation

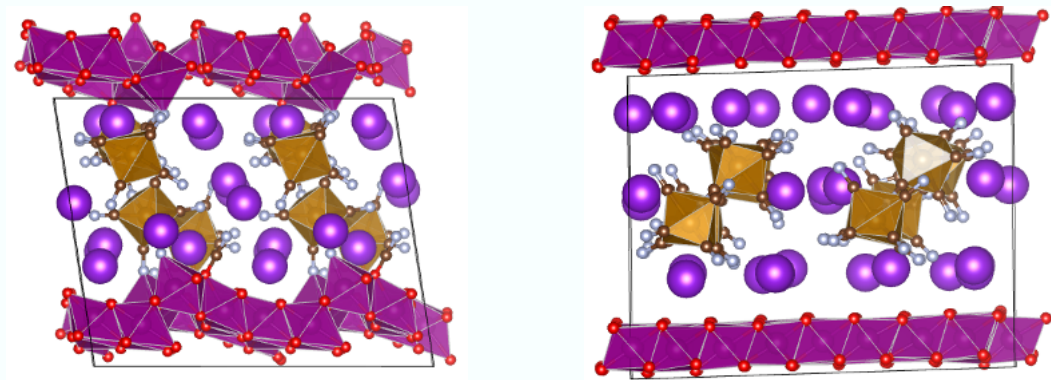
Project period: 2020-2022

Principal Investigator: S.V. Savilov

Most of commercial supercapacitors (SCs) are based on electrochemical double layer (EDL) mechanism, providing specific power as high as 20 kW/kg but a relatively low energy density of 5~8 Wh/kg (6~10 Wh/L), which severely limit the widespread application of SCs. To minimize the energy gap between SCs and other widely used high energy storage devices (rechargeable batteries, fuel cells, etc.), Faradaic processes involved SCs, also called Pseudocapacitors, have emerged as research focus toward the alluring features: high energy as well as large power with long cycling life. The Faradaic charge transfer between electrolyte and (sub)surface of suitable transition metal oxides /hydroxides (TMOs) is crucial to the pseudocapacitors.

Among various TMOs, MnO₂ has been extensively reported as a promising electrode material for supercapacitors due to its low cost and nontoxicity. It has been proved that the surface modification of MnO₂ not only enables fast electronic & ionic transport but also confines the redox electrolyte ions around the electrode surface to provide highly efficient pseudocapacitance with low self-discharge rate. Yet, the coupling mechanism between modified MnO₂ and redox electrolyte in microscale (molecular or atomic level), regulation strategy, and pseudocapacitive mechanism are still not clear. Therefore, in this project, the solid liquid interface modification is proposed to reinforce the coupling between MnO₂ and redox electrolyte ions, aiming at increasing pseudocapacitive sites and improving corresponding reaction kinetics in electrode & electrolyte system for high energy & power density. Efficient surface modification methods will be developed for targeted coupling. The mechanism of coupling, energy storage, and self discharge improvement in electrode & electrolyte systems will be clarified by studying the associated chemical structure of surface modified MnO₂ with mono or multilayer of targeted redox electrolyte molecules during charge/discharge process. Accordingly, the optimized MnO₂ based negative electrode redox electrolyte system with high electrochemical performance will be fabricated. Finally, advanced asymmetric supercapacitors with high energy density (> 10 kWh/kg) as well as high power density will be assembled by rational integration of negative and positive electrodes in redox electrolytes. The successful implementation of this project will provide theoretical guidance and technical support for advanced and practical asymmetric supercapacitors.

PROJECTS IN FOCUS



Interfaces δ -MnO₂ [001]- K₃[Fe(CN)₆] [111] (left) and δ -MnO₂ Delta [001] K₄[Fe(CN)₆] [111] (right) "C" configuration

- The mechanisms of interaction, energy accumulation, and self-discharge in the electrodes / electrolyte system will be thoroughly studied by the investigation of the structure and properties of the modified electrode material surface based on MnO₂, incl. upon the contact with redox electrolyte molecules and during charging / discharging processes;
- Modification methods the electrode material surface will be developed. Their use will allow not only the introduction of reactive active surface centers that take part in the implementation of pseudo-capacitive interactions, but also aimed at obtaining an electrode material with developed porosity and high values of the specific surface area;
- The synthesis ways of redox electrolytes will be proposed. The electrochemical properties of these systems will be also studied;
- The advanced asymmetric supercapacitors with high energy density (> 10 kWh/kg), high power density as well as long cycling (>1000 0 cycles) will be assembled.

These results will make it possible to implement new technologies for the production of safe and inexpensive supercapacitors with high power and energy characteristics corresponding to the world level. This will lead to the creation of new industries and the organization of jobs, which indicates the high social significance of the project.

PROJECTS IN FOCUS

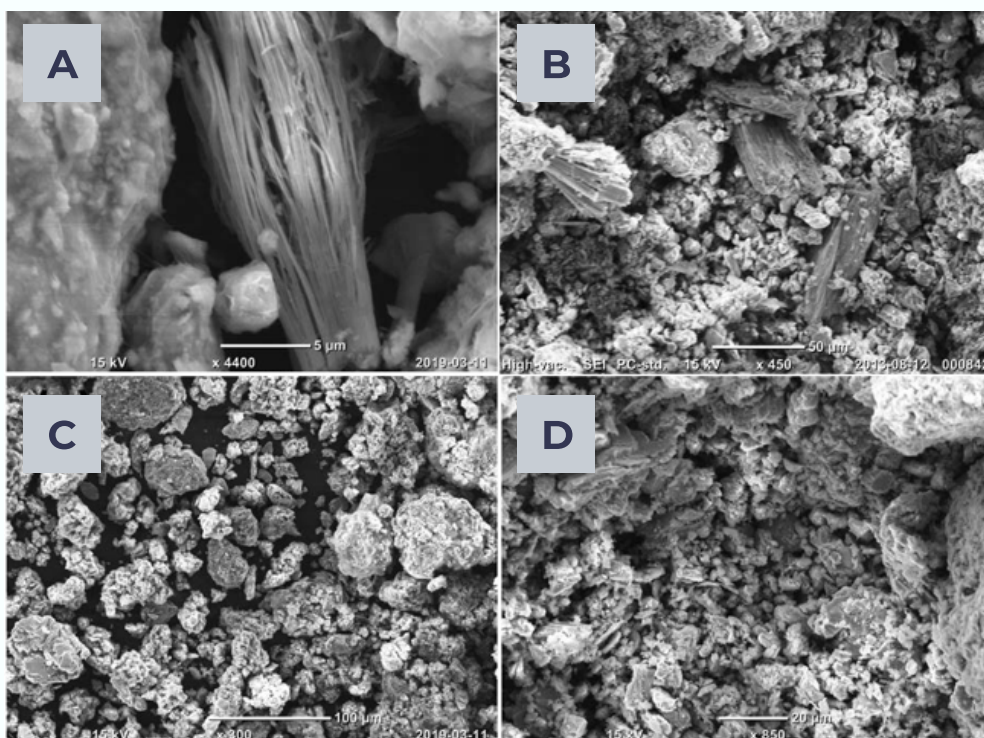
New 2D materials as electrodes for energy storage systems

Funding: Russian Foundation for Basic Research Project

Project period: 2019-2021

Principal Investigator: E.V. Suslova

The project is aimed at development of highly efficient devices for energy storage and assumes a comprehensive approach for their implementation based on various types of two-dimensional materials. The project participants have the experience in both-synthesis and characterization of electrode materials and electrolytes, as well as in the assembling and testing of electrochemical devices. Project is focused on the use of the 2D layered materials – graphene derivatives and MXenes - for supercapacitors with non-aqueous electrolytes, as well as lithium and sodium-ion batteries. The implementation of this project will allow to develop new energy storage devices with high capacitance, power and performance characteristics, increase their safety. It is important that there are a lot of young participants in the team, and getting the project will allow them to gain a foothold in the scientific community, establish close international relations.



PROJECTS IN FOCUS

Visualization and quantitative analysis of biopolymers in vivo via photon counting computed tomography enhanced by nanocomposite contrast agents

Funding: Russian Science Foundation

Project period: 2022-2024

Principal Investigator: G.A. Chelkov, E.V. Suslova

The study of biopolymers (for example, receptors or enzymes) and the quantitative analysis of their content and activity in various tissues and organs are necessary for the study of biochemical processes and pathogenesis of various diseases, as well as for the study of potential drugs.

This problem can be addressed in experimental settings (with possible subsequent implementation in clinical diagnostics) can be the use of multi-energy computed tomography (CT). This method allows to assess not only the overall X-ray density of the tissues and organs under study, but also to identify and visualize up to 6 compounds that differ in the spectral lines of their constituent elements. Thus, multi-energy CT allows simultaneous direct in vivo study of biopolymer systems that is unattainable with other methods.

Effective use of CT requires the use of contrast agents (CA). CA must satisfy several requirements, namely, have a high content of an element with an atomic number of more than 28, have known and controllable pharmacokinetic characteristics, have a high affinity for the target biopolymers, and also do not require a unique synthesis process (which is critical given the need to work with several CAs simultaneously to realize all the multi-energy CT capabilities). Those that satisfy all of the above requirements are virtually absent.

In this project we propose to develop and implement composite CAs constituted by lanthanide (Ln) nanoparticles deposited on nano-scaled matrix structures based on carbon and/or SiO₂, covalently bonded to low-molecular “anchor” compounds with high affinity to target biopolymers. The use of matrices will allow stabilizing Ln nanoparticles, simplifying synthetic processes, and facilitating development of CAs with the required pharmacokinetic parameters. The use of Ln will make it possible to synthesize series of CAs (differing in Ln included in the composite) using similar synthetic processes. In the future, this technique can also be adapted as a method of controlled delivery of low molecular weight drugs to the target tissue, which will lead to the creation of fundamentally new methods of pharmacotherapy.



MARS BioImaging multi-energy computed tomograph

PROJECTS IN FOCUS

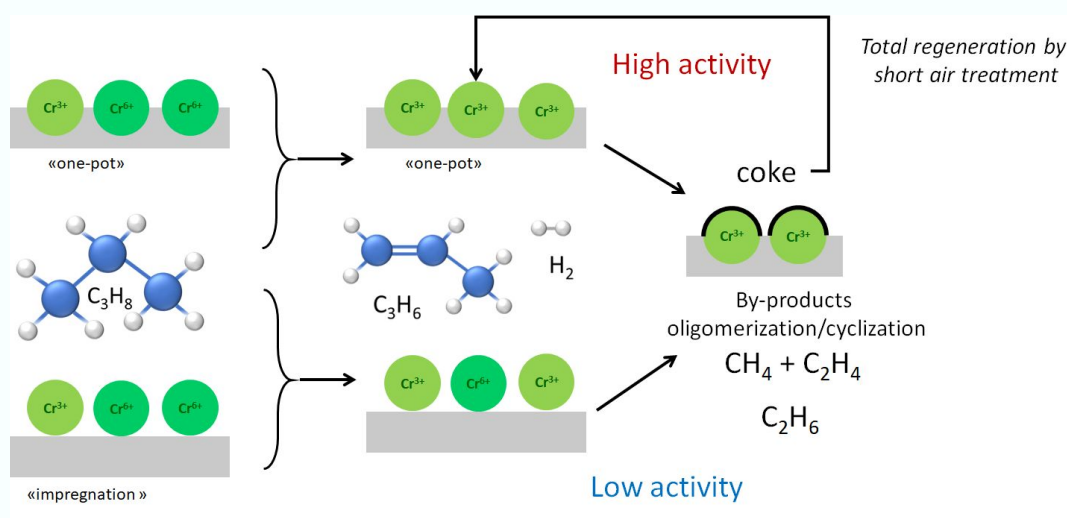
Design structured oxide catalysts with ultra-low content of active components for non-oxidative dehydrogenation of propane

Funding: Russian Science Foundation

Project period: 2022-2023

Principal Investigator: E.V. Golubina

The project is aimed at finding and researching new ways to form a catalytically active phase based on Cr_2O_3 and precious metals in order to reduce the amount of the active component while maintaining or increasing the efficiency of catalytic systems in the non-oxidative dehydrogenation of propane. The advantage of non-oxidative dehydrogenation of propane in comparison with oxidative dehydrogenation is the exclusion of raw material loss due to irreversible oxidative processes. The urgent task is to develop highly efficient and selective catalysts that suffer less from decontamination as a result of coking and form fewer by-products. The solution of this problem is possible on the way of more efficient structural organization of catalytic systems, which allows to reduce the number of cracking and oligomerization centers leading to the formation of coke, optimization of the electronic state of active centers and surface structure, which makes it possible to achieve rapid desorption of the target product of the reactor.



PROJECTS IN FOCUS

Transformation of halogen-containing ecotoxics on microparticles in the atmosphere, hydrosphere and pedosphere

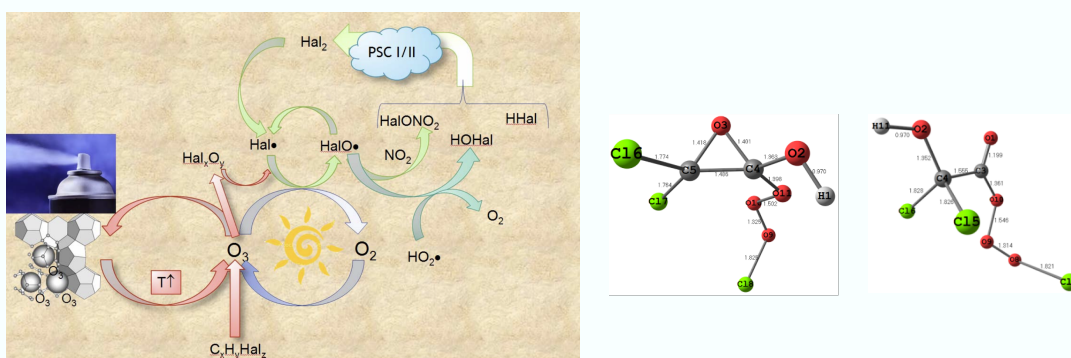
Funding: Russian Foundation for Basic Research Project

Project period: 2020-2022

Principal Investigator: S.V. Savilov

The constantly increasing human impact on natural ecosystems stimulates the study of finely dispersed objects in these ecosystems. Thus, atmospheric aerosols can have a significant impact on the stratospheric ozone depletion, climate change, transport and chemical reactions of environmental pollutants. Numerous atmospheric transformations of organochlorine compounds initiated by hydroxyl radicals result in the formation of various types of toxicants in the atmosphere.

The systematic study of the physical and chemical properties of a large number of atmospheric components using the most modern instrumental approaches allowed supplementing the climatic models of the atmosphere of our planet, in particular, emphasizing the role of non-photolytic processes of stratospheric ozone destruction.



Ab-initio quantum-chemical calculations resulted in the equilibrium geometries of the several intermediates.

The interaction of chloroacetic acids with ozone was studied under conditions close to stratospheric using low-temperature IR Fourier-spectroscopy.

PROJECTS IN FOCUS

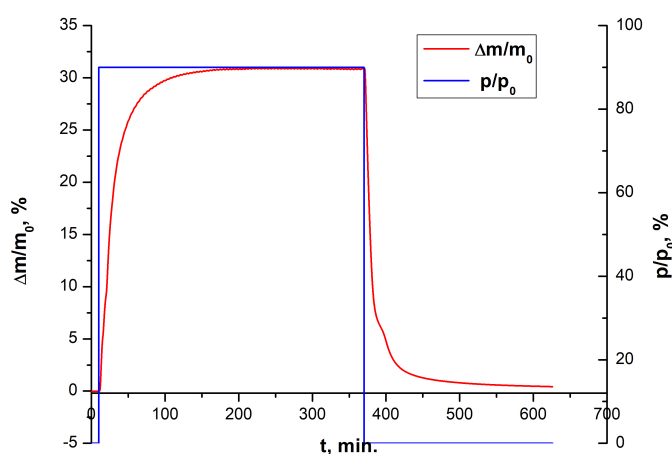
Features of organic solvents adsorption on modified carbon materials

Funding: Ministry of Science and Higher Education of the Russian Federation

Project period: 2022-2023

Principal Investigator: S.Yu. Kupreenko

The aim of the project is to study the effect of doping and oxidative functionalization of carbon nanomaterials (CNM) on the kinetics of volatile organic compounds (VOC) vapour sorption. First it is necessary to study adsorption on model structures. Carbon nanotubes (CNT) and few-layer graphene nanoflakes (GNF) were chosen as model structures. These materials contain graphene layers twisted into tubes or stacked, respectively. The introduction of heteroatoms (N, S, Si...) leads to appearance of many defects and adsorption centers on the CNMs surface, a change in the surface conductivity, which affects the organic solvent vapour sorption. Oxidative functionalization increases the polarity of the surface, which promotes the adsorption of polar molecules, but this reduces the volume available for adsorption. After investigation of all factors influencing the sorption kinetics, one can proceed to the study of inexpensive porous carbons using the example of carbons obtained by the pyrolysis of rice husk, agricultural waste. It should be noted that there are no works devoted to research the effect of doping with various elements and functionalization of the surface on the kinetics organic solvent vapour sorption by CNMs. Adsorption on some new doped materials (S-GNF, Si-GNF) has not been studied. The obtained fundamental regularities can be used in various adsorption technologies (air purification from VOCs vapours, vapour sensors), heterogeneous catalysis (catalytic conversion of alcohols) and electrochemistry (selection of the optimal pair of electrode material and electrolyte in energy storage devices).



Dependence of the relative change in mass of CNT $\Delta m/m_0$ on time with a change in the vapour pressure p/p_0 of toluene and linear approximation of mass versus time for estimation of the diffusion rate D (d – diameter of CNT).

PROJECTS IN FOCUS

Creation of new antiarrhythmic drugs – potassium channel blockers based on indole-3-carboxylic acid derivatives

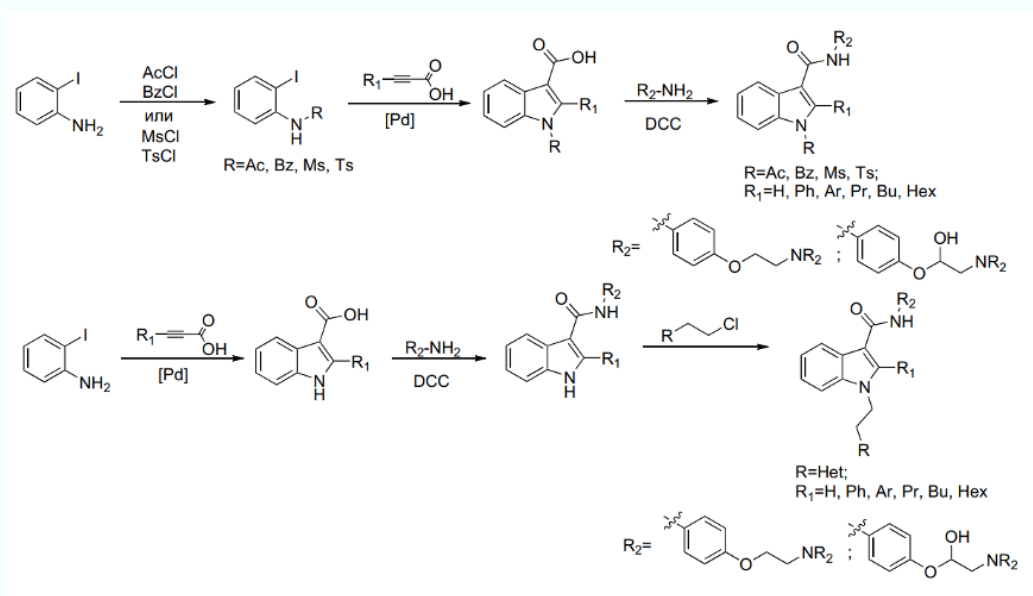
Funding: Russian Science Foundation

Project period: 2022-2023

Principal Investigator: A.N. Volov

Cardiac arrhythmias are one of the most frequent and severe complications of various cardiovascular diseases – coronary heart disease, myocarditis, rheumatic malformations, cardiomyopathy, hypertension, etc. Arrhythmia and ventricular fibrillation are observed in 94% of cases in patients with a heart attack and, as a rule, are the direct cause of death. The variety of forms of cardiac arrhythmias and conduction disorders, their high prevalence, danger to life are the main reasons for creating new, more effective and safe medicines for the prevention and treatment of arrhythmias.

The project is aimed at creating new and effective antiarrhythmic drugs - blockers of hERG potential-dependent potassium channels based on indole-3-carboxylic acid derivatives. During the Project, new 1,2-disubstituted derivatives of indole-3-carboxylic acid will be synthesized and their antiarrhythmic activity on different groups of animals with different methods of administration will be investigated. The affinity of the obtained compounds will be determined by radioligand binding with the corresponding biomimetic (hERG potential-dependent potassium channels) and the results obtained will be compared with those for the drug amiodarone, which is the most effective among antiarrhythmic drugs today. Then the leading compounds will be selected (based on data obtained as a result of radioligand binding) and their antiarrhythmic activity on various animal species and with different methods of administration (intravenous, intramuscular, oral) will be investigated.



PROJECTS IN FOCUS

New anti-tuberculosis drugs based on 5-alkynyl-substituted pyrimidine nucleosides

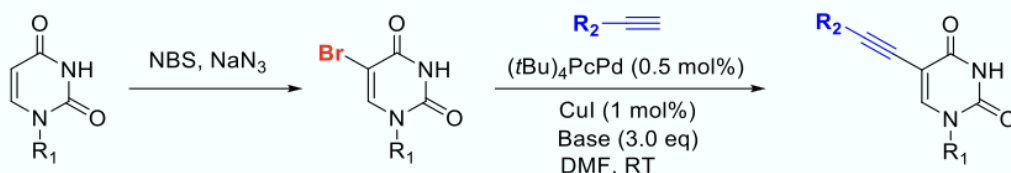
Funding: Ministry of Science and Higher Education of the Russian Federation

Project period: 2022-2023

Principal Investigator: Ya.B. Platonova

According to the World Health Organization, tuberculosis is an extremely socially dangerous disease that claims millions of lives around the world every year. It should be noted that new strains of mycobacteria are constantly appearing, responsible for the infection and development of tuberculosis in biological objects (*Micobacterium tuberculosis*, *Mycobacterium bovis* and *Micobacterium avium*), which are partially or completely resistant to existing antimycobacterials.

The aim of this work is to synthesize a number of new 5-alkynyl-substituted pyrimidine nucleosides proposed as promising highly effective anti-tuberculosis drugs for the treatment of multidrug-resistant tuberculosis and having improved pharmacological characteristics compared to known anti-tuberculosis drugs such as rifampicin, cycloserine and isoniazid. In the course of the Project, the design of compounds and preliminary molecular docking of ligands with biomishen will be carried out, a synthetic approach to new 5-alkynyl-substituted pyrimidine nucleosides based on uracil containing various sugars in their structure will be developed, and their in vitro antimycobacterial activity in comparison with known anti-tuberculosis drugs will be investigated, as well as in vivo experiments on different groups of animals.



PROJECTS IN FOCUS

Modified by silicon, manganese and copper oxides catalysts based on mesoporous ceria and zirconia: the scientific basis of template synthesis and catalytic properties in the oxidation of carbon monoxide and catalytic properties in the oxidation of carbon monoxide

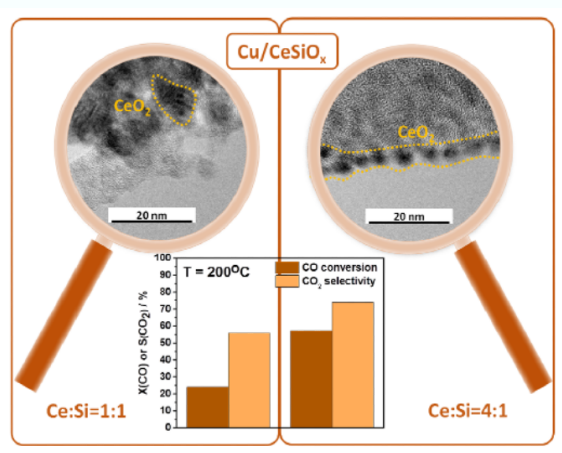
Funding: Russian Foundation for Basic Research

Project period: 2020-2022

Principal Investigator: I.Yu. Kaplin

The aim of this project is the development of scientific basis for the preparation of new highly efficient oxide catalysts based on modified oxides of cerium or zirconium for the preferential CO oxidation in the presence of excess hydrogen (CO-PROX).

For this purpose, three-component composite materials comprising CeSiO_x or ZrSiO_x and copper or manganese oxides as additional modifiers have been prepared using template methods. The effect of template synthesis conditions on the texture, structure and other properties of oxide catalysts important for the catalysis have been studied using a set of modern physical-chemical methods. The features of the formation of active centers in these catalytic systems have been studied. Catalytic tests in CO-PROX have been performed using reaction mixtures with variable $\text{CO}:\text{H}_2$ ratios. The effect of other gas additions - carbon dioxide and water vapor - has also been studied. A detailed study of the kinetic parameters of the reaction in a continuous flow system and their comparison with the results of the physicochemical characterization of catalysts made it possible to propose a mechanism for the processes occurring in the course of the reaction. Based on the results obtained, directions for modifying the methods for the synthesis of oxide catalysts are proposed, which make it possible to increase their efficiency in CO-PROX reaction.



PROJECTS IN FOCUS

Orientation ordering of layers in graphite oxide membranes. Determination by the spin probe method.

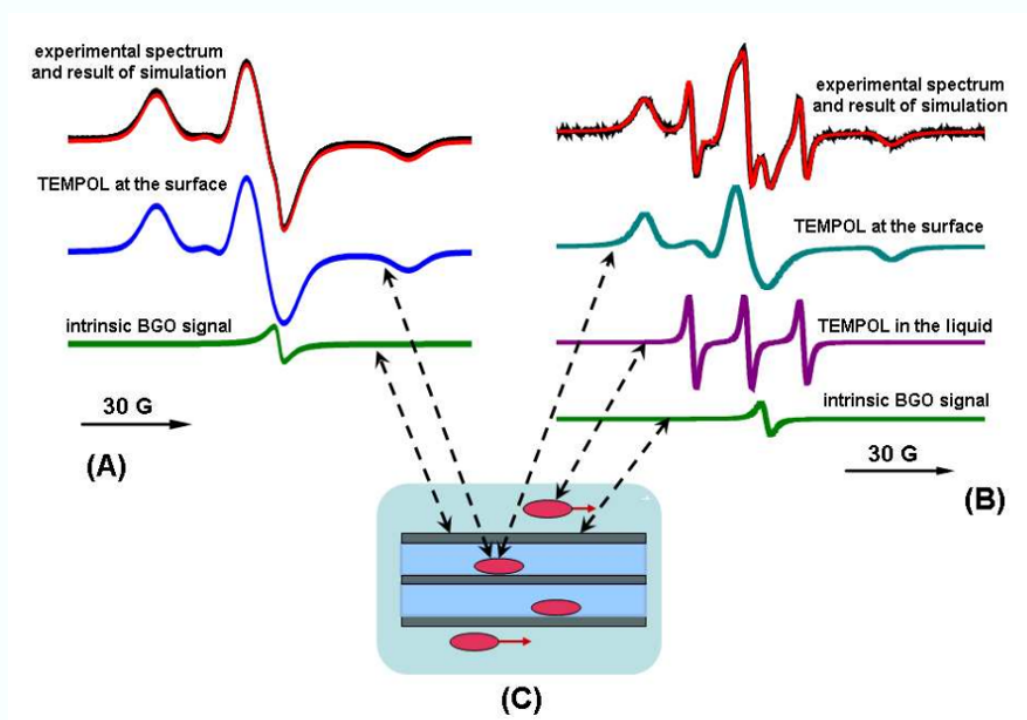
Funding: Russian Science Foundation

Project period: 2021-2023

Principal Investigator: A.T. Rebrikova

Graphite oxide membranes are of increasing interest of the scientific community due to their highly selective permeability of liquids and gases and the possibility to use them for separation of polar mixtures. Manufacturing method, thickness, interplanar distance and sorption capacity of the membrane are used to specify graphite oxide membrane. At the same time, inner structure of the membrane (order of graphite layers, presence of pores and defects) is practically not considered due to the lack of suitable experimental methods. The main scientific problem is to establish the relationship between the morphology of graphite oxide membranes and method of preparation and its thickness.

The main objective of this fundamental project is to develop the spin probe method for determining the orientation parameters of the graphite layers order in graphite oxide membranes and for establishing the relationship between the orientation order of the membranes and their properties. It was experimentally shown orientational alignment of the membranes affects strongly the sorption capacity: the higher ordered membranes don't sorb acetonitrile but easily sorb water.



PROJECTS IN FOCUS

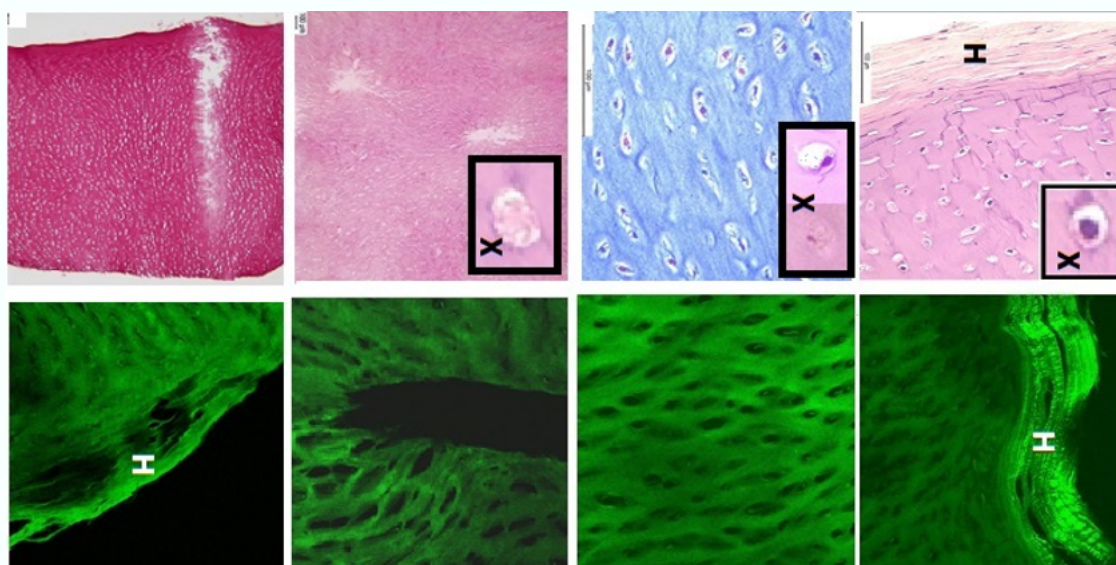
Transformation of the nasal septum cartilage into the tissue engineering construction for orthopedics using infrared laser radiation

Funding: Russian Foundation for Basic Research Project

Project period: 2019-2021

Principal Investigator: N.Y. Ignatyeva

The project is aimed at developing a new approach to human tissue repair, which consists of creating a biomimic supporting structure (scaffold) based on animal tissue. We propose using cartilage of the nasal septum, including hyaline cartilage, transitional zone and perichondrium. After a complex treatment with moderate intensity IR radiation and chemical reagents, the non-immunogenic and multilayer scaffold will have the necessary elastic-mechanical properties and will provide the necessary differentiation of the cells in different parts. The effect of photothermal and photomechanical effects of IR laser radiation of moderate intensity on the damage of cellular structures in a solid matrix and on the change in the matrix of a complex composition will be evaluated.



PRIVATELY-FUNDED R&D PROJECTS

ADVANCED ELECTROCHEMICAL MATERIALS CHARACTERIZATION

Funding: Global SO

Project period: 2012 - 2022

Principal Investigator: S.V. Savilov

VERIFICATION AND REFINEMENT OF TECHNOLOGICAL SOLUTIONS FOR THE PRODUCTION LINE OF AMORPHOUS SILICON DIOXIDE AND ACTIVATED CARBON, AS WELL AS CUSTOMIZATION OF THE PRODUCT LINE ACCORDING TO CUSTOMER REQUIREMENTS

Funding: Rice HT

Project period: 2018 - 2021

Principal Investigator: R.Yu. Novotortsev

IMPROVEMENT OF THE PLASTIC LUBRICANTS PROPERTIES

Funding: Intesmo (Lukoil group)

Project period: 2018 - 2021

Principal Investigator: S.V. Savilov

RESEARCH WORK ON THE STUDY AND DIRECTED MODIFICATION OF THE PROPERTIES OF COMMERCIALY OBTAINED COMPOSITIONS BASED ON WATER-RETAINING ACRYLATE GELS

Funding: ChemRusAgro

Project period: 16 March 2020 - 31 December 2022

Principal Investigator: S.V. Savilov

DEVELOPMENT OF FUNDAMENTALS AND TECHNOLOGICAL SOLUTIONS FOR THE PRODUCTION OF MODIFIED AMORPHOUS SILICA DERIVATIVES

Funding: Rice HT

Project period: 1 February 2021 - 31 December 2021

Principal Investigator: S.V. Savilov



Биоселтек
ГК ХИМУСАГРО



ХИМУСАГРО
ГРУППА КОМПАНИЙ



СПЕКТРОСКОПИЧЕСКИЕ СИСТЕМЫ



RESEARCH

CARBON NANOMATERIALS SYNTHESIS, INVESTIGATION AND APPLICATIONS

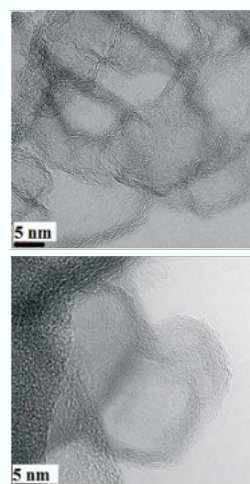
Scientists involved to the topic:

S.V. Saviolov, E.V. Suslova, S.A. Chernyak, A.S. Ivanov, S.V. Maximov, S.Yu. Kupreenko, R. Yu. Novotortsev, S.V. Dvoryak, N.A. Tabarey, E.A. Arkhipova, N.N. Kuznetsova

A scientific team of the leading researcher Dr. habil. Serguei V. Saviolov provides a wide range of researches connected with carbon nanomaterials and their applications. Besides he takes part in various collaboration projects with universities all over the world. The continuous growth of the scientific interest to carbon nanomaterials (CNMs) deals with their application perspectives in different spheres on industry. Numerous of studies are devoted to their synthesis and investigation of physico-chemical properties as well as experimental search for the materials with the optimal parameters for certain areas. Nevertheless, only small part of researches is devoted to their fundamental characteristics. That is why the data on correlations between structure, composition and thermophysical parameters of different types of CNMs sometimes are contradictory. Group members summarize them as well as provide original experimental results demonstrating the dependence of burning temperatures, heats of combustion and enthalpies of formation on structure, type and amount of functional groups of CNMs. Original experimental results on thermochemical and structural features as well as surface chemistry of different types of carbon-based nanostructures were obtained by adiabatic bomb calorimetry, thermal analysis, XRD, NMR, EPR, HRTEM, XPS and Raman spectroscopy. It was demonstrated for the first time that heats of formation and burning temperatures are extremely sensitive to the structure, specific surface area, heterosubstitution as well as presence of functional groups and adsorbed species. They also provide the wide practical use of CNMs. Group members applied them as an effective fillers in polymer composites and plastic lubricants, component of metal alloys, catalysts, electrode materials for supercapacitors, ion-istors and metal-ion batteries.



Serguei Saviolov



RESEARCH

CARBON NANOTUBES AND GRAPHENE NANOFLAKES FOR CATALYSIS APPLICATIONS

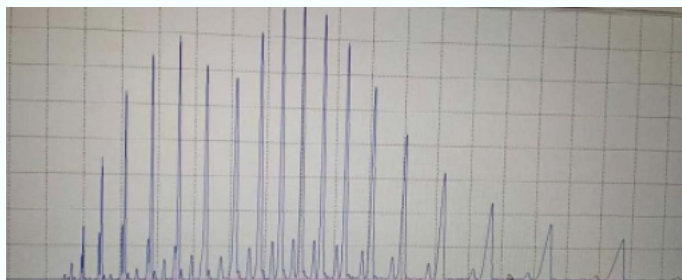
Scientists involved to the topic:

S.A. Chernyak, S.V. Maximov, R. Yu. Novotortsev

Research interests of Senoir Researcher Dr. Sergei Chernyak could be divided in three areas:

- **Long-term study of Co-based Fischer-Tropsch catalysts supported on oxidized carbon nanotubes (CNTs).**

High stability of this system was observed: CO conversion did not decrease during 3 weeks of catalytic tests. TEM monitoring of Co particle size during the experiment revealed that metal crystallite diameter grew at the induction period of 2-3 days from less than 4 nm to optimal value of 8-15 nm. Such increase promotes the high activity and selectivity of the catalyst.



Chromatogram of liquid fraction obtained during the Fischer-Tropsch synthesis (FTS).

- **Effect of nitrogen doping of graphene nanoflakes (GNFs) on the structure and catalytic properties of Co/GNF FTS catalysts.**

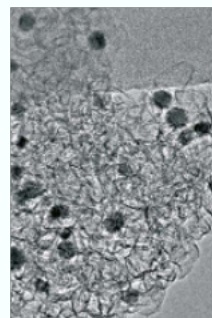
It was found that N-doping of carbon support by pyrrolic, pyridinic, and graphitic nitrogen increase catalyst activity by 2-3 times. XPS studies of initial N-GNFs, annealed and reduced catalysts allowed us to determine the mechanism of thermal transformations of nitrogen functionalities.

- **Synthesis of catalytically active materials using spark plasma sintering technique (SPS).**

Metal-CNT frameworks contained Co, Fe, Ni, and Cu were obtained by SPS treatment of CNTs decorated with nanoparticles of appropriate metal oxides. Metallic phase formed during the synthesis because of oxide reduction by carbon and graphitic shells and were observed on the nanoparticle surface after the experiments. It was shown that metal addition increases the electrical conductivity of CNTs. Moreover, resulted samples demonstrated ferromagnetic properties. Co-based structures exhibited noticeable catalytic activity in FTS and carbon shells around the metal particles allowed us to skip the catalyst reduction stage.



Sergei Chernyak



TEM image of Co/N-GNF catalyst.

RESEARCH

3D FRAMEWORKS OF CARBON NANOMATERIALS

Scientists involved to the topic:

E.V. Suslova, A.P. Kozlov, Z.O. Zoirova

Senior Researcher Dr. E.V. Suslova and A.P. Kozlov work on creation and investigation of 3D frameworks of carbon nanomaterials as well as study of the thermochemical properties. She adapts synthesis conditions and concentrations of frameworks' precursors.

Group members study the application of spark plasma sintering (SPS) to multiwalled carbon nanotubes and nanoflakes, which was found to be an effective route to their compactisation for further use in catalysis and as electrode materials for energy storage devices. It was found that the increase of temperature and pressure during SPS increased the density of the sintered samples and decreased their surface area. It is accompanied by appearance of the mesopores. Raman spectroscopy, TG and X-ray data show that the defectiveness of the CNTs decreased during SPS. Using a focused beam of the transmission electron microscope in-situ experimental simulation of the CNT consolidation and their crosslinking was successfully performed together with Dr. A.V. Egorov for the first time.

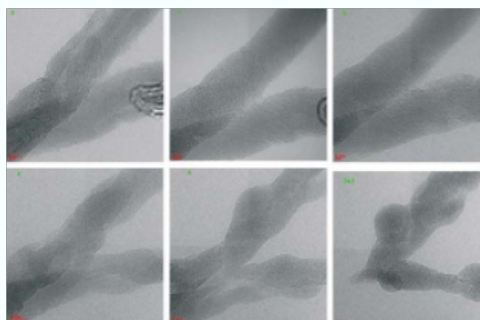
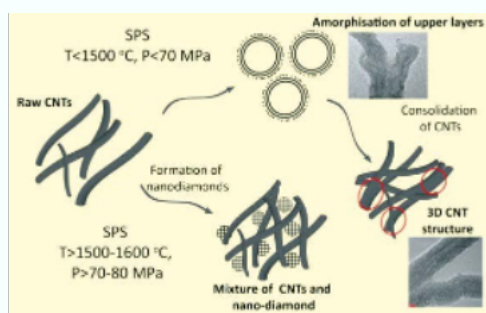
Together with colleagues she performed systematic investigations and stressed sufficient correlations between structure, composition and properties of carbon nanomaterials and their N-doped derivatives. The adiabatic bomb calorimetry technique was used for determination of these values, together with elemental and thermal analysis, electron microscopy, Raman and X-ray photoelectron spectroscopy applied for structure and composition analysis. The contributions of surface and bulk components in the values of enthalpies of formation for different CNMs were estimated for the first time. It is shown that the first one is highly influenced by the surface area while the latter — is defined by the number and homogeneity of inner layers, conformable to graphite structure. In the case of nitrogen-doped CNMs heat of formation is influenced not only by the nitrogen content but by coordination of heteroatom; substitutional nitrogen demonstrate higher effect comparing to pyrrolic and pyridine-like ones.



Evgenia Suslova



Alexey Kozlov



RESEARCH

DEVELOPMENT OF COMPLEX CATALYSTS FOR HYDRODECHLORINATION OF CHLOROBENZENE AND CO OXIDATION

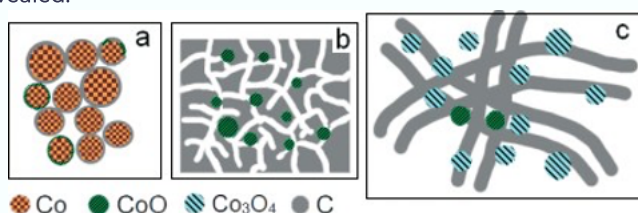
Scientists involved to the topic:

E.S. Lokteva, E.V. Golubeva, S.V. Klovov, A.N. Kharlanov, A.V. Fionov, L.V. Voronova

Leading researcher Prof. Ekaterina Lokteva and Associate professor Dr. Elena Golubina work with different composite materials including cobalt and carbon, comparing their properties in gas-phase hydrodechlorination of chlorobenzene in flow-type fixed-bed system. The role of different oxidized Co particles in catalytic activity was revealed.



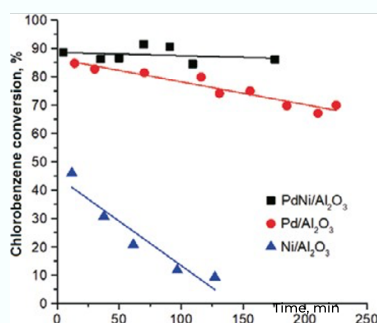
Ekaterina Lokteva



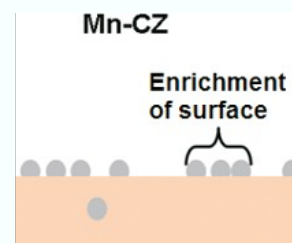
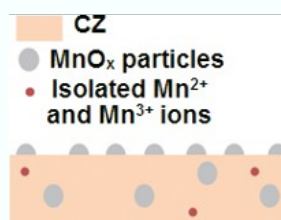
The scheme of structure of Co@C (a), Co/C (b) and Co/CNT (3) composites on the base of TEM, XPS and TPR data

For the first time bimetallic NiPd systems with average particles size of 1 nm synthesized by laser electrodispersion (LED) were tested in hydrodechlorination reaction. The NiPd/Al₂O₃ bimetallic catalyst at 150–350°C is superior in gas-phase hydrodechlorination of chlorobenzene not only to nickel, but also to palladium monometallic analogue, as a result of the formation of new bimetallic active centers at the contact of PdO and NiAlOx.

Oxide catalysts Ce_{0.8}Zr_{0.2}O₂ (CZ), MnO_x-Ce_{0.8}Zr_{0.2}O₂ (Mn-CZ), CeO₂ and MnO_x were produced by co-precipitation from the corresponding salts solution using CTAB as the template, and tested in CO total oxidation. Both catalysts despite the big difference in SBET values are nearly equally effective in the wide temperature range in CO oxidation.



Chlorobenzene conversion vs reaction time at 200°C in the presence of mono- and bimetallic LED catalysts.



Elena Golubina

WATER VAPOR ASSISTED SYNTHESIS OF OXIDE POWDERS FOR CERAMICS AND GLASSES

Scientists involved to the topic:

M.N. Danchevskaya, Yu.D. Ivakin, A.A. Kholodkova and G.P. Muravieva

A research group focused its interests on the processes occurring in solid oxides exposed to the media of water vapor or supercritical water. Interaction between oxide matrix and water molecules was revealed to induce chemical and physical transformations resulting in formation of new complex phases, recrystallization, and low-temperature ceramics sintering. The directions of the recent research by Dr. M.N. Danchevskaya, Dr. Yu.D. Ivakin and Dr. A.A. Kholodkova are the following:

- Synthesis of oxides in water vapor (SiO_2 from amorphous silica particularly obtained from rice husk; Yb_2O_3);
- Synthesis of complex oxides in water vapor ($\text{K}_{0.5}\text{Na}_{0.5}\text{O}_3$, BaTiO_3 , CaSnO_3 , BaSnO_3) for further applications in functional ceramics manufacturing;
- Functional and technical (porous) ceramics fabricating by different shaping techniques (pressing, casting, 3d-printing);
- Cold sintering of ceramics in water medium (ZnO , alumina).

The use of water medium discloses the opportunities of mild and environmentally benign production of single-phase crystalline powders with a controlled morphology. The formation of the oxides listed above occurred “one-pot” in a temperature range of 150-300°C without addition of any toxic auxiliary substances or waste compounds generation. The synthesized powders showed high ability for shaping and sintering by different approaches from traditional to recently developed. This technology of synthesis could be scaled up from laboratory to industrial level as it was previously performed for SiO_2 and Al_2O_3 production.

Cold sintering process is based on the mechanisms similar to those realized in water vapor during the synthesis of metal oxides. This cutting-edge approach in ceramics manufacturing counts a little over a decade and allows a decrease in the sintering temperature of about 1000°C. Dr. Yu.D. Ivakin and Dr. A.A. Kholodkova are focused on the study of grain growth mechanisms under these conditions in model systems such as ZnO and alumina.



Anastasia Kholodkova



Dr. Yu.D. Ivakin and Dr. A.A. Kholodkova with SiO_2 glass produced from fine-crystalline powder

RESEARCH

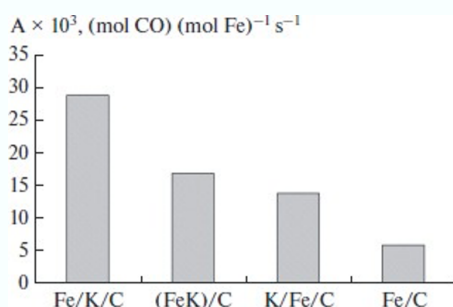
METAL-SUPPORTED FISCHER-TROPSCH SYNTHESIS CATALYSTS

Scientists involved to the topic:

P.A. Chernavskii, G.V. Pankina, V.I. Bogdan, I.I. Mishanin

During the last 5 years a research team under Prof. Peter Chernavskii supervision has been researching some of topochemical processes accompanying the synthesis and operation of metal-supported Fischer-Tropsch synthesis catalysts. A number of new results were obtained.

It was found out that the sequence of the supporting of active components onto potassium-promoted iron catalysts affected a number of their physicochemical and catalytic properties.



Dependence of the specific activity on the type of catalysts

Moreover, this team is working on developing a new direction in the synthesis of composite materials based on traditional carriers and carbon. New carbon-silica composite support was prepared by soaking of silica in water solution of glucose followed by drying and calcinations in inert atmosphere. This material was successfully used for the preparation of iron Fischer-Tropsch synthesis catalysts.

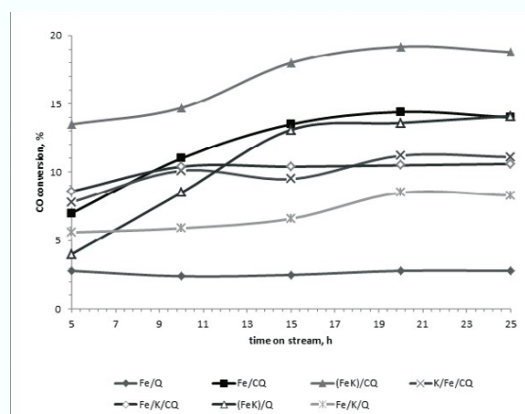
Dr. Chernavskii suppose that for the composite support the extent of iron silicate formation is less since at least some of the iron oxides are initially located on the carbon substrate. Additionally, the presence of carbon in the support promotes conversion of iron oxides to carbides. Carbon-silica composite support has a beneficial effect on catalytic activity of iron in CO hydrogenation. Other advantages of the new catalysts are suppression of methane formation and higher value of chain growth parameter. In fig. below CQ means composite material C/SiO₂.



Peter Chernavskii



Galina Pankina



Carbon monoxide conversion as function of time on stream.

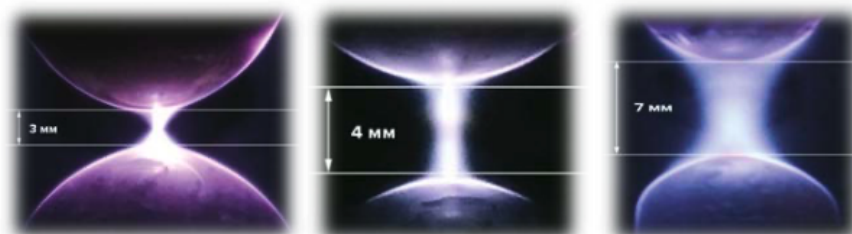
FILAMENTARY AND DIFFUSE BARRIER DISCHARGES IN NOBLE GASES WITH ADMIXTURES OF MOLECULAR GASES

Recently Dr. Kozlov K.V. and Abramovskaia E.A. reported the results of the plasma diagnostics of the barrier discharges in argon with admixtures of acetone. These discharges were found to be diffuse only for a limited range of acetone concentration, the latter corresponding to the local minimum of the burning voltage. In the year 2018, they have proposed a semi-empirical physical model for the barrier discharges in inert gases with small admixtures of molecular gases, that accounts for the experimental findings mentioned above, and that provides a simple method to prognosticate the possibility of the diffuse mode appearance for any chosen combination “noble gas + molecular gas (admixture)”.



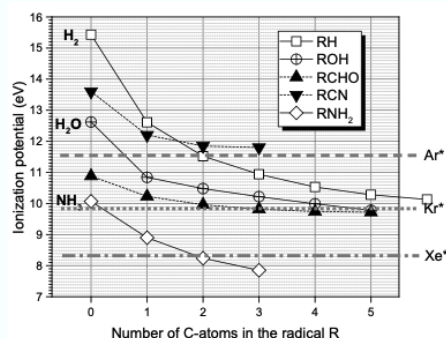
Kirill Kozlov

The model is based on the assumption of the Townsend mechanism of initial (pre-breakdown) phase of the microdischarge development and of the validity of the Paschen law for the breakdown voltage. Certain additional assumptions concerning electron energy distribution functions in the gas mixtures under consideration should be made. Then qualitatively, our model is able to explain the experimentally observed dependencies of the burning voltage upon the content of molecular admixture, as well as a transition of the discharge to the diffuse mode within a certain concentration range of molecular gases.



Transition from the filamentary mode to the diffuse mode of the barrier discharges in argon with admixtures of ethanol. Concentrations of ethanol: 0.005% (left), 0.06% (center), 0.5% (right).

To explain the latter exception, as well as an absence of the diffuse mode in the barrier discharges in humid argon, we assumed that the diffuse mode is impossible if ionization potential of the molecular admixture exceeds the energy of the metastable levels of argon, and included the corresponding limitation into the proposed physical model. Schematically, this hypothesis is presented. For all the points located below the dashed line, small admixtures of the corresponding chemical compounds to argon can cause a transition of the filamentary barrier discharge to the diffuse mode.



Comparison of the ionization potentials of selected inorganic and organic compounds with the energies of the lowest metastable excited states of argon, krypton and xenon.

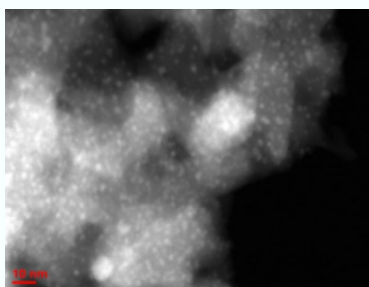
RESEARCH

METHANATION OF CARBON DIOXIDE ON NICKEL CATALYSTS APPLIED TO RICE HUSK PRODUCTS

The main goal of the research group consisting of Vyacheslav Rodin, Roman Novotortsev and Dmitry Stolbov is the synthesis and testing of nickel catalysts applied to rice husk products in the CO₂ methanation process.

Rice husk, calcined in air and in an inert atmosphere, and pure amorphous SiO₂ isolated from rice husk ash by alkaline treatment followed by precipitation are used as carriers. After impregnation, the samples were annealed at 300 °C for 2 hours in a nitrogen current. The reduction was carried out at 350-500 °C for 2-4 hours in a current of N₂/H₂ mixture.

During catalytic tests it was shown that the maximum conversion of CO₂ up to 95% was achieved at temperatures of 325-375 °C. It was found that the alkali and alkaline-earth metal impurities contained in the rice husk ash acted as promoters at temperatures of 250 - 350 °C and promoted the formation of CO by the water gas reverse conversion reaction. The sample on the carbon-containing carrier showed low activity values. It was found by TEM method that the reason for this is the low degree of interaction of carbon with the metal and, as a consequence, the low stabilization of the particles. The best results in activity and stability showed catalyst on precipitated pure SiO₂ (Fig. 1): 95% conversion at 350 °C.



Ni/SiO₂ catalyst TEM image



Viacheslav Rodin



Dmitri Stolbov

RESEARCH

TARGETED SYNTHESIS OF MODIFIED SILICA USING ORGANIC MODIFIERS

Researchers Yana Platonova and Roman Novotortsev are engaged in research in the field of surface modification of SiO_2 particles in order to obtain preassigned properties. Modification with the use of organic modifiers allows you to control the surface properties and significantly expand the scope.

To use SiO_2 as sorbents, the scientific group carried out a modification using γ -APTES and DMDCS as a modifier. In addition to the classical solvent method, a completely new method of modifying the SiO_2 surface has been developed that eliminates the use of solvents. It is shown that the new method makes it possible to obtain chemically modified silica with a grafted monomolecular layer of organic or organoelement compounds.

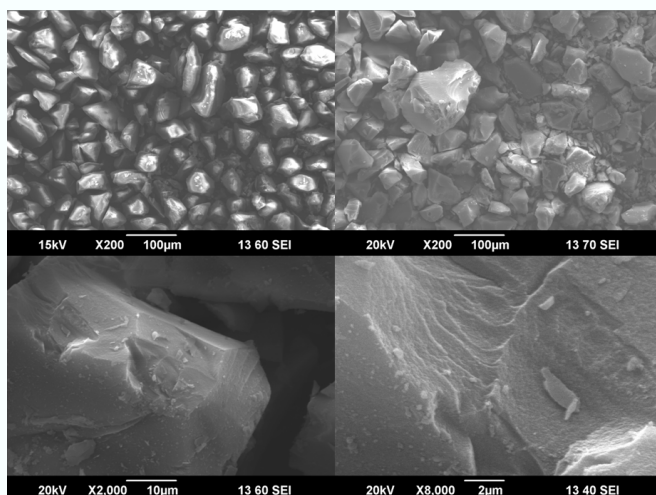
SiO_2 particles can be used as a support for catalysts, including photocatalysts. We have carried out the immobilization of tert-butyl-substituted palladium(II) phthalocyanine by adsorption from solution on silica, and also studied the physicochemical properties of the obtained material.



Yana Platonova



Roman Novotortsev



(t-Bu)PcPd/SiO₂ material SEM image

FINE-CRYSTALLINE MATERIALS FOR CERAMICS PRODUCTION

Scientists involved to the topic:

M.N. Danchevskaya, V.A. Kreisberg, Y.D. Ivakin, B.S. Lunin, A.V. Kholodkova, Dr. G.P. Muravieva

Leading Researcher M.N. Danchevskaya, Dr. V.A. Kreisberg and Dr. Y.D. Ivakin study the quality of ceramics that could be obtained with original method of synthesis of fine-crystalline oxides in hydrothermal conditions in sub- and supercritical water fluids with the help of which fine-crystalline simple and complex oxides were obtained. The content of water and gases in the crystalline raw materials for the production of high-quality ceramics are the most important criteria for the quality of ceramics. Using the method of kinetic thermodesorption mass spectrometry, it was possible to quantify the gas content, gas release and diffusion characteristics of alumomagnesium spinel for the first time. This allows them to estimate the degassing time of the spinel with a certain degree of dispersion and ceramics made of it, and thereby promote the production of high-quality ceramics.

The kinetic curve of water evolution of the spinel sample, which is shown in Fig. 1, consists of the regions of a sharp increase in the water flow with a rapid increase in temperature and isothermal sections, when the flow of water released falls. The temperature dependence of the coefficient of water diffusion for spinel at temperatures of 500, 600 and 700 °C is represented in the Arrhenius coordinates in Fig. 2. The activation energy of water diffusion E is 146 ± 5 kJ/mol. Fig. 2 also presents the results of previously studied fine-crystalline samples of undoped corundum and quartz.

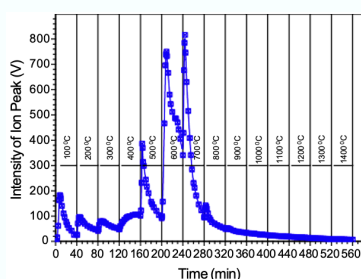


Fig. 1. Kinetics of the change in the intensity of molecular peak of water during stepwise vacuum heating of the weighted (0.1275 g) fine-crystalline spinel in mass spectrometric experiment at a sensitivity of $1 \text{ V} = 2.03 \cdot 10^{-4} \mu\text{g H}_2\text{O/s}$.

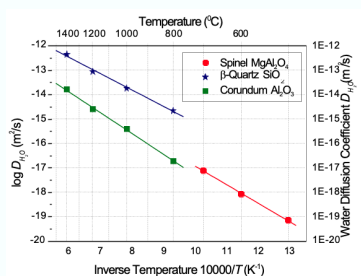


Fig. 2. Temperature dependence of the water diffusion coefficients for spinel, β -quartz and corundum.



Marina Danchevskaya



Valery Kreisberg



Yuri Ivakin



Galina Muravieva

DESIGN OF NEW CATALYTIC SYSTEMS BASED ON PHTHALOCYANINE METAL COMPLEXES

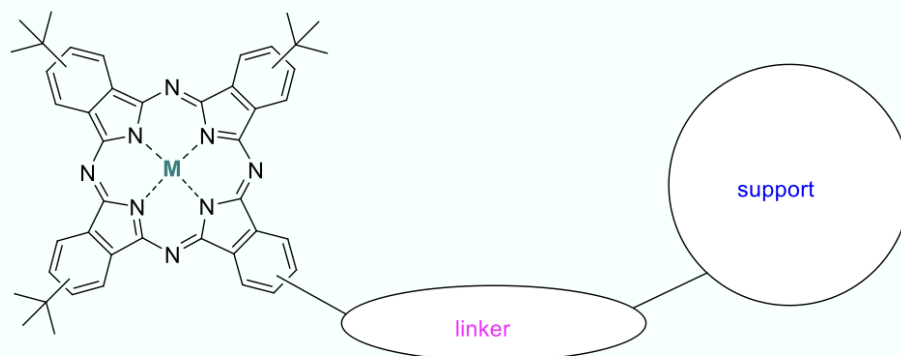
Scientists involved to the topic:

Ya.B. Platonova, A.N. Volov, V.A. Kirillova

The scientific group consisting of researcher Yana Platonova and researcher Alexander Volov is engaged in the synthesis of phthalocyanine metal complexes and catalysts based on them.

The areas of practical application of phthalocyanine complexes are numerous and diverse. Due to their unique properties, phthalocyanines are widely used as chemical and biochemical sensors, catalysts for various processes, components of semiconductors, solar cells and liquid crystals, in molecular electronics and in photodynamic cancer therapy (PDT).

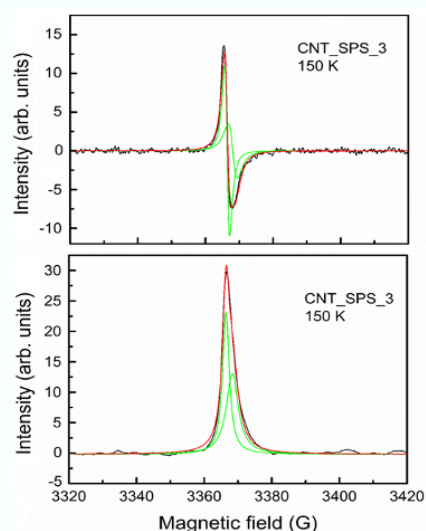
Catalytic processes using phthalocyanine metal complexes as catalysts were studied in homogeneous and heterogeneous versions by depositing metal complexes on various surfaces. The following support were used as substrates: melamine sponges, Nafen nanofibers, modified hyper-crosslinked polystyrene, and amorphous SiO_2 .



For oxidation processes, heterogeneous catalysts showed greater activity and stability compared to homogeneous ones. Also, heterogeneous catalysts are less susceptible to photodegradation, which makes them promising for use in wastewater treatment.

A- AND B- SITE SUBSTITUTED PEROVSKITES LIKE ABO_3 MANGANITES, AND SELF- (OR VACANCY) DOPED $\text{Ln}_{1-x}\text{MnO}_{3+\Delta}$ OXIDES

Carbon nanotubes (CNTs) and manganites attract considerable attention due to their unique electronic, magnetic and surface properties, and various field of application. Here we describe the peculiarities of properties of noted materials.



Raw and absorption EPR spectra of CNTs consolidated by spark plasma sintering and oxidized for 3 h show narrow and broad lines with different g-factors. This testify the different surrounding of paramagnetic centers associated with the lines. Temperature dependence of spin numbers, associated with the narrow line, transfers from Curie-Weiss law to Curie law with increasing temperature.

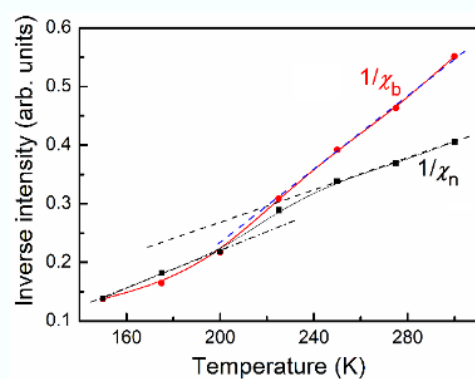
High similarity of the XPS spectra of the samples with different Nb doping is probably a result of the self-organization of terminal layers.



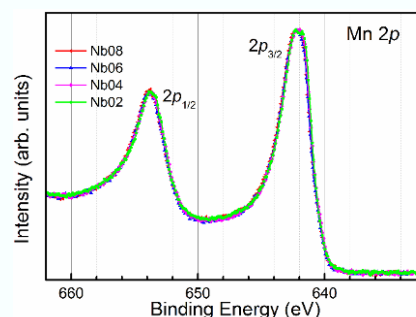
Alexander Ulianov



Nikolai Taibarei



Temperature dependence of inverse EPR susceptibility, associated with the narrow line, transfers from Curie-Weiss law to Curie law with increasing temperature. EPR susceptibility, associated with the broad line, can be attributed to a paramagnetic matrix with superparamagnetic inclusions.



Normalized Mn 2p XPS spectra for $\text{CaMn}_{1-x}\text{Nb}_x\text{O}_3$ ($x = 0.02, 0.04, 0.06$ and 0.08) perovskites.

PHYSICOCHEMICAL STUDY OF PLANT BIOMASS DELIGNIFICATION BY OZONE

Present topic is developed by Senior researchers Dr. E.M. Benko, Dr. N.A.Mamleeva and leading researcher Dr. habil V.I. Bogdan. The aim of the study is to elaborate an effective and environment friendly method of delignification plant materials by ozone in relation to the subsequent fermentation in sugars and ethanol.

For these purpose the effect of various parameters on the kinetics of ozonation of lignin-cellulose material (LCM), structural changes in samples of ozonation, reactivity of ozonated samples in enzymatic hydrolysis processes under the cellulase complex are studied.

A summary of the obtained experimental data makes them to draw conclusions on the optimal ozone usage for plant raw materials:

- Moisture content in the sample is a key factor for the ozone consumption rate;
- Content of residual lignin and sugars yield are governed by ozone consumption;
- Ozonation of biomass causes a degradation of lignin and partially hemicelluloses and cellulose;
- Ozone treatment leads to noticeable structural changes of plant materials;
- The process of lignin removing in the course of ozonization is directed from the secondary to the primary cell shell.
- There are common patterns of ozone pretreatment for biomass of different types. This allows us to predict the optimum dose of ozone for biomass pretreatment. (2- 3 eq. O₃/PPU). At an average content of lignin in plant materials 25-35% the re- quired amount of ozone (O₃ : LCM) corresponds to 10-15 wt. %.
- Methods of lignin extraction using a soxhlet apparatus as a high value-added product have been investigated and optimized.
- Browns lignin extraction method was optimized for industrial use. This method makes it possible to obtain lignin for use in the pharmaceutical industry.



Elena Benko



Nadezhda Mamleyeva



Denis Bikkulov

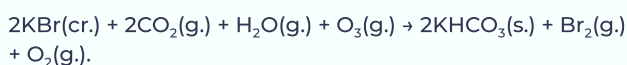


Maria Paslova

STUDY OF OZONE REACTIONS WITH CRYSTALLINE HALOGENIDES

Associate professor Dr. A.V.Levanov and Senior Researcher Dr. O.Y.Isaikina work on the sources and mechanism of activation of bromine in the troposphere that can interact with ozone while being in dry or wet marine aerosol containing bromide ions. The purposes of this study are to investigate the interaction of gaseous ozone and $O_3 + CO_2$ mixtures with polycrystalline potassium bromide, determining the composition of products released into the gas phase and remaining in the solid phase, establishing quantitative kinetic patterns of their formation, and to identify a possible mechanism for this process. It was found that $KBrO_3$ was the only nonvolatile product of the interaction of solid KBr with gaseous ozone, and the kinetic laws of its formation were determined.

It was discovered for the first time, that $KHCO_3$ and $KBrO_3$ are formed in the solid phase, and molecular bromine Br_2 is released into the gas phase, when solid KBr interacts with gaseous ozone in the presence of significant amounts of carbon dioxide.



A kinetic scheme has been proposed that satisfactorily explains all the kinetic patterns established in the experiments. The formation of Br_2 and bicarbonate is due to the interaction of hypobromite ion, the primary oxidation product of bromide, with carbon dioxide and water, according to the equation



First reaction can be considered as the primary source of active bromine in the troposphere. In atmospheric conditions, its rate does not depend on the concentration of carbon dioxide (as it is in considerable excess), but directly proportional to the concentration of ozone.



Alexander Ivanov



Oksana Isaikina

OZONE APPLICATION FOR WATER TREATMENT

Scientific interests of Professor Sergey N. Tkachenko and Dr. Ilia S. Tkachenko are physical chemistry, kinetics and catalysis, ozone production and application, homogeneous and heterogeneous ozone decomposition, water treatment, ozone-catalytic oxidation, air treatment, ozone technologies.

New technologies have been developed in the group to clean water and air from man-made contaminants, which effectively use ozone in combination with other methods. Creation of systems for removal and destruction of residual ozone after various technological processes. Carrying out of physical and chemical studies of the developed series of high-efficiency catalysts for ozone decomposition and oxidation of toxic organic compounds (goptalymys of goptalyum catalysts GT and GTT grades with different content of oxides of transition metals of different compositions), including the reaction of complete oxidation of methane and oxidation of carbon monoxide. Investigation of ozone synthesis by surface barrier discharge by numerical simulation method. All research and developments take into account the application of «green chemistry» principles.

Recently developed goptalyum catalysts of GT and GTT brand have been put into operation and work effectively at more than 50 enterprises of the Russian Federation and abroad. Ozone-sorption station of water treatment for purification of underground waters of compounds of iron on JSC WIMM-BILL-DANN (PepsiCo); Residual ozone removal and destruction system at Zapadnay and Rublevskay water treatment stations in Moscow are designed, produced and operated. The goptalum catalyst of GTT grade works effectively at the ATLAS device in the Grand Hadron Collider, CERN, (Geneva).

In 2018 Lunin V.V., Tkachenko S. N., Tkachenko I.S. with colleagues were the laureates of the Russian Government Prize in science and technology.



Ilia Tkachenko



Sergey Tkachenko

VERY IMPORTANT PERSONS IN LABORATORY LIFE



Valery Vasiliev



Natalia Kuznetsova



Maxim Yurenkov



Nikolai Osipov



Sergey Maximov



Stanislav Dvoryak



Elena Kuzovkina



Eleonora Gorodkova



Valentina Levkina

LAUREATES

Laureate of the Russian Federation President scholarship

The scholarship was awarded for a series of scientific works devoted to the new generation energy storage devices based on modified carbon nanostructures derived from the products of processing rice husk products



E.A. Arkhipova

Laureate of the Moscow University Scholarship

The scholarship is given for a cycle of scientific works devoted to the study of carbon nanomaterials.



D.N. Stolbov

Laureate of the Moscow University Scholarship

The scholarship is given for the synthesis and study of new electrolytes based on ionic liquid solutions.



M.M. Levin

Laureate of the Moscow University Scholarship

The scholarship is given for a cycle of scientific works devoted to the study of catalytic oxidation of CO and propane dehydrogenation.



I.Yu. Kaplin

Laureate of the Moscow University scholarship

The scholarship is given for significant results in teaching and research activities.



S.Y. Kupreenko

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calorimeter



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implemented video-
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(TG+DSC) system with quadruple
mass and IR spectrometers for gases
detection



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