MODERN RESEARCHES AND PROSPECTS OF THEIR USE IN CHEMISTRY, CHEMICAL ENGINEERING AND RELATED FIELDS

The conference is dedicated to the 60 th anniversary of
R. Agladze Institute of Inorganic Chemistry and Electrochemistry

International Scientific Conference
September 21-23, 2016, Ureki, Georgia

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თსუ რაფიელ აგლაძის არაორგანული ქიმიისა და ელექტროქიმიის ინსტიტუტი
TSU R. Agladze Institute of Inorganic Chemistry and Electrochemistry

ივანე ჯავახიშვილის სახელობის თბილისის სახელმწიფო უნივერსიტეტი
Iv. Javakhishvili Tbilisi State University

შოთა რუსთაველის ეროვნული სამეცნიერო ფონდი
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Modern researches and Prospects of their Use in Chemistry, Chemical Engineering and Related Fields

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თანამედროვე კვლევები და მათი გამოყენების პერსპექტივები ქიმიაში, ქიმიურ ტექნოლოგიასა და მომიჯნავე დარგებში

კონფერენცია ეძღვნება რ. აგლაძის არაორგანული ქიმიისა და
ელექტროქიმიის ინსტიტუტის 60 წლისთავს.

International Scientific Conference
September 21-23, 2016, Ureki, Georgia

საერთაშორისო სამეცნიერო კონფერენცია
21-23 სექტემბერი, 2016, ურეკი, საქართველო

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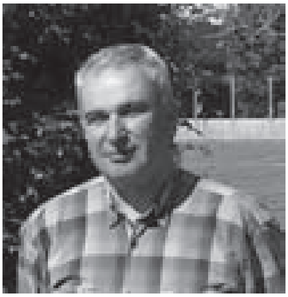

Dear colleagues!

I greet you at our Conference and thank you for your attention and participation.

Development of any country is impossible without innovative economics, based on high level science and education. Enterprise, education, science is a triangle bringing to a new level of socio-economic status.

Moreover, development and adoption of new technology in any economic sector can't do without help of specialists in the sphere of chemistry and chemical technology.

In the light of the aforesaid, it is difficult to overrate topicality and the significance of our Conference.

I believe, that our forum will become a platform for advanced knowledge exchange and innovation approaches. Also, the Conference will promote strengthening of connections between our scientific communities, organizations and countries.

I believe, that such dignified and diverse composition of participants will facilitate productive connection between science and practice.

I wish you fruitful work and constructive discussions. I hope, that obtained results will be wholesome for all participants.

The work will be conducted in different forms: plenary and sectional sessions, poster reports, round tables. The organizing committee of the conference will do everything possible to make your stay in Ureki useful and unforgettable.

In the end, I wish you further success in research work and practical activities.

G. Tatishvili G. Ta

Chairman of the Organizing
Committee of the Conference

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CONTENT

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Venue

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Phone: (+995) 99205445, 99205452
kolkhida.hotel@gmail.com

Emergencies

Any urgent question, please call: 112

Message Board

A message board will be available next to the registration desk. Please check it regularly for possible messages. Also you can leave a message if you have any to other participants.

Computers will be available next to registration board. Wi-Fi will work at the hotel

Transportation

The conference site is located in a town Ureki, resort on the Black Sea coast of Georgia. The railroad connects Ureki to Batumi (60 kilometers). The train station is about 1.5 km from the beach.

PROGRAM

	WEDNESDAY, 21 SEPTEMBER
13:00 – 15:00	**Registration,** *Lobby of the Hotel Kolkhida*
15:00 – 16:00	**Welcome address,** *Hall A*
16:00 – 16:30	**Coffee break,** *Hall of the Hotel Kolkhida*
	PLENARY, ***Hall A***
	Chair: **Dr. N. Vaszilcsin,** University Politehnica Timisoara, Romania
16:30 – 17:00	**V. Beschkov**, Institute of Chemical Engineering, Bulgarian Academy of Sciences, Bulgaria
	BIOWASTE AND HYDROGEN SULFIDE – PERSPECTIVE RENEWABLE FUELS
17:00 – 17:30	**V. Tsitsishvili,** Ivane Javakhishvili Tbilisi State University, Georgia
	NEW GENERATION ZEOLITIC ADSORBERS
19:00 – 21:00	**Welcome Reception,** *Café of the Hotel Kolhida*
	THURSDAY, 22 SEPTEMBER
	PLENARY, ***Hall A***
	Chair: **Dr. V. Beshkov**, Institute of Chemical Engineering, Sofia, Bulgaria
8:30 – 9:00	**K. Dossumov,** Center of Physical and Chemical Methods of Research and Analysis al-FarabyKazNU, Kazakhstan
	CONVERSION OF METHANE OVER THE OXIDE CATALYSTS
9:00 – 9:30	**T. Agladze,** Georgian Technical University, Georgia
	NOVEL TECHNOLOGY PLATFORM FOR SYNTHESIS OF MULTIFUNCTIONAL HYBRID NANOCOMPOSITES
9:30 – 10:00	**N. Vaszilcsin,** University Politehnica Timisoara, Romania
	ENHANCEMENT OF CATHODIC HYDROGEN EVOLUTION REACTION USING PROTON CARRIERS
10:00 – 10:30	**Coffee break**
	NEW METHODS FOR ECOLOGICAL AND RADIATION SAFETY, MEDICAL AND AGRARIAN RESEARCHES, ***Hall A***
	Chair: **Dr. S. Kirillov**, Joint Department of Electrochemical Energy System, Kyiv, Ukraine
	Co – chair: **Dr. M. Tsitsagi,** TSU Petre Melikishvili Institute of Physical and Organic Chemistry, Georgia
10:30 – 10:45	**A. Mansourizadeh,** Department of Chemical Engineering, Islamic Azad University, Iran
	OILY WASTEWATER TREATMENT USING BLEND PSF-SPEEK HOLLOW FIBER MEMBRANE
10:45 – 11:00	**M. Tsitsagi,** TSU Petre Melikishvili Institute of Physical and Organic Chemistry, Georgia
	UTILIZATION OF AGRO-INDUSTRIAL WASTE MATERIALS BY USING SEQUENTIAL SUPERCRITICAL FLUID AND ULTRASOUND EXTRACTION METHODS
11:00 – 11:15	**S. A. Kirillov**, Joint Department of Electrochemical Energy Systems, Ukraine
	PHOSPHATE SCAVENGERS FOR REMEDIATION OF GROUNDWATERS AND TREATMENT OF HYPERPHOSPHATAEMIA IN ANIMALS AND HUMANS: REVIEW AND COMPARISON

11:15 – 11:30	**A. Surmava**, M. Nodia Institute of Geophysics, Georgia
	NUMERICAL SIMULATION OF DISTRIBUTION OF ARSENIC DISCHARGED TO TSKHENISTSKALI AND LUKHUNI RIVERS FROM INDUSTRIAL WASTE
11:30 – 11:45	**M. Mirtskhulava**, National Center for disease control and Public health, Georgia
	ULTRASOUND IN MEDICINE, BIOLOGY, BIOTECHNOLOGY
11:45 – 12:00	**D. Gventsadze**, LEPL R. Dvali Institute of Machine Mechanics, Georgia
	TECHNOLOGY OF ECO-FRIENDLY HIGH TEMPERATURE HEAT-INSULATOR MATERIALS ON THE BASIS OF LIQUID GLASS AND FOAMED PERLITE
12:00 – 12:15	**N. Kvirkvelia**, TSU R. Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia
	OZONE USE IN AGRICULTURE
12:15 – 13:15	**Free time**
	Chair: **Dr. E. H. Ismailov**, Institute of Petrochemical Processes, Baku, Azerbaijan
	Co-chair: **T. Chachibaia,** TSU, Tbilisi, Georgia
13:15 – 13:30	**T. Chachibaia,** TSU Faculty of Madicine, Georgia, University of Santiago de Compostela, Spain
	NMR TECHNOLOGY FOR ASSESSMENT OF SOCIETAL, ENVIRONMENTAL AND CHEMICAL RISKS OF AMMONIUM NITRATE
13:30 – 13:45	**I. Chikvaidze,** TSU, Georgia
	REGARDING SOME STEPS OF E. FISCHER REACTION MECHANISM
13:45 – 14:00	**E. H. Ismailov**, Institute of Petrochemical Processes of Azerbaijan National Academy of Sciences, Azerbaijan
	HYDROGENATION OF CARBON DIOXIDE OVER Fe-Zr/Al AND Fe-Ni/Al OXIDE CATALYSTS
14:00 – 14:15	**T. Varazi,** Durmishidze Institute of Biochemistry and Biotechnology of Agricultural University of Georgia, Georgia
	ABOUT ALGAE SPIRULINA’S ECOLOGICAL POTENTIAL FOR THEIR APPLICATION REMEDIATION TECHNOLOGIES
14:15 – 14:30	**V. Bakhtadze**, R. Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia
	OXIDE-MANGANESE CATALYSTS FOR SOLVING OF ECOLOGICAL PROBLEMS
14:30 – 14:45	**M. V. Panchvidze**, R. Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia
	ABOUT RADIOPROTECTIVE PROPERTIES OF SULFUR-ORGANIC COMPOUNDS
14:45 – 15:45	**STUDENT SESSION, *Hall A***
	Chair: **MSc**. **M. Soselia**, IICE, Georgia
14:45 – 15:00	**K. Kharaishvili**, TSU, Georgia
	SEPARATION OF ENANTIOMERS WITH SUPERFICIALLY POROUS SILICA MODIFIED WITH POLYSACCHARIDE DERIVATIVES AS EFFECTIVE CHIRAL STATIONARY PHASES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY
15:00 – 15:15	**M. Shavgulidze**, Iv. Beritashvili Experimental Biomedicine Centre, Georgia
	CHANGES OF LEARNING MOTIVATIONAL AND EMOTIONAL BEHAVIOR AND PASSIVE AVOIDANCE IN DEPRESSIVE RATS

15:15 – 15:30	**L. Khvichia,** Akaki Tsereteli State University
	QUANTITATIVE DETERMINATION OF TOTAL MANGANESE IN ZESTAFONI SOIL AND DRINKING WATER AND ABNORMALITIES CAUSED BY ITS ABUNDANCE
15:30 – 15:45	**Z. Samkharadze**, R. Agladze Institute of Inorganic Chemistry and Electrochemistry
	OXIDATION OF MANGANESE NITRATE SOLUTIONS BY OZONE - AIR MIXTURE
15:45 – 16:15	**Coffee break**
	NANO PROCESSES AND NANOTECHNOLOGIES, *Hall B*
	Chair: **Dr. G.Ya. Kolbasov**, V.I. Vernadskii Institute of General and Inorganic Chemistry of National, Academy of Sciences of Ukraine, Ukraine
	Co-chair: **Dr. N. Nioradze**, TSU, IICE, Georgia
10:30 – 10:45	**O. Ruzimuradov**, Turin Polytechnic University in Tashkent, Uzbekistan
	SECOND-GENERATION POROUS TiO_2 BASED PHOTOCATALYTIC NANOMATERIALS: SYNTHESIS AND PROPERTIES
10:45 – 11:00	**L. Tsereteli**, Max Planck Institute of Colloids and Interfaces, Germany
	AN ACCURATE COARSE-GRAINED MODEL FOR POLYSACCHARIDES IN SOLUTION
11:00 – 11:15	**M. Ersoz,** Selcuk University, Advanced Technology Research&Application Center, Turkey
	NANOSTRUCTURE FABRICATION BY USING OF BLOCK COPOLYMERS
11:15 – 11:30	**V. Bregadze**, TSU, Andronikashvili Institute of Physics, Georgia
	SORPTION CHARACTERISTICS OF ORGANIC MATERIALS IN METAL ION REDUCTION REACTION AND NANOTECHNOLOGY
11:30 – 11:45	**M. Rukhadze,** TSU, Faculty of Exact and Natural Sciences, Georgia
	STUDY OF STRUCTURE OF CONFINED WATER NANODROPLETS
11:45 – 12:00	**G. Ya. Kolbasov**, V.I. Vernadskii Institute of General and Inorganic Chemistry of National Academy of Sciences of Ukraine, Ukraine
	NANOMATERIALS AND PHOTOELECTROCHEMICAL SYSTEM FOR PRODUCTION OF SOLAR HYDROGEN
12:00 – 12:15	**N. Nioradze**, TSU, R. Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia
	SCANNING ELECTROCHEMICAL MICTROSCOPY OF NANOSTRUCTURED CARBON MATERIALS
12:15 – 13:15	**Free time**
	ENERGY SOURCES, CONVERSION AND STORAGE, *Hall B*
	Chair: **Dr. M. N. Abdikarimov,** KazNTU, Kazakhstan
	Co-chair: **Dr**. **G. Tsagareli,** R. Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia
13:15 – 13:30	**E. Kachibaia**, TSU R. Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia
	SPINELS $LiM_XNi_{0.5-X}Mn_{1.5}O_{4-}$ – TYPE (M=CO+CR, AL AND CU; 0<X≤0.4) AS PROMISING CATHODE MATERIALS FOR Li- ION BATTERIES
13:30 – 13:45	**M. N. Abdikarimov**, KazNTU, Kazakhstan
	PHOTOVOLTAIC MODULE

13:45 – 14:00	**S. I. Abasov,** Institute of Petrochemical Processes of Azerbaijan National Academy of Sciences, Azerbaijan
	THE FORMATION OF INTERMOLECULAR C-C BONDS AS A FUNCTION OF TEMPERATURE WITH PARTICIPATION OF C3-C4 ALKANE
14:00 – 14:15	**P. Nikoleishvili**, R. Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia
	SYNTHESIS OF TiO_2 NANOTUBES BY Ti FOIL ELECTROCHEMICAL DISSOLUTION FOR DYE-SENSITIZED PHOTOELECTROCHEMICAL SOLAR CELL
14:15 – 14:30	**N. Khetsuriani,** TSU, Institute of Physical and Organic Chemistry, Georgia
	PRODUCTION OF BIODIESEL USING SUPERCRITICAL FLUIDS TECHNOLOGY
14:30 – 14:45	**G. Tsagareli,** R. Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia
	THE PREPARATION OF THE ACTIVE MANGANESE DIOXIDE POWDER BY ELECTROCHEMICAL METHOD FOR CURRENT SOURCES
14:45 – 15:45	**STUDENT SESSION, *Hall A***
15:45 – 16:15	**Coffee break**
16:15 – 17:15	**POSTER SESSION, Hotel Kolkhida Lobby**
	FRIDAY, 23 SEPTEMBER
	PLENARY, *Hall A*
	Chair: **Dr. V. Tsitsishvili**, TSU, Tbilisi, Georgia
8:30 – 9:00	**G. A. Tsirlina**, Moscow State University, Russia
	PLATINUM FREE ELECTROCATALYSTS BASED ON MANGANESE OXIDES FOR ELECTROCHEMICAL DEVICES
9:00 – 9:30	**S. A. Kirillov,** Joint Department of Electrochemical Energy Systems, Ukraine
	HIGH-RATE LITHIUM-ION BATTERIES: RECENT ADVANCES
9:30 – 10:00	**T. Marsagishvili,** R. Agladze Institute of Inorganic chemistry and Electrochemistry, Georgia
	SOME ASPECTS OF MODELING OF PHOTOCATALYSIS PROCESS
10:00 – 10:30	**Coffee break**
	NEW METHODS FOR ECOLOGICAL AND RADIATION SAFETY, MEDICAL AND AGRARIAN RESEARCHES, *Hall A*
	Chair: **Dr. L. Gorniak**, Industrial Chemistry Research Institute, Warsaw, Poland
	Co-chair: **Dr. I. Rubashvili**, Aversi-Rational Ltd, Quality Control Laboratory, Georgia
10:30 – 10:45	**M. N. Abdikarimov,** KazNTU, Kazakhstan
	INVESTIGATION OF POSSIBLE CHEMICAL WASTE DISPOSAL
10:45 – 11:00	**L. M. Gorniak,** Industrial Chemistry Research Institute, Warsaw, Poland
	CHEMICAL SECURITY AS A SYNTHESIS OF SCIENCES
11:00 – 11:15	**M. Labartkava,** University “Geomedi”, Georgia
	THE USE OF MODERN PHYSICAL-CHEMICAL METHODS OF SUBSTANCE ANALYSIS IN THE ANALYSIS OF GEORGIAN RED WINE
11:15 – 11:30	**M. Nalbandyan,** NAS RA Institute of Geological Sciences, Yerevan, Armenia

	TECHNOLOGY OF PURIFICATION OF IRRIGATION WATER WITH A HIGH SALT CONTENT IN ORDER TO PREVENT SECONDARY SALINIZATION OF ARARAT VALLEY
11:30 – 11:45	**Ch. Stahl**, NaralexMaschinen UG, Germany
	BIO BRIQUETTES POTENTIAL IN GERMANY
11:45 – 12:00	**V. V. Tkach**, Chernivtsi National University, Ukraine
	A MATHEMATICAL REPRESENTATION OF ELECTROANALYTICAL FUNCTION OF THE SAFRANIN-MODIFIED RADICALLY-PRETREATED MATERIAL TO HYDROQUINONIC COMPOUNDS
12:00 – 12:15	**I. Rubashvili**, Aversi-Rational Ltd, Quality Control Laboratory, Georgia
	DEVELOPMENT AND VALIDATION OF SAMPLING AND QUANTITATIVE DETERMINATION METHODS OF CARVEDILOL RESIDUES USING HIGH PERFORMANCE LIQUID CHROMATOGRAPHY FOR CLEANING VALIDATION
12:15 – 13:15	**Free time**
	Chair: **Dr. N. Durgaryan**, Institute of Geological Sciences of NAS of Armenia, Yerevan, Armenia
	Co-chair: **Dr**. **M. Mantskava**, Society of Rheology, I. Beritashvili Center of Experimental Biomedicine, Georgia
13:15 – 13:30	**M. Karchkhadze**, TSU, Georgia
	ENANTIOSEPARATION OF CHIRAL ANTIMYCOTIC DRUGS IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY WITH POLYSACCHARIDE-BASED CHIRAL COLUMNS
13:30 – 13:45	**N. Durgaryan**, Yerevan State University, Yerevan, Armenia
	SYNTHESES OF NH2/NH2 CAPPED ANILINE OLIGOMERS AND THEIR DERIVATIVES
13:45 – 14:00	**M. Mantskava**, Society of Rheology, I. Beritashvili Center of Experimental Biomedicine, Georgia
	THE SIGNIFICANCE OF THE NEW PROPERTIES OF BEMIPARIN FOR APPLIED MEDICINE
14:00 – 14:15	**A. Mskhiladze,** Faculty of Natural Sciences and Healthcare, Sokhumi State University, Georgia
	SOME CHARACTERISTICS OF THE SEPARATION OF ENANTIOMERS OF BETA-BLOKER DRUGS USING POLYSACCHARIDE BASED CHIRAL COLUMNS IN HPLC
	FUNDAMENTAL AND TECHNOLOGICAL ASPECTS OF PROCESSING OF MINERAL PRODUCT AND SECONDARY RAW MATERIALS
	Chair: **Dr. G. Magalashvili**, GTU, Tbilisi, Georgia
	Co-chair: **Dr. Ali A. Jazie**, Alqadissiya University, Iraq
10:30 – 10:45	**L. Gurchumelia**, TSU, R. Agladze Institute of Inorganic Chemistry and Electrochemistry
	ELABORATION OF NEW TYPES, ECO-SAFE, INEXPENSIVE, HIGHLY EFFICIENT FIRE- PROTECTIVE MATERIALS
10:45 – 11:00	**G. Zakharov,** Ferdinand Tavadze Institute of Metallurgy and Materials Science
	OBTAINING LIGATURES FROM FINE GRAINED PARTICLES OF MANGANESE WASTE BY TECHNOLOGY -SHS METALLURGY

11:00 – 11:15	**D. Gogoli**, TSU R. Agladze Institute of Inorganic Chemistry and Electrochemistry
	ELECTRODEPOSITION AND CHARACTERIZATION OF Mn-Cu-Zn ALLOYS FOR CORROSION PROTECTION COATINGS
11:15 – 11:30	**L.G. Shamanauri**, R. Dvali Institute of Machine Mechanics
	COMPOSITES BASED ON POLYESTER LACQUER AND MINERAL FILLERS
11:30 – 11:45	**Ali A. Jazie,** Alqadissiya University, Iraq
	OPTIMIZATION OF BIODIESEL PRODUCTION FROM MUSTARD OIL
11:45 – 12:00	**G. Magalashvili,** Georgian Technical University
	ASCERTAINMENT OF THE MECHANISM OF FORMING OF ZONAL CONCENTRIC “AGATE STRUCTURES”
12:00 – 12:15	**B. Godibadze**, LEPL, G. Tsulukidze Mining Institute, Georgia
	EXPLOSIVE CONSOLIDATION OF Cu–W COMPOSITES IN HOT CONDITION
12:15 – 13:15	**Free time**
	Chair: **Dr. A. Peikrishvili**, F. Tavadze Institute of Metallurgy and Materials Science, IICE, Georgia
	Co-chair: **Dr. T. E. Machaladze,** TSU, R. Agladze Institute of Inorganic Chemistry and Electrochemistry
13:15 – 13:30	**A. Peikrishvili**, F. Tavadze Institute of Metallurgy and Materials Science, IICE, Georgia
	SHOCK WAVE ASSISTED CHEMICAL REACTIONS AND CONSOLIDATION OF Ta-Al INTERMETALIC COMPOUNDS
13:30 – 13:45	**L. Gabunia**, Caucasian Alexander Tvalchrelidze Institute of Mineral Resources, Georgia
	RESEARCH OF THE POSSIBILITY OF RECEIVING ACID AND HEAT-RESISTANT CONTINUOUS FIBER GLASS WITH USE OF MANGANIFEROUS WASTE PRODUCTS
13:45 – 14:00	**T. Machaladze,** TSU, R. Agladze Institute of Inorganic Chemistry and Electrochemistry
	THERMAL CHARACTERISTICS OF SPINEL-TYPE COMPLEX OXIDES $Me_{1-X}Zn_{X}Fe_{2}O_{4}$ (WITH Me= Cu OR Mg)
14:00 – 14:15	**E. Shapakidze**, TSU, Caucasian A. Tvalchrelidze Institite of Mineral Resources, Georgia
	RESEARCH OF INFLUENCE OF THE MODIFYING BaO AND SO_3 OXIDES ON PROPERTIES OF CEMENT CLINKER
14:15 – 15:15	**POSTER SESSION, *Hotel Kolkhida Lobby***
	ROUND TABLE; ***Hall A***
15:15 – 15:30	**L. Chobanyan**, Georgian Technical University, Institute TECHINFORMI
	ANALYSIS OF SCIENTIFIC PRODUCTIVITY AT THE MESO- AND MACRO-LEVELS
15:30 – 16:00	**M. Kutsia,** National Intellectual Property Center of Georgia – Sakpatenti
	PATENTING IN CHEMISTRY
16:00 – 16:15	**Discussion**
16:15 – 17:15	**CLOSING THE CONFERENCE, *Hall A***

PLENARY (PL) AND ROUND TABLE (RTL) LECTURES

PL-01

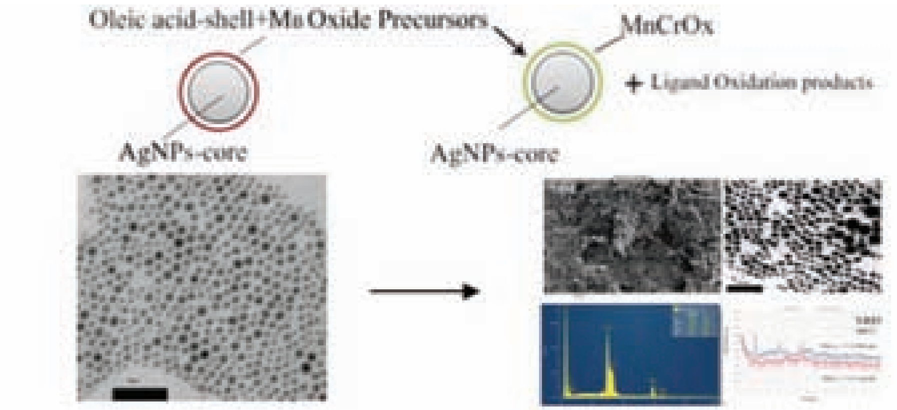
NOVEL TECHNOLOGY PLATFORM FOR SYNTHESIS OF MULTI-FUNCTIONAL HYBRID NANOCOMPOSITES

T. Agladze, M. Donadze, M. Gabrichidze, P. Toidze

Georgian Technical University, 77 Kostava Str., Tbilisi 0175, Georgia
t.agladze@gtu.ge

The nanohybridisation strategy provides material economy contributing to a cleaner and safe environment. The presentation highlights the recent studies curried out in the GTU on the bottom-up nanoarchitectonic design strategy for multicomponent hybrid (MH) nanomaterials using metal core/ organic shell nanoparticles (M_ANPs) as starting building blocks. MH nanomaterials has attracted much attention owing to their unique catalytical, biomedical, magnetic, and electrical properties compared to their bulk counter parts. Designed $M_A M_B O_x$- type (A ≡ Ag, B ≡ transition metals) inorganic materials exhibit a range of tunable functionalities such as bactericidal activity, green adsorption, and catalytic conversion of organic liquids and gases. Here we present novel surface technology for synthesis binary and ternary nanomaterials spatially stabilized by organic shell molecules via selective oxidation of shell material by precursors [1-3].

Synthesis of binary Ag/MnO_2 and ternary AgMnCrOx nanohybrids by the Ligand Oxidative Substitution (LOS) reaction. The hybrid colloidal soles were synthesized in hexane by electrochemical deposition of stabilized by ligand (oleic acid) Ag NPs and subsequent oxidation of the oleic acid molecules by metal oxide precursors $(MnO_4)^-$ and $(Cr_2O_7)^{2-}$:



Hybrid nanomaterials were characterized by means of XRD, DLS, FTIR, UV, SEM, TEM, ICPES and XRF technique. Implementation of MH nanomaterials for clean environment discussed.

References:
[1] M. Donadze, M. Gabrichidze, S. Calvache, T. Agladze, Trans. of the IMF, **94** (2016) 16-23.
[2] T. Agladze, M. Donadze, M. Gabrichidze , P. Toidze, J.Shengelia , N. Boshkov, N. Tsvetkova, Z. Phys. Chem. **227** (2013) 1187–1198.
[3] Proceedings of the 2nd International Conference “Nanotechnologies”, Tbilisi, 2012.

PL-02

BIOWASTE AND HYDROGEN SULFIDE – PERSPECTIVE RENEWABLE FUELS

V. Beschkov

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vbeschkov@yahoo.com

The enormous economical growth in a global scale in the last century has lead to extensive use of fossil fuels, like coal, oil and natural gas. The result was strong emissions of carbon dioxide and greenhouse effect with the consequent climate changes. The extensive use of fossil fuels formed and stored underground for millions of years has made impossible for the present vegetation on Earth to treat the emitted carbon dioxide by photosynthesis.

One of the ways to cope with this global problem is to close the carbon cycle in nature by the use of renewable fuels enabling recycling the sources of biological origin by energy production and consumption the resulting carbon by photosynthesis. Such biofuels are biogas (a mixture of methane and carbon dioxide) generated by anaerobic digestion of organic waste, ethanol, produced by fermentation of carbohydrates and biodiesel, produced by trans-estherification of lipids. The main feature of these approach is the utilization of organic waste as energy thus leading to multiple benefits for environment: waste treatment with energy production, closing the natural carbon cycle and saving of fossil fuels.

Another perspective source of energy is the hydrogen sulfide accummulated in the deep waters of the Black Sea. It can be converted into electric energy by sulfide-driven fuel cells. The generated energy could be directly used or employed for hydrogen generation by electrolysis fed by the produced electric energy.

The present work demonstrates all of these opportunities based on own experimental data and the available scientific results.

Acknowledgement. The support of projects HYSULFCEL (bs.era-net, FP7) and DFNI E02/16 (NSF-Bulgaria) is gratefully acknowledged.

CATALYSTS FOR SELECTIVE DECOMPOSITION OF METHANE

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The catalytic conversion of natural gas into motor fuel component, the raw material for the petrochemical industry and organic synthesis for over 20 years, the subject of intensive research are driven by the problem of reducing the resources of hydrocarbons of petroleum origin. Of particular interest in this respect are the partial oxidation of methane to synthesis gas and an oxidizing dimerization of methane to C_2 hydrocarbons. Syngas is a feedstock for the oxygenates production (methanol, dimethyl ether, etc.) and for producing liquid and solid hydrocarbons by the Fischer-Tropsch process [1]. C_2-C_4 olefins are of considerable interest as a raw material for industrial organic synthesis, which are widely used for the preparation of polymeric materials, plastics, alcohols, esters, carboxylic acids, components of motor fuels etc. Production of ethylene ranked first in terms of production among basic petrochemicals [2]. For countries with large reserves of cheap natural gas, the practical implementation of these processes today seems economically justified. Therefore, the creation of highly efficient, selective and stable catalysts for processing light hydrocarbons to produce valuable products of petrochemical synthesis is an important practical and strategic goal [3].

We report here on the activity of silicon and aluminum oxides, and a new series of catalysts on the base of $H_8[Si(W_2O_7)_6]\ nH_2O$ and NiO-La_2O_3, supported on SiO_2 and Al_2O_3 to be tested in partial oxidation processes and oxidative dimerization of methane. Experiments to test the catalytic activity of the catalysts developed carried out on an automated flow set to 600-850^{o}C temperature range, at atmospheric pressure. The results of the study showed that changing the composition of the catalyst and the conditions of the oxidation of methane can obtain valuable products such as synthesis gas, and ethylene. Supporting of tungsten heteropolyacid on alumina leads to improved selectivity on ethylene. Using as active phases of nickel and lanthanum oxides supported on alumina results in a mixture of hydrogen and carbon monoxide (synthesis gas). Introduction of the lanthanum oxide into the Ni / Al_2O_3 catalyst increases the textural characteristics of the catalyst and enhances catalyst stability to coke deposition. For Ni-La / Al_2O_3 catalyst is observed the highest catalytic activity in the reaction of partial oxidation of methane with oxygen. The conversion of methane was 95%, the yield of hydrogen and carbon monoxide 46 and 40%, respectively.

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PL-04

HIGH-RATE LITHIUM-ION BATTERIES: RECENT ADVANCES

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To be prospective for automotive applications, lithium-ion batteries must ensure the starting acceleration of a vehicle. Their power density is significantly governed by the diffusion of lithium ions into (and within) the grains of an electrode material. It is considered [1] that obtaining nanosized electrode materials is beneficial from the point of view of the accessibility of theoretical capacities and high speed of discharge of lithium-ion batteries. Contrary to this expectation, numerous microsized materials demonstrate excellent electrochemical performance; it is even stated that no difference exists between microsized and nanosized samples.

During the past years, in Joint Department of Electrochemical Energy Systems, significant efforts have been undertaken towards synthesis, characterization and electrochemical testing of numerous micro- and nanosized materials serving as cathode and anode materials in high-rate lithium-ion batteries. In particular, titanium derivatives (TiO_2 and $Li_4Ti_5O_{12}$) have been probed as anode materials. Olivines (e.g., $LiFePO_4$) and neat and substituted spinels ($LiMn_2O_4$, $Li_{1\pm\delta}Mn_2O_4$, $LiNi_{0.5}Mn_{1.5}O_4$) have been studied as cathode materials.

In this presentation, based on literature data and our works, we discuss the high-rate electrochemical applications of electrode materials [2]. In particular, specific capacities and rate capabilities are analyzed and a conclusion is drawn that these materials often demonstrate extremely high capacity retention in heavy-duty tests and at the same time show shortage in capacity at small current loads. In order to uncover the origin of such behavior, the following requirements to electrode materials are formulated. An ideal electrode material should consist of nonaggregated, nanosized, perfect single crystals. The absence of aggregation would provide an access to the whole surface and whole volume of the crystals for the lithium ions migrating from the bulk of an electrolyte solution to the electrode and diffusing inside the electrode. Nanodimensionality would be the prerequisite of achieving the minimal possible times of diffusion in the solid material. The perfectness of the crystals would guarantee the absence of defect regions inaccessible to the lithium ions, i.e. would ensure the attaining of theoretical capacity. Therefore a balance between high rate properties and capacities should be determined not only by the size of crystals but also by their perfectness and ability to aggregation.

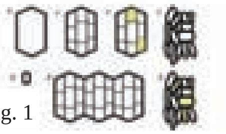
Fig. 1

These requirements can be illustrated by Fig. 1. Electrode materials made of perfect crystals of either micrometer (a) or nanometer dimensions (b) must be able to be discharged with great currents, at the same time demonstrating specific capacities close to theoretical values. In well-shaped microsized and nanosized crystals, such imperfections as dislocations, domain boundaries, etc., should not cause significant resistance to the diffusion of the lithium ions (c). These crystals will be able to be discharged with great currents and demonstrate high specific capacities. The same is probably applicable for regularly accreted well-shaped crystals of any size (d). The possible presence of defect domains and non-conductive crystallites (e, colored regions) decreases specific capacity but does not influence the speed of diffusion. In chaotically accreted, aggregated crystals, an access of the electrolyte to the inner part of aggregates will be hampered. This will greatly decrease specific capacity. However, ability to the fast discharge may be secured by external crystals and will not be reduced significantly (f). Even greater capacity lowering will occur in aggregates of partly imperfect crystals (g).

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SOME ASPECTS OF MODELING OF PHOTOCATALYSIS PROCESS

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A model system which is condensed medium with dissolved reagents is considered in the work. In order to neglect direct interaction of reagents with each other and to take into account interaction of the groups of particles, which cause reaction, we assume, that the concentration of particles-reagents is very low. We assume also, that the photon flux acts on the system. Absorption of one photon is one act of photo-transfer, as a result of which reagent in an excited state is obtained. Generally it is supposed, that interaction of reagents with medium is either weak or so strong, that reagents from complexes or these complexes are considered as reagents.

Charge photo-transfer process between dipole-active polarizable particles in non-regular condensed medium is considered. Interaction of intramolecular vibrations with polarization of medium is taken into account. Spatial and frequency effects of the medium are also considered. Spatial effects must be described by different model functions. Modeling of frequency dispersion function may be realized on the basis of the absorption spectrum of medium. During theoretical calculations of photocatalytic chemical reactions methods of theoretical and mathematical physics have been used – multiparticle temperature Green functions of polarization operators of the condensed medium.

Reorganization energy, transition dipole moment, the reorganization energy of quantum subsystem, the rate constant of charge photo-transfer process, etc. were calculated in introduced models. In order to simplify the calculations of the rate constant we will contemplate the case when intramolecular vibrations may be considered as classical. We assume also, that at the beginning and at the end of the process the number of reagent’s degrees of freedom is the same.

PL-06

PLATINUM FREE ELECTROCATALYSTS BASED ON MANGANESE OXIDES FOR ELECTROCHEMICAL DEVICES

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MnO_x oxides with various crystallographic structures are reported in respect to their electrocatalytic behavior in oxygen reduction, oxygen evolution, and hydrogen peroxide reactions. The dual role of carbon in carbon-oxide composite electrodes is discovered (conductive binder and a source of intermediate peroxide species) [1]. Mechanistic features of reactions under study are addressed using rotating disc and rotating ring disc electrodes [1-3]. Correlation of Mn(IV/III) interfacial redox potential and catalytic activity is found. α-Mn_2O_3 (bixbyite structure) is the most active in the series [4]. Microkinetic model is applied to estimate the rate constants of various reaction steps [4,5]. The most pronounced difference of rate constants is found for the steps with participation of di-oxygen species sensitive to surface crystallography.

The specific activity of α-Mn_2O_3 is less than an order lower as compared to Pt, and this material is a real candidate for the alkaline fuel cell cathode. However more ambitious goal is to find the material for regenerative fuel cells, which requires much higher stability under anodic polarization. In this context, carbon-free electrodeposited MnO_x is considered. The challenge is to arrange deposition at as high pH as possible, to provide the material stable under operation in alkaline media. New data on manganese oxide potentiostatic electrodeposition from neutral and alkaline media are reported, and deposition potential is demonstrated to affect crystal structure, dispersion, and specific activity of oxide.

The reported work is supported by 16-53-76014 EraNet.Rus project (collaboration with the Universities of Strasbourg and Antwerpen).

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NEW GENERATION ZEOLITIC ADSORBERS

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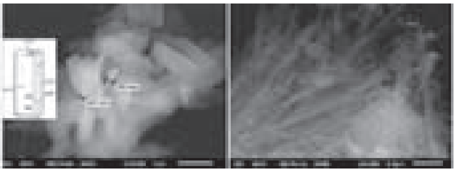
Wide application of zeolites in industry, agriculture, environmental protection and other areas led to interest in new synthetic materials with zeolite-like molecular sieve, sorption, ion exchanging, catalytic, and other properties. Through the synthesis wide range of structures can be obtained, not existing in nature or possessing different properties. For example, synthetic mordenite has the ability to accept ions or molecules larger than 4.5Å, while natural mordenit deprived this ability. On the other hand, due to the well-developed mesoporous structure, natural zeolites have a number of useful properties, including possibility to bond macromolecules and even microorganisms. Synthetic zeolites are usually prepared in the form of crystallites with sizes ranging from hundreds of nanometers (“nano-zeolites”) to tens of micrometers, without secondary porosity. However, the mesoporous structure can be reproduced synthetically.

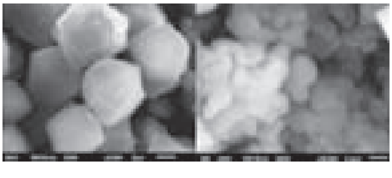
Synthetic mordenite (UPAC chemical formula $|Na^+_8\ (H_2O)_{24}|$ **[**$Al_8Si_{40}O_{96}$**]-MOR**) was prepared using Georgian natural zeolite (clinoptilolite-heulandite-containing tuff from the Rkoni plot of Tedzami deposit, Kaspi region) of **HEU** type ($|Ca_4\ (H_2O)_{24}|$ **[**$Al_8Si_{28}O_{72}$**]-HEU**) in following steps: preparation of raw materials and suspension including acid treatment; gel formation by sodium hydroxide; gel aging; crystallization in the Teflon flasks at 100-110^{o}C; separation and cleaning of target product.



According to the SEM images (Jeol JSM6510LV equipped with Oxford Instruments X-Max 20 analyzer), it is possible to produce mordenite prismatic crystals having width in a range of 0.15 – 0.45 μm and length up to 3 μm (left), as well as mordenite fibrous aggregates characterized by fiber diameter from 40 nm to 90 nm and length up to 10 μm (right), an imitation of non-regular mesoporous structure.

Among widely applied in industry adsorbents and ion exchangers, synthetic zeolites of type A (UPAC chemical formula $|Li^+_4\ (H_2O)_4|$ **[**$Al_4Si_4O_{16}$**]-ABW**) remain popular, and getting them in micro- and nano-powder forms by a simple path from the available and relatively inexpensive raw materials is quite true.

Samples of the sodium form NaA have been prepared by two-stage re-crystallization of the same natural zeolite firstly to the sodalite structure ($|Na_8Cl_2|$ **[**$Al_6Si_6\ O_{24}$**]-SOD**), and then in the target structure: **HEU → SOD → ABW**, in following stages: preparation and acid treatment of raw material; gel formation and its aging; hydrothermal crystallization; separation of intermediate product, new gel formation and its aging; crystallization and separation of target product, its washing, drying and packaging.



SEM images testify the possibility of obtaining both size (av. 5 μm, left) and nanoscale crystallites (150 – 250 nm, right) depending on the crystallization rate and other parameters of gel preparation and crystallization processes; selection of conditions makes possible to receive samples with narrow distribution of the crystallite sizes.

The proposed methods are based on the use of natural silica-alumina raw materials and inexpensive reagents (HCl, NaOH), are characterized by the relative rapidity, low energy expenditures and low Sheldon’s factor R.

PL-08

ENHANCEMENT OF CATHODIC HYDROGEN EVOLUTION REACTION USING PROTON CARRIERS

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The paper is a review on the enhancement of hydrogen evolution reaction using proton carriers. Results obtained in a studies concerning catalytic effect of amines on the cathodic hydrogen evolution are presented.

The approach of this topic is justified by the fact that hydrogen is still considered an excellent energy carrier and a fuel of the future because in the combustion process in engines results only water without carbon dioxide. Unfortunately, most widely used methods for hydrogen production are based on coal gasification, or hydrocarbons cracking and reforming, having as a result not only hydrogen, but also a huge amount of carbon dioxide.

Water splitting by electrolysis is a clean (*green*) procedure, but it is limited by an important electric energy consumption. This is the reason why the research on the cathodic hydrogen evolution is still beneficial. The great majority of studies on the enhancement of water electrolysis process approach the electrocatalytic effects of materials on both anodic and cathodic processes: oxygen and hydrogen evolution respectively. In these circumstances, the enhancement of hydrogen evolution using catalysts in the electrolyte solution has been studied much less. Such effect was noticed in polarography, because on mercury the overpotential of hydrogen evolution is outstanding. Albumin was the first proton carrier studied as catalyst for hydrogen evolution. Later, Heyrovsky M et al extended this study using other type of peptides or proteins [1]. Mechanism of protonated amines effect on hydrogen evolution was proposed by Frumkin A.N. According to his explanation, protonated amines take part directly in the cathodic charge transfer process, a second step been a chemical reaction in which molecular hydrogen is produced [2]. A mechanism in which the overall process occurs in four consecutive steps was proposed by Stackelberg et al [1,3].

Recently, the catalytic effect of amines on hydrogen evolution has been studied using metals on which the overpotential is lower than on mercury. For example, on copper cathode, in 1 M H_2SO_4, the exchange current (i_o) of $4.38\cdot10^{-4}$ A m^{-2} has been obtained, whereas in the presence of 0.1 M benzylamine, i_o increased almost 100 times ($4.74\cdot10^{-2}$ A m^{-2}) [1]. A thorough study on the catalytic effect of methylamine, aniline and 4-chloroaniline on gold cathode in the same solution was carried out [4]. Interesting results, with practical implementation perspectives, have been obtained on platinum. In this case, an increase of i_o from 2.9 A m^{-2}, in blank H_2SO_4, to 67.6 A m^{-2}, in the presence of 10^{-2} M aniline, was emphasized. In the same time, activation energy for hydrogen evolution decreased to times [5].

As well, a correlation between molecular parameters of proton carriers and catalytic effect for hydrogen evolution reaction has been accomplished [1, 5].

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ANALYSIS OF SCIENTIFIC PRODUCTIVITY AT THE MESO- AND MACRO-LEVELS

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The most important instrument for solving science management problems is analysis of scientific activity efficiency at both the microlevel, that is for an individual researcher as well as at the meso- and macro levels:for scientific groups and departments, large scientific collectives (universities, institutes, etc.) and the State as a whole.

The formal analysis on the basis of such quantitative parameters can produce a distorted picture of the scholar's scientific activity. In order to obtain a real characteristic of the researcher's activity independent expert opinions need to be used [1,2], whereas in calculating the quantitative scientometric characteristics, of most importance is to take into account such parameters as self-citation (direct and indirect), number of co-authors, time distribution of published works, etc.[3,4]

In our opinion, of special importance is the taking into account the scientific field/discipline of the researcher. An average number of citations per article in the world flow of publications can, depending on the discipline, differ more than seven times. For Georgian chemist, depending on research area, an average number of citations per article is also significantly differ: for Chemistry, Analytical – 17,5 citations per article, Chemistry Applied – 1,7, Chemistry, Physical -4,6. As a result, the formal analysis of their activity will give a distorted account [5,6]

Similar problems arise when comparing scientific activity characteristics at the meso- and macro levels.

On the basis of conducted experimental research authors have arrived to a conclusion that the effective citation index I* obtainable by modernization of the I-index concurrently introduced by Kosmulski [7] and Prathap [8] is the most expedient for analyzing the efficiency of scientific activity at the meso- and micro-levels.

A complete solution of a problem of scientometric support of the Georgian science management system requires that the articles published by Georgian scientists in the Georgian scientific periodicals need also be analyzed.

This will require standardization of the processes of preparation and publication of the Georgian scientific periodicals as well as the development of a Georgian Science Citation Index.

The works on the implementation of the aforesaid tasks are intended to start on the basis of scientific periodical published at the Georgian Technical University and to be extended, in the future, to the publications of other universities, research centers and publishers of Georgia.

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NPN

NANO PROCESSES AND NANOTECHNOLOGIES

NPN-O-01

SORPTION CHARACTERISTICS OF ORGANIC MATERIALS IN METAL ION REDUCTION REACTION AND NANOTECHNOLOGY

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Our aim is to applicate adsorption and sorption characteristics of DNA, PAMAM (Polyamidoamine) – dendrimere, cellophane membranes, human hair and cotton fibber in copper and silver ion reduction to atomic state. Based on DNA – silver complex interactions of structures having identical chromophore and hard structure are demonstrated widening of DNA-silver absorption spectra [1]. Interactions of silver ions with DNA are characterized by inter – cross type of links which reduce dynamic properties of double helix and make it harder.

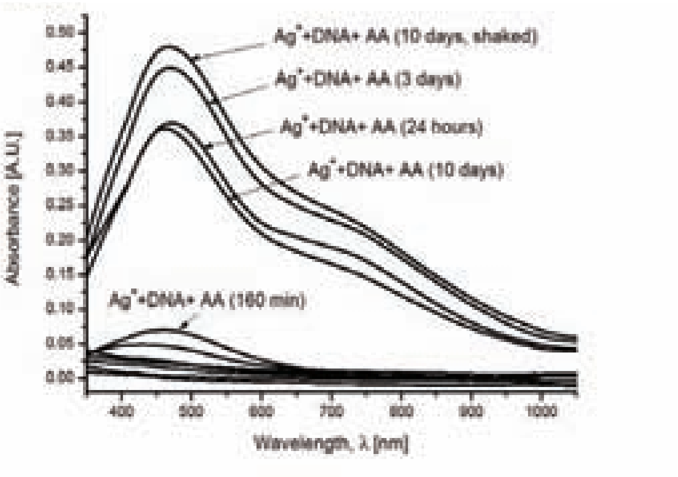

Figure. Spectra for silver ion reduction (AA - Ascorbic acid) in complexes.DNA-$AgNO_3$-AA. [DNA]-$5.9 \cdot 10^{-4}$ M(P), [$AgNO_3$]-$1.2 \cdot 10^{-4}$M, [AA]-$2.4 \cdot 10^{-4}$M, [$NaNO_3$]-10^{-2}M.

The reason for spectrum widening is further condensation of reduced silver ions in clusters and nanoparticles with the size of more than 50 nm.

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NPN-O-02

NANOSTRUCTURE FABRICATION BY USING OF BLOCK COPOLYMERS

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Digital electronics is one of the key factor for contributing to world economic growth. For electronic industry, miniaturisation has been driving forces in the last two decade. Moore's law describes a driving force of technological and social change, productivity, and economic growth. As it has been observed by Moore who predicted that the number of transistors in a dense integrated circuit doubles approximately every two years. This development has been made very clear in the semiconductor industry which is moving below 22 nm in pitch and has been scheduled to hold the 10 nm width in late 2017 [1].

Block copolymers (BCPs) have attracted increasing interest with a promising future in the nanoelectronics industry due to their ability to self-organize at nanometer scales. BCPs have been used as a template for generating periodic nanopattern on the surfaces and as self-assembled nano-lithographic resists for patterning/templating front-end nanodevices. BCPs. When the strength of the repulsive interaction between blocks is sufficiently large, two or more chemically distinct homopolymers tethered to each other, leads to microphase separation of dissimilar polymer chains into periodic domains in the transition state. Typical dimensions of these microdomains range from 7 to 50 nm, a span that encompasses those required by the semiconductor industry for the fabrication of future integrated circuits [2].

In this perspective, procedures for achieving nanopatterning, as well as orientation order of microdomain patterns, and how BCPs could be used as a form of selected area deposition and lead to process complexity reduction in device fabrication. Moreover, the recent advances in the chemical and physical aspects of patternable block copolymers, and highlight some of the challenges in promising nanostructure fabrication for electronic applications will be presented.

Acknowledgements

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NANOMATERIALS AND PHOTOELECTROCHEMICAL SYSTEM FOR PRODUCTION OF SOLAR HYDROGEN

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For use as electrodes in photoelectrochemical systems for solar energy converting, semiconductor materials which have high photosensitivity are promising in the visible spectrum, in particular GaAs and CdSe. To improve the photoconversion efficiency, various surface modification techniques may be used, for example, the deposition of metal nanoparticles and creation on the basis of their semiconductor nanoheterostructures and other nanostructure systems. We studied single-crystal epitaxial films of n-GaAs and heterostructures TiO_2 - Cd chalcogenide / graphene oxide (GO). The heterostructures were obtained by combined (electrochemical, chemical, mechanical) methods on the Ti -framework with specially formed layer of TiO_2 nanotubes (NT). It is shown that such structure provides good adhesion the CdSe layer to the substrate, reduced the leakage of cathode dark currents and increases the efficiency of the photoelectrodes.

The aqueous dispersion of GO was obtained using the modified Hammers methods from multiwalled carbon nanotubes, and acetylene black [1, 2]. On the electrodes surface were deposited nanoparticles of Zn, CdS, Au, Pt and the particles of Nb_2O_5. There were investigated the photoelectrochemical properties, the recombination processes, the surface structure of nanocomposites films and heterostructures, as well as their efficiency in photoelectrochemical systems for hydrogen production.

It was established that the modification the surface of CdSe-, GaAs- electrodes reduces the density of recombination centers, which are formed by surface defects, located in the zone of three-phase contact [3], and an increase the characteristic relaxation time of photopotential and growth its amplitude, i.e. increase the electrode photosensitivity. Modification of the semiconductor surface is also led to an increase in the photoelectrochemical current quantum yield η_i in a wide spectral range. The greatest increase η_i was observed in the case of CdS nanoparticles and the smallest - to Pt. Increasing η_i in the visible spectrum after surface modification CdS, Zn, and Pt can be explained by an increase of the surface photocatalytic activity (increasing the anode reaction rate) and the decrease rate of surface recombination of holes and, as a consequence, increase the hole photocurrent [3]. We found that the modification the surface of the semiconductor electrode with Nb_2O_5 increases the load parameters NT-TiO_2 / CdSe- electrode on 10 ÷ 20%, and reduces the relaxation processes related to adsorption processes, slow processes of recombination and carrier capture of charges at the electrode surface.

Obtained values of photopotential shows, that the developed by us photoanodes provide the hydrogen evolution on Pt and are promising for use in the electrochemical systems for the solar energy conversion. As cathode materials were tested nanocomposites based on carbon nanotubes, and reduced graphene oxide with catalytically modified surface. It is found that the characteristics of these materials in the hydrogen evolution reaction exceed the values on the smooth platinum.

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NPN-O-04

SCANNING ELECTROCHEMICAL MICROSCOPY OF NANOSTRUCTURED CARBON MATERIALS

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Nanostructured carbon allotropies (fullerene, carbon nanotubes, graphene) have attracted great interest due to their capability to be exploited in various fields such as energy, environment, water, or biomedicine. Herein we apply scanning electrochemical microscopy (SECM) to demonstrate quantitatively electroactivity of carbon nanostructured surfaces: graphene and highly organized pyrolytic graphite (HOPG). Scanning electrochemical microscopy is a powerful electroanalytical tool to investigate heterogeneous electron transfer (ET) reactions at interface of different phases [1]. In standard SECM measurements, a disk ultramicroelectrode (UME) tip is positioned near a target surface to monitor ET kinetics at the local substrate area under the tip.

Study of HOPG, important electrode material as a structural model of graphitic nanocarbons, by SECM-based nanogap voltammetry [2] in (ferrocenylmethyl)trimethylammonium ($FcTMA^+$) solution showed the higher electrochemical reactivity of the HOPG surface as the aqueous concentration of organic impurities, i.e., total organic carbon (TOC), is decreased from ~20 to ~1 ppb. In ~1 ppb-TOC water, SECM-based nanogap voltammetry yielded very high standard electron-transfer rate constants, k^0, of ≥17 and ≥13 cm/s for the oxidation and reduction of the $FcTMA^{2+/+}$ couple, respectively, at the respective tip−HOPG distances of 36 and 45 nm. Anomalously, k^0 values and nanogap widths were different between the oxidation and reduction of the same redox couple at the same tip position, which is ascribed to the presence of an airborne contaminant layer on the HOPG surface in the noncontaminating water [3].

Apart from HOPG, we used nanogap voltammetry based on scanning electrochemical microscopy to find that heterogeneous electron transfer can be remarkably fast at graphene electrodes grown by chemical vapor deposition (CVD) that are fabricated without using the conventional poly(methyl methacrylate) (PMMA) for graphene transfer from a growth substrate. Very high standard rate constants, $k^0 \geq 25$ cm/s for ferrocenemethanol (FcMeOH) oxidation at polystyrene-supported graphene, which are at least 2–3 orders of magnitude higher than those at PMMA-transferred graphene, were obtained [4]. SECM-based nanogap voltammetry also revealed that the high reactivity of a graphene surface can be readily compromised by its airborne contamination.

Adventitious organic impurities must be eliminated from the surface of a target electrode to study its intrinsic electroactivity. This task, however, is highly challenging for advanced electrochemical measurements. SECM-based nanogap voltammetry of clean carbon nanomaterials and graphite will enable us to reliably address relationships between their electrochemical reactivity and electronic structures.

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STUDY OF STRUCTURE OF CONFINED WATER NANODROPLETS

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The wide spectrum of applications of microemulsions is mainly stipulated by their flexibility, viz. by ability of microemulsions to change their internal structure under the influence of different additives [1]. The doping of most widely used sodium bis (2-ethylhexyl) sulfosuccinate (AOT) reverse micelles interface by nonionic surfactants results in the changes in elastic rigidity of the interface, which in turn stipulates the changes in water solubilization capacity and microviscosity of entrapped water. Mixing of surfactants influence also the dynamics of water in RM [2].

The goal of the proposed work was to study the influence of additives of anionic sodium cholate (SCh) and cationic cetyl trimethyl ammonium bromide (CTAB) introduced in the Brij-30 (polyoxyethylene (4) lauryl ether) non-ionic reverse micelles on the: ratio of the bound, free and trapped water fractions, values of critical micellar concentration, binding process of optical probes with reverse micelles, sizes of the water droplets, density of the water core, etc. with infrared and UV-visible spectroscopy, dynamic light scattering, viscosity measurements, etc.

The O-H stretching vibrational absorption spectra in the region of 3000-3800 cm^{-1} were fitted into three subpeaks with the help of a Gaussian curve fitting program. The microenvironment Brij-30 mixed reverse micelles was investigated by UV-visible spectroscopy via o-nitroaniline and methylorange as optical probes. The change in Gibbs free energy at the micellization process were calculated on the basis of determined values of critical micellar concentration. Kinetic viscosity of the reversed mixed micellar solutions was measured with an Ostwald viscometer.

The revealed changes in: a) ratio of the free, bound and trapped water fractions; b) values of critical micellar concentration; c) Gibbs free energy at the micellization; d) sizes of water droplets and e) binding constants of molecular probe with reverse micelles under the influence of additives of anionic and cationic surfactants may be will introduce some insight in the complex structure of nonionic reversed micelles.

Results may be useful in the investigations of the interface features of reverse micelles as models for biomembranes i.e. in the investigations of water structure, when it is confined to nanometer-scale cavities, viz. in biological systems.

Results can be of considerable pharmaceutical interest in the field of drug delivery, also in the extraction processes via mixed reversed micelles.

Results may be informative in the investigations of reverse micelles since several features of reverse micelles remain to be solved, e.g. water structure close to the interface, water activity, internal pH in the water nanocage, etc.

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NPN-O-06

SECOND-GENERATION POROUS TiO_2 BASED PHOTOCATALYTIC NANOMATERIALS: SYNTHESIS AND PROPERTIES

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A research interest in obtaining and studying of nanoscale porous powders and monoliths on the basis of titanium dioxide has been significantly increased for the last decades. This is due to the fact that the specific surface area of titanium dioxide increases at particle size attenuation, allowing to quantitatively increasing the number of reaction sites on the surface. Besides, the distance to the surface reaction sites can be reduced at the expense of particle size decrease, leading to more effective separation and transfer of photo-generated charge carriers. The versatility of the properties of clusters and nanoparticles synthesized in the last decade has allowed using them in the processes of deep oxidation of organic compounds, including eco-pollutants.

Researches on the development of nanostructured porous adsorption-photocatalytic systems and their application in the field of environmental technology and adsorption purification of wastewater have been active carried out in several world research centers. Preparation of porous photocatalytic materials and investigation of their physic-chemical characteristics are carried out by following priority directions: improvement of phase separation mechanisms in the formation of porous materials; fabrication of photocatalysts with improved properties on the base of nanosized-heterostructured TiO_2, which is active in ***Visible light***; formation of new generation of nanomaterials and aslo bimodal meso-macroporousphotocatalysts for using in sorption-catalytic processes. One issue that has taken some time to be resolved is the notion of how we can make better use of sunlight's visible radiation seeing that the absorption edge of TiO_2 is at 387 nm (ca. 3.2 eV – the band gap energy) for the anatase polymorph. A successful strategy that is gaining some momentum is to dope this metal oxide with suitable dopants (e.g., metal ions and/or non-metals) to shift the absorption edge to longer wavelengths. Doping has been achieved using various physical and chemical strategies, which have led to materials whose absorption edges have been red-shifted to wavelengths ~550 nm (and beyond in some cases).

In present work, we will discuss about purposeful synthesis of novel porous titania based nanomaterials and perspective ways of their modification (Figure):development of the versatile way for the fabrication of perovskite monoliths $ATiO_3$ containing alkaline-earths (A = Mg, Ca, Sr and Ba) with hierarchical pore structures, to control the formation of porous alkaline-earth metal titanates with narrow pore size distributions; fabrication of nitrogen-doped TiO_2 and its hetero-structured monoliths with well-defined porous structure and bicrystalline framework using sol-gel reaction accompanied by a phase separation followed annealing under a modest flow of ammonia gas [1,2].

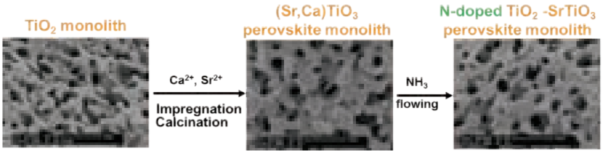

Figure. General scheme for the facile formation of porous TiO_2 based nanostructural materials.

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AN ACCURATE COARSE-GRAINED MODEL FOR POLYSACCHARIDES IN SOLUTION

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Computational models can provide detailed information about molecular conformations and interactions in solution, which is currently unachievable for experimental techniques. Here we provide efficient and precise model for studying conformational properties of long chain polysaccharides in water solution, under different physico-chemical conditions (pH, ionic strength) as well as interactions with various surfaces (Lipid Bilayers, Vesicles, Silica Nano particles etc.). Our model is validated against experimental data for Chitosan polysaccharides with various degree of deacetylation and is applicable to any polysaccharide in a good solvent.

Within our work we developed Coarse Grained (CG) Force Field (FF) with bottom-up approach [1]. Multiscaling was based on Molecular Dynamic (MD) and Metadynamic simulations performed with Amber Glycam All-Atom (AA) FF for the polysaccharides. Pivot Move (PM) Monte Carlo (MC) simulations of CG polysaccharides were used for characterizing the properties of the sugar polymers in implicitly solvent. All available experimental data could be closely reproduced.

We were able to characterize microscopic and mesoscopic structural properties of the long polysaccharide molecules at various pH and ionic strength of the solvent. Consider cooperative impact of the relative stiffness of the particular glycosidic angles and steric interactions. Determine protonation rate and pKapp of the polymer, radius of gyration, persistence length and characteristic ratio.

After the successful characterization of the polymers in good solvent, studies of their interactions with various surfaces of interests were performed. Fully titratable models for the interactions with liposomes with various DOPG/DOPC ratio was employed (Figure 1).

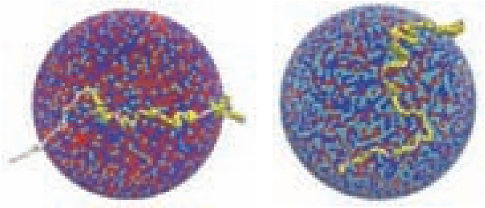

Figure 1. Chitosan adsorbed on Large Unilamellar Vesicles with diameter of 100 nm; Vesicle: Red – DOPC head group; Cyan – DOPG negatively charged head group; Blue – DOPG neutral head group Chitosan: Yellow – Neutral (NH2) monomer; Pink – Acetylated (NAc) monomer; White – Protonated (NH3) monomer. Left image: pH 2, DOPC/DOPG ratio 1/1, Ionic strength of the solutions 0.001. Right image: pH 5, DOPC/DOPG ratio 1/10, Ionic strength of the solution 0.001.

Adsorption on surfaces of various metal oxides was studied with constant charge density of the surface. Currently we are able to simulate systems as dense as composed out of 10 vesicles and 100 polymers each of 1000 monomer unit length. Considering the system size the model achieves a very high level of chemical accuracy.

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NPN-P-01

STRUCTURAL, ELECTRICAL AND OPTICAL PROPERTIES OF INDIUM TIN OXIDE (ITO) AND CDS THIN FILMS WITHIN GLASS / ITO/ AAO/CDS SYSTEM

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Glass- ITO – alumina (G/ITO/ AAO) and Glass/ITO/CdS thin film and nanostructures was manufactured on transparent Soda lime glass substrates for solar cell application. The dependence of structural, electrical and optical properties of ITO, CdS and AAO on fabrication condition was studied. Moreover, the contribution of an each component of Glass/ ITO/AAO/CdS structure on properties of the whole structure during the temperature treatments which it undergoes during conventional fabrication of solar cell in order was evaluated.

Both ITO and aluminum thin films were fabricated by r-f magnetron sputtering at different oxygen content of the plasma in the sputter chamber. The procedure for preparing the AAO layer were prepared by anodic oxidation of Al films in oxalic and sulfuric acids under constant voltage of 40 V at 5º C. Then, AAO samples were subject to etching in 5% phosphoric acid for 30 min at room temperature. The CdS thin films were electrochemically deposited on indium tin oxide (ITO) coated glass substrates from non-aqueous solution of 0.055M $CdCl_2$ and 0.19M elemental sulfur, dissolved in dimethyl sulfoxide (DMSO) at 110º–120°C. The co-deposition kinetics of cadmium and sulfur has been investigated by combination of cyclic voltammetric and potentiostatic techniques. The mechanism of the electrode reactions for the investigated substance have been evaluated and proposed.

As grown ITO and CdS films deposited on conducting glass substrates under identical conditions were treated at 200, 400 and 500ºC in Argon and in air ambient.

The morphology, structural, electrical and optical properties of synthesized thin films was performed by various techniques like scanning electron microscope (SEM), Energy Dispersion X-ray analysis (EDX), X-ray diffraction, sheet resistance measurements, optical transmission and resonance Raman spectroscopy at room temperature at wavelength range from 200nm to 800 nm. The mean sizes of CdS and ITO grains were calculated by using Debye-Scherer formula.
X-ray diffraction measurement of CdS and analysis indicated a hexagonal phase rather than the cubic phase. The XRD and UV-Vis absorption spectroscopic studies reveal the relationship between the thermal treatments and the bandgap and crystallinity of the synthesized films. It was revealed partially, that while the transparency of the ITO films is directly proportional to the oxygen content of the plasma in vacuum chamber and increased with annealing temperature, the sheet resistance is inversely proportional to it.

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PHYSICAL-CHEMICAL TRANSFORMATIONS ON THE LASER IRRADIATED POLYMER SURFACES

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Physical-chemical processes both in the polymer surfaces and ones doped with different substances (metallic, ceramic and polymer micro/nano powders) by laser irradiation with use of modern physical experimental methods are studied. It is established the regularities of the functional dependences between laser beam parameters and polymer structures and physical-chemical properties of laser irradiated polymer materials. There are investigated the following effects of laser irradiation in the polymer materials:

1. Creation of electric conducting materials both in pure polymer surfaces and in polymer part of doped layers. The process of transition of type dielectric - conductor initiated by laser radiation is due to formation of the conjugated double bonds in the polymer macromolecules (formation of infinite clusters), which have semiconducting character of p-type (at moderate laser beam energy) and n-type (at more high energies).
2. Creation of the surfaces with improved sliding properties (anti-frictional materials) on the basis of formation of cross-linking bonds in the macromolecular systems and the annealing of some structural defects. Besides of the selecting of the base polymer, doping substances and doping laser mode allow us to get a surface with good sliding properties.
3. On the basis of carbon chain and siloxane polymers mixtures with nano-dispersive inorganic fillers the composites have been obtained characterizing by both high adhesion to the construction materials both anti-icing properties. The methods of regulation of adhesion and anti-icing properties of these materials have been fond with using of optimization of content and selection of the conditions of laser irradiation.
4. It is shown that after laser irradiation of polymer materials doped with different substrates effectively scatter and even absorb super high frequency (higher 1 GHz) electromagnetic waves. Such properties indicate both the plates/films fully processed by laser irradiation with definite energy and diffraction gratings with selected parameters, formed with combination of conducting channels on some polymer surfaces obtained by laser irradiation with selected diameter of laser beams.

NPN-P-03

SILVER IONS SORPTION BY DNA DOUBLE HELIX AS A MULTISTEP NANOMOLECULAR ADSORPTION PROCESS

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Soft ions in particular Cu+, Ag+, Pt++, Hg++ ions are able to form the so-called inter-strand crosslinks in DNA. Let's consider the process on the example of Ag+. First, silver ions are adsorbed on DNA major groove (N7G or chelate complex N7G and O6G). At small silver ion concentration on DNA does not cause ejection of AO and EB. On the other hand, silver ions at interaction with DNA induce double proton transfer in GC pair. Chelate complex with silver ions makes it easy to unfold DNA double helix with wrong Watson-Crick GC pair. The work presents electron configuration of GC atom pairs taking part in H-bonds before and after DPT. In the last process Guanine's atom O6 is in enol form, Nitrogen atom N1G is in pyridine state and N3C in pyrole state. After unfolding of double helix in neutral water solution N3C atom cannot keep enol state in a long time and it should transfer into its usual pyridine state. At the same time silver ions can with definite possibility attack nitrogen atoms N1G still existing in pyridine state. During the following folding of double helix inter-cross link formation between N1G (rare tautomeric form of bases) and N3C takes place. This way the process of inter-cross link formation can be considered as such a simple process as: 1. Silver ion adsorption on DNA (N7G) and double proton transfer of GC pair with the life-time $\tau1$, 2. Unfolding of double helix, formation of N1G - Ag+ binding, HN3C transfer to N3C and formation of link between N1G - Ag+ - N3C. Total time of the process is $\tau2$, 3. DNA folding with formation of stereoscopically distorted double helix with inter-cross links ($\tau3$). So, in the case of DNA compound absorption process of inter-cross link formation can be reduced to a multi-stage adsorption process consisting of several simple adsorption processes named above with the total time of $\tau1+\tau2+\tau3$.

NICKEL-IRON MAGNETIC COMPOSITES AT THE ETHANOL CONVERSION

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Preparation of nano-sized transition metal of the iron group and their mutual two-component systems are among the most urgent and promising directions. Increased attention to these objects caused to a large extent the features of the magnetic properties of both bulk and fine systems - high values of the saturation magnetization in a relatively low magnetic fields in conjunction with small times of magnetization reversal, the possibility of variation in doping compositions magnitude of the coercive force. For these reasons, highly dispersed (including nano-sized) powders of metals of the iron group stand out as a very promising mainly for production of magnetic materials, including subminiature junctions and elements, magnetic wire, magnetic fluids [1]. Also, transition metal (Fe, Co, Ni) nanophase composites are widely used as catalysts, in the utilization of solar energy systems [2], they are used in the composition of the supported catalysts, in the systems of the magnetic recording and storage of information, power sources and a number of other directions.

The most popular method of producing nanoparticles of magnetite - a liquid phase chemical condensation, which is based on the deposition of bi- and trivalent iron salts, by concentrated aqueous ammonia solution [3].

In this paper for the preparation of magnetic composites impregnation method of bases(carrier) for magnetite on water absorption was used. Thus obtained nickel-iron magnetic composites have magnetic properties. As a precursor of the active components used nickel nitrate, iron nitrate or acetate. It is known that one of the factors influencing the activity of particle precursors is the nature of the salts used. Therefore, in this work the effect of the iron oxide precursor to its state in the composite and catalytic activity in the conversion of ethanol was studied

For the synthesis of the nickel-iron magnetite used the nitrate $Ni(NO_3)_2{\bullet}6H_2O$ "chem. pure" iron nitrate $Fe(NO_3)_3{\bullet}9H_2O$ "chem. pure", iron acetate 4-aqueous $Fe(CH_3COO)_2{\bullet}4H_2O$ and microspheres oxide alumina gamma modification $\gamma-Al_2O_3$. Composites were prepared by impregnating a carrier (alumina) by incipient wetness. The heat treatment is conducted at a temperature 400-500° C during 3 hours.

Test of catalytic activity of magnetic composites in the ethanol conversion performed on an automated flow catalytic unit (1 PKU). The reaction products were identified on the apparatus "ChromosGC-1000" using an absolute calibration method and a thermal conductivity detector. Study of oxidized forms of the active phase of the magnetic composite was determined by temperature-programmed reduction with hydrogen ($TPRH_2$).

The study of the influence of a precursor (ferric nitrate and acetate) of iron oxide on the catalytic change of magnetic nickel-iron composites showed that the use of iron nitrate leads to the formation of 20 vol.% hydrogen and 17 vol.% ethylene. Application of iron acetate to produce iron oxide in the iron-nickel composite leads to the formation of 23 vol.% aromatics. This is due to the formation of a new phase in the low-temperature (T_{max} = 350° C) region of TPR. TPR method determined that in the case of iron oxide supported on aluminum oxide can be observed consistent recovery: $Fe_2O_3 \rightarrow Fe_3O_4 \rightarrow FeO \rightarrow Fe$ and increased dispersion of the composite particles with the addition of a nickel oxide

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NPN-P-05

MODIFIED GRAPHENE OXIDE BY ALUMOORGANIC COMPOUNDS

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Graphene oxide, obtained by oxidation of graphite contains oxygen functional groups (-COOH, -OH, -O-O-, -CHO), after reduction of which reduced graphene oxide (rGO) is received, in which C:O ratio increases due to partial removal oxygen atoms (deoxygenation). Many organic and inorganic compounds are used as reducers. As a result of reduction oxygen containing graphene functional groups OH groups are formed. By using this method, we have obtained graphene structure containing pressing powdery composites [graphene]-O-AlR-O-$[Al_2O_3]$, where graphene oxide and alumina were connected by alumoorganic compounds. Powder composites consolidation has been conducted by SPS method (at 1450-1700^0C) for 5-10 minutes.

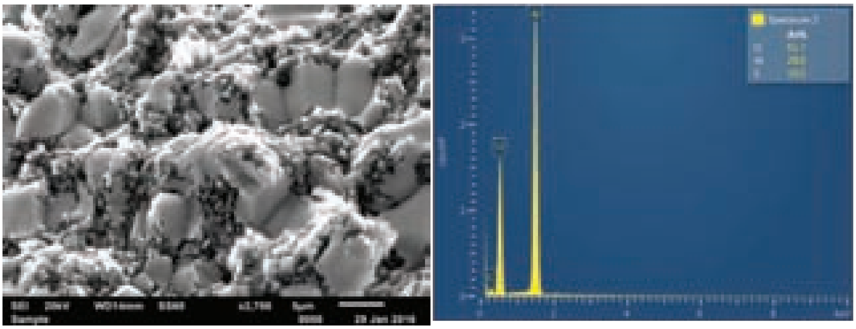

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Fig 1. SEM micrograph (I) and EDS (II) graphene/alumina ceramic composites

During the work the following devices have been used: SPS synthesis device, Glove box, Electronic scanning microscopes Nikon ECLIPSE LV 150, Analysette 12 Dyna sizer, planetary mill Pulverisette 7 *premium line*, SHIMADZU Dynamic Ultra Micro Hardness Tester DUH-211S.

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PREPARATION OF CONDUCTING COMPOSITE POLYMERIC MATERIALS CONTAINING MICRO- AND NANOPARTICLES AND THEIR ELECTROCHEMICAL ALUMINIZING

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The scientific-technical progress requires the necessity of preparation of new materials. Metalized plastics are considered as such materials. Metalizing of plastics allows preparation of the materials with distinguished functional and decorative properties. It is well-known that replacement of light metal by metalized plastics increases the affordability to 20-40% and the heat-resistance increases by 10-15%.

Innovation technology for direct electrochemical metalizing (aluminizing) of polymeric materials will be presented instead of existing chemical - galvanic technology the main disadvantage of which is a difficult formation of current - conducting layer on the polymers surfaces.

The technology of preparation of conducting composite polymeric materials, containing various current-conducting and non-conducting fillers of micro- and nanosize on the basis of phenol formaldehyde resin will be elaborated. The ratio between conducting (graphite, carbon black, metal powders, graphite fiber) and non-conducting (caolin, andesite and etc.) fillers will be determined for revealing of synergic effect which provides the required conductivity and mechanical properties of polymeric material.

The effect of the fillers concentration, of the ratio between them and of the particles dispersion on the conductivity, thermal stability and, what is of important, on the materials operative properties as well as their physical - mechanical properties and electrical characteristics will be studied. The following will be investigated: specific weight of the samples, hardness at impact and compression, water absorption, the specific electrical resistance of the materials and etc.

Primarily in the practice the direct electrochemical aluminizing of prepared conducting composite polymeric materials, the thermal stability of which exceeds 393K, will be carried out from the relatively low-temperature (373-393K) halide melt of our elaboration. Mentioned method is of importance since the preparation of aluminum electroplating is impossible at higher temperatures because of un-stability of polymeric materials. Optimal parameters of the technological process (duration, temperature, current density) will be determined. Their chemical and physical-mechanical properties will be studied. Structural research of prepared plating will be performed.

Obtained innovative materials will be widely used in mechanical engineering, aviation, cosmonautics, electronics, electrical engineering, as well as in medicine and food industry.

Presented innovative technology will significantly reduce the operative costs and improve the eco-safety, will considerably extend the sphere of the use of the polymeric materials.

NPN-P-07

NANOSTRUCTURAL CATALYSTS FOR SYNTHESIS OF N-VINYLMORFOLINE

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In last years, a great progress in construction and investigation of properties modified nanostrutural heterogeneous catalysts for vinylation of organic compounds having in their composition active atoms of hydrogen has been reached.

Vinyl derivatives of heterocyclic compounds also as aromatical hydrocarbons can be synthesized by different methods for example by action of acetylene.

More detail reaction of vinylation of morpholine in presence of KOH with using super base systems KOH-DMSO and KOH-DMPhA and also for comparison without solvent has been investigated. Experimental data have shown that in absence of aprotonic dipolayric solvents also vinylmorpholine was formed with low yield (2.0 % and below). In solution of DMPhA obtained product at 70 ^{o}C and duration of reaction before 4 h. was formed with yield 8-10 %.

Displacement of DMPhA on DMSO has increased yield of forming N-vinylmorpholine. At the same conditions it's yield has reached of maximum – 22 %. In all cases with increasing duration of reaction before 4 h. yield of product was increased and in case of absence of solvent it's changed insignifically.

Investigation of kinetics of morpholine vinylation by acetylene at atmospheric pressure in the presence of system KOH-DMSO carring out at different duration and temperatures has been investigated. By kinetical data graph of dependence on logariphm of rate (lgW) from temperature (1/T) has been constructed and the activation energy (E) of morpholine vinylation was calculated which was equaled 55.6 kDj/mole.

For reaction of morpholine with acetylene nanostructural matrixes of activated coal were elaborated as catalytical systems. Initial dimensions of particles of activated coal which was used as bearer of catalyst at synthesis N-vinylmorpholine by reaction of morpholine with acetylene have been determined.

Dispersion analysis by method of microscopy has been carried out. For this with aim of decreasing of particles dimensions of activated coal fractionation samples were undergo to ultra-sound treatment. For this water dispersion of activated coal (150 ml H_2O:5 g of activated coal) was undergo to ultra-sound treatment in regime 0.6 A, 38 кGc during 60 min.

Analysis of obtained results has shown that dimensions of dispergated particles of activated coal were equaled 700-900 nm. Determination of sedimentational fractionation of particles of activated coal during 20, 30, 40 and 60 min. has shown that in investigated intervals of time their dimensions were changed in great degree. Particles dimensions of obtained fraction after 20 min. of dispergation were in range 500-750 nm. Dimentions of particle of fractions after 30, 40 and 60 min. dispergation were equaled 300-550, 200-320 and 200-250 nm correspondenly.

Heterogeneous-catalytical reaction of acetylene with using catalyst on the base of nanostructural activated coal with dimension of particles 200-250 nm has been investigated. Conditions of carring out of reaction were the same as in presence catalytical system activated coal-KOH. Quantity of KOH in composition of this system was equaled 30 mass %. Influence of temperature on reaction of acetylene with morpholine in heterogeneous conditions in the presence of above-mentioned catalyst has been investigated.

Thus heterogeneous-catalytical reaction of acetylene with morpholine in the presence of catalysts: activated coal AU-L/KOH and nanostructural activated coal/KOH has been investigated. It was shown that in both cases N-vinylmorpholine was formed. Activity of catalytical system nanostructural activated coal/KOH was higher in comparision with catalyst AU-L/KOH. Yield of N-vinylmorpholine in their presence was equaled 38.2 and 31.7% correspondently.

INHIBITION OF THE PHOTOOXIDATIVE DEGRADATION OF CdTe NANOPARTICLES

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The photooxidative degradation of CdTe nanoparticles in the double solvent DMSO/water (ϕ（DMSO)=φ(H_2O）has been investigated for a series of inhibitors including 6-{[(3-hydroxypropyl)N,N-dimethylammonium]methyl}-5-etoxycarbonyl-4-phenyl-3,4-dihydropyrimidine-2-on bromide (Compound I) and ionole. A suspension of the 30 nm CdTe nanoparticles in the solvent containing an inhibitor has been exposed to irradiation of the 405 nm laser. An integral photoluminescence intensity is decreasing under the influence of Compound I (concentration 0.31-5 mmol/l) 50-60 % slowly in comparison to the decrease caused by ionole of the same concentration. The total photoluminescence decrease during the one hour photooxidation of the suspension containing the nanoparticles and Compound I is not deeper than 25 % at 292 K. It is supposed that the lactam-lactym tautomerization and the positive charge of nitrogen atom are responsible for inhibition of photooxidation of the nanoparticles suspension by Compound I.

NPN-T-01

CREATION OF CELLULOSE ACETATE MEMBRANE ON THE BASIS OF DIFFERENT COMPOSITIONS

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Today polymer membranes are widely used to filter solutions. They constitute 80 % of the world production of membranes.The usage of polymers is due to their physical structure and their chemical properties. The Goal of polymermodification is to obtain the membrane with a structure desired for the particular process of filtering.

Properties of polymer membrane in exploitation depends on polymer, its concentration, composition of the polymer solution, solvent type and the concentration of nonsolvent.

Cellulose Acetate areoften used for preparation of membranes [1]. Their properties are moderate hydrophilic, inertto filtering components of the solution and relatively cheap raw materials.

The researchwas conducted on solutions with different concentration of cellulose Diacetate (5-7%) in DMAc/LiCl for creation of Cellulose Acetate membranes in the Engineering Institute of Membrane Technology [2]. The study of the process ofphase inversion ofobtained solutions indifferent correlation conditions ofsolvent and nonsolvent revealed that the range of this correlation forCoagulation bath is 0-20%.

The research was conducted on the automated laboratory instrument created in the Institute. The instrument allowed to control the membrane precipitation process by regulating bath temperature and the speed and angle of immersing of the polymer solution in the bath.

The morphology of the obtained samples is studied by the microscope which is equiped with a digital camera (x5000). The structures of obtained membranes differ. The pore size of some microfiltration membrane is 0, 3-0,45 µm.

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NPN-T-02

VOLTAMMETRIC STUDIES OF SULPHITE ANODIC OXIDATION IN ALKALINE SOLUTIONS ON SMOOTH NICKEL BASED 3 LAYERS PLATINUM NANOPARTICLES ELECTRODE

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This paper presents studies on electrochemical behavior of sulphite ions in aqueous alkaline solution on smooth nickel based 3 layers platinum nanoparticles electrode (Ni-Pt) prepared by spray-pyrolysis [1] in order to understand the oxidation mechanism and to determine the optimal parameters for the sulphite oxidation process in anodic domain.

Nanoparticles are the key components in the development of energy technologies. Therefore, new strategies are necessary for preparing nanoparticles in large volume by techniques that are advantageous in terms of costs. They are widely used in reformers for hydrogen production from solid material, liquid or gaseous energy carriers [2], in electronics and optics [3], enzyme immobilization [4], for industrial synthesis of nitric acid [5], reduction of exhaust gases from vehicles [6] and as catalytic nucleating agents for synthesis of magnetic nanoparticles [7].

Electrochemical behavior of sulphite ions has been studied by cyclic voltammetry on Ni-Pt electrode as a function of sulphite concentration at different polarization rate.

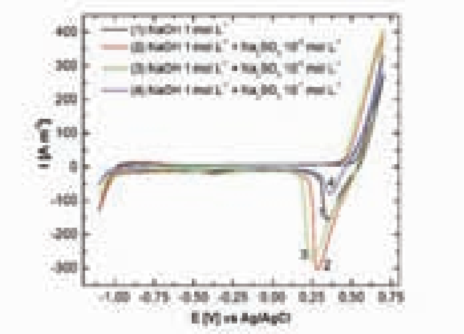

Figure 1. Cyclic voltamograms recorded on Ni – Pt electrode in 1 mol L^{-1} NaOH wihout/with different concentration of Na_2SO_3 at 500 mV s^{-1}.

Based on Tafel method, kinetic parameters (transfer coefficient - α and exchange current density - i_o) for electrochemical oxidation of sulphite to sulphate in alkaline solution on Ni – Pt electrode have been calculated.

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NPN-T-03

MODIFICATION OF CHROMIUM STEEL BY NANO-OXIDE COMPOSITE

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Medium-carbon chromium steel, which contains C – 0.37–0.45, Mn – 0.30–60, Si – 1.20–1.60, Cr – 1.30–1.60, S – ≤0.035 and P – ≤0.035, is applied in mechanical engineering for the production of high-strength and wear -resistant special-duty parts (shafts, fingers, rack-wheels, etc.).

In the development of nano-technology of modification highly-carbon-manganese austenitic steel by a nano-reagent, it's turned out that the effectiveness of the nano-particles impact essentially depends on the uniformity of their distribution in the metal.

For the purpose of this, the briquettes containing iron and nano-Al_2O_3 were manufactured. Namely, a well-mixed powder of carbonyl iron (particles size of 160–200 microns) and nano-Al_2O_3 (nano-particles size of 30–100 nm) in the ratio of 5:1 briquetted by utilizing a double-acting 100-ton press.

Melting of the medium-carbon chromium steel was carried out in an induction furnace.

The study showed the positive effect of the modification by nano-Al_2O_3 on precipitation strengthening of medium-carbon chromium steel. It increases the hardness of steel after rolling or forging in average be 25.5%.

Study of wear- stability was carried out on a rotary machine in conditions of dry friction. The studies did not include the impact-dynamic effect on the sample. Nevertheless, they are acceptable for comparative analyzes. Wear resistance of cast metal modified by nano-Al_2O_3 increases by 26%.

The structure of both steel is ferrit-factured. It's clearly that the steel modified by nano-Al_2O_3 is fine-grained in more extent.

By the electron microscopic ((ultra-high-resolution FESEM for SE and BSE) examination of the rolled speciment it was found that nano-particles of Al_2O_3 existing in the steel structure are located in the boundary zones of the particles, where, presumably, intense diffusive processes (in two, three and higher orders of magnitude more intense than in the similar classic structure) take place. In result, grain boundaries are strengthened.

HOT EXPLOSIVE CONSOLIDATION OF NANOSTRUCTURED Ta-Ag COMPOSITES

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The Different composition of nanostructured Ta-Ag blend powders were consolidate near to theoretical density using the hot explosive consolidation technology (HEC). The percentage of consisting phases were changed between the 10-90%. In order to consolidate Ta-Ag powders and maintain nanostructured billets there were used tantalum precursors with grain sizes 80nm. As a matrix phase, the powders with grain size 5μ were applied. The temperature of heating and loading during the processing was changed too and was up to 1000^0C. The intensity of loading was under 10GPa. The investigations showed that the application of nanostructured Ta-Ag blends of powders and their further explosive consolidation up to 1000^0C allows fabricating high dense cylindrical billets near to theoretical density without cracks and maintaining nanoscale tantalum grains.

The consolidated samples are characterized with good integrity, and good electrical properties. The structure and characteristics of obtained samples depends on the phase content, distribution of phases and conditions of consolidation. Additionally there was established that the electrical properties (resistance and dependence of the susceptibility) of the consolidated Ta-Ag composites are changed depending on phase content and density of consolidated samples too.

The observation of microstructures shows that the consolidated samples have high density and good integrity between the Ag matrix and nanoscale tantalum grains. The investigation of hardness for HEC composites shows strong dependence of hardness value from content of composition. With increasing of matrix phase of Ag, the value of hardness decreases at high temperature consolidation. But the composites with high concentration of Ta (80-90%) have high value of hardness between the 600-700Hv. The mentioned effect may be explained by plastic deformation and fragmentation of individual tantalum grains maintained after HEC due to their high value of recrystallization temperature.

The above mentioned and other features of preparing Ta-Ag Nano-structural precursors to obtain high dense cylindrical billets with perfect structure and uniform distribution of consisting as well as the detail description of HEC technique will be discussed and presented.

FTA

FUNDAMENTAL AND TECHNOLOGICAL ASPECTS OF PROCESSING OF MINERAL PRODUCT AND SECONDARY RAW MATERIALS

RESEARCH OF THE POSSIBILITY OF RECEIVING ACID AND HEAT-RESISTANT CONTINUOUS FIBER GLASS WITH USE OF MANGANIFEROUS WASTE PRODUCTS

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The possibility of working out the new initial compounds of continuous glass fiber on the base of raw material of manganese containing waste products has been studied. By determining the melting of the waste products' raw material, homogenization and boiling properties has been stated the necessity of correcting the waste products by adding quartz sand.

The combination in the compounds of the optimal correlation between oxides SiO_2 and MnO simultaneous existence of several species of twovalent oxides in the compound of CaO, MgO, ZnO and modifying additions provided easier melting property of the experimental glasses, good working and data and high physical and chemical properties both of the glasses and elementary fibers.

The study of the properties of the worked out glasses revealed their lower crystallizing notivity - one of the most important parameters of glass for working out continuous glass fiber. It enable us to form the fibers in the laboratory equipment at reduced temperature and high stability of the working out process, which actually went on without breaking within a wide temperature interval.

The worked out fibers are marked with high acid stability in the area of 1N HCl and 1N H_2SO_4 and also temperature resistance within the range of 400-500 C^o.

As a result of the research the new compounds of chemical and thermoresistant glasses for the glass fiber on the base of non-deficit waste products, containing manganese in order to work them out in the textile filtered materials to be used for the filtration of the products of burning hot and chemically aggressive gasses and liquids.

FTA-O-02

EXPLOSIVE CONSOLIDATION OF Cu–W COMPOSITES IN HOT CONDITION

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The alloys of W-Cu have been growing industrial interest for superior thermal managing and as microwave materials due to the high thermal conductivity of copper and the low thermal expansion coefficient of tungsten [1]. W–Cu alloy parts are generally fabricated by Cu infiltration into W skeleton or liquid phase sintering of W–Cu powder mixtures [2]. However, because of the W–Cu system exhibits mutual insolubility, W–Cu powder compacts show very poor sinter-ability [3]. The Physical-mechanical properties of the composite largely depend on both microstructure and composition relating to fabrication methods and synthesis conditions.

In this work a new approach for the preparation of Cu-W composite materials was proposed, the essence of which is the joint reduction of tungsten and copper oxides by energy saving combustion synthesis or self-propagating high-temperature synthesis (SHS process) method [4] using Mg+C mixture as combined reducer. The latter will allow controlling the reaction temperature in a wide range, and performing complete reduction of both oxides synthesizing W-Cu composite powders in a controllable combustion mode. The combustion experiments in the $CuO\text{-}WO_3\text{-}xMg\text{-}yC$ quaternary system were performed based on the preliminary thermodynamic calculations made for that system, as well as considering the experimental results of binary and ternary systems. It was shown that at certain amount of reducers and slow propagation of combustion wave, it becomes possible the joint and complete reduction of both oxides. According to XRD analysis results, at optimal conditions combustion products contain only - W, Cu and MgO. After the acid treatment (10%wt. HCl) of the product obtained at optimal conditions, it represents a desired W-Cu composite with particles submicron sizes. EDS analysis certifies the homogeneity of obtained W-Cu composite material with similar distribution of both metals.

W-Cu precursors developed by CS process were subjected to consolidation into cylindrical rods using hot explosive consolidation (HEC) technology and hot vacuum compaction (HVC) process. The consolidation temperature was changed up to 1000 °C at the shock wave loading intensity under 10 GPa. The investigations showed that fine W-Cu precursors obtained by combustion-coreduction process and their further explosive consolidation allows to fabricate high dense cylindrical billets near to theoretical density without cracks and uniform distribution of consisting phases. The consolidated samples are characterized with good integrity, which depends on the distribution and size of the W and Cu particles. It was further established that the electrical properties (resistance and dependence of the susceptibility) of the consolidated W-Cu composites are changed depending on phase content and density of the consolidated samples.

It was demonstrated that combination of CS and HEC undoubtedly has advantages compared to other technologies and may be considered as an alternative way to fabricate novel Cu–W composites with enhanced properties.

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ELECTRODEPOSITION AND CHARACTERIZATION OF Mn-Cu-Zn ALLOYS FOR CORROSION PROTECTION COATINGS

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Mn-Cu-Zn alloys were electrodeposited from sulfate bath, containing citrate or EDTA and their mixtures as complexing ligands. The influence of bath composition and deposition parameters on alloys composition, cathodic current efficiency and structural and electrochemical properties were studied. At a higher current density (≥ 37.5 A dm$^{-2)}$ a uniform surface deposit of Mn-Cu-Zn was obtained (Fig.1, a). Optimal pH of electrolyte (0.3 mol dm^{-3}Mn^{2}+ + 0.6 mol dm^{-3} $(NH_4)_2SO_4$ + 0.1 mol dm^{-3} Zn^{2+}+0.005 mol dm^{-3} Cu^{2+}+ 0.05mol dm^{-3} Na_3Cit + 0.15mol dm^{-3} ЭДТА; $t=30^0C$; $\tau=20$ min) for silvery, nonporous coating of Mn-Cu-Zn alloy is within 6.5-7.5; coating composition: 71-83% Mn, 6-7.8% Cu, 11.5-20% Zn, current efficiency 33 -36%.

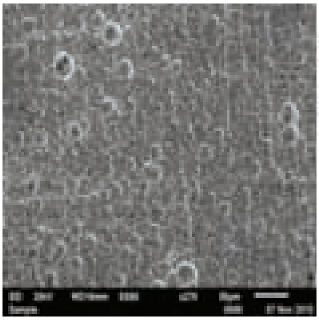

Fig.1, a

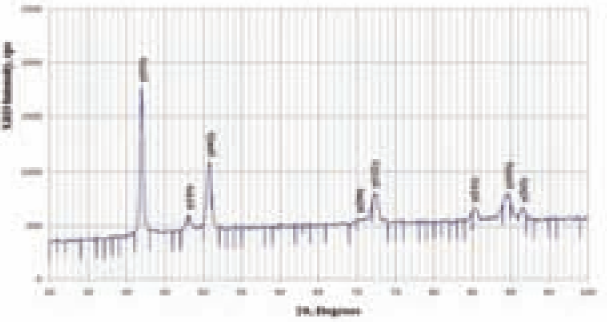

Fig.1,b

XRD patterns (Fig.1,b) reveals BCT (body centered tetragonal) γ-Mn solid phase solution (lattice constants a=2.68 Å; c=3.59 Å) . Corrosion measurements of deposited alloys were performed in aerated 3.5% NaCl solution. The corrosion current density (i_{corr}) of the electrodeposited alloys on carbon steel (analog of Russian Ст3) was 10 times lower than corrosion rate of pure zinc and manganese coatings. Triple alloy coatings corrosion potential (E_{corr} = -1140mV vs. Ag/AgCl) preserved negative potential value longer (more than three months) compare to carbon steel substrate (E_{corr} = -670 mV vs. Ag/AgCl). Tafel polarization curves taken on Mn-Cu-Zn alloy coating (Fig.2) in aerated 3.5% NaCl solution did not show a typical passivation behavior which can be explained by formation of low solubility, adherent corrosion products on the alloy surface.

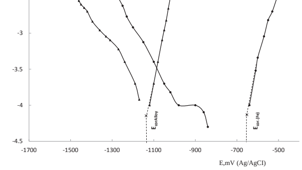

Figure 2. Tafel polarization behavior of carbon steel and electrodeposited Mn-Cu-Zn alloys on carbon steel substrate in aerated 3.5 % NaCl solution, t=25oC.

FTA-O-04

ELABORATION OF NEW TYPES, ECO-SAFE, INEXPENSIVE, HIGHLY EFFICIENT FIRE- PROTECTIVE MATERIALS

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Elaboration of new types, eco-safe, highly efficient fire-protective materials, by the use of local mineral raw materials are discussed in the article. The technology for production of these materials differs from the serial production technology. Such fire-protective materials are manufactured only by mechanical mixing of binders and fillers, does not need addition of expensive flame retardants, which is reflected in low cost price of fire-protective materials in comparison with imported analogues.

Organic as well as inorganic compounds are used as binders. The high-dispersed composite powders of mineral raw materials were used as fillers. Raw materials: zeolite, clay shale and perlite were selected according their high operating properties and due to the factors indicating the reduction of burning processes. This is enabled by means of thermo-gravimetric analysis and Investigating their fire-extinguishing ability [1,2]. On the basis of experimental results it is stated that, composite powders of zeolite, clay shale and perlite on flame zone perform homogenous as well as heterogeneous inhibition of combustion process and in surface zone they form protective layer, which hinders heat transfer to combustive material and excludes direct contact of combustive material with air. Hence, they are characterized by high inhibition properties similarly to flame retardants [2, 3]. Therefore, such powders we used as fillers, which in composite materials are functioning, in itself, as efficient inert flame retardants. Mentioned fillers, similarly to serial inert flame retardants, don’t participate in the process of polymer preparation and in contrast to them are characterized by high operating properties.

Operating properties as well as fire-resistance of obtained fire-protective materials, were studied by standard laboratory methods. Investigation of fire-resistance is possible by various standard methods of fire testing. We use the method of “fire tube”, which is exploited for building materials for establishing of combustibility group [4].

Experimental results show, that fire-protective materials prepared on the basis of such composite powders and of polyurethane resins are characterized by high operating properties as well as fire-resistance. Thus, obtained materials may be used for protection against fire of practically all types of building materials and construction and provide fire-safety of surface as well as of underground buildings.

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FTA-O-05

OPTIMIZATION OF BIODIESEL PRODUCTION FROM MUSTARD OIL

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Mustard oil is one of the promising future raw material for biodiesel production in India. Biodiesel yields from mustard oil was comparable with other raw material e.g., canola and soybean oils that has been reported in the literature. Thus, the transesterification process to produce biodiesel from mustard oil was studied. Biodiesel yields were analyzed using the FTIR (Mid-IR) spectroscopy method. Biodiesel yields from mustard oil at different conditions were investigated in order to optimize the process. Response surface methodology (RSM) was used to optimize the process parameters of the transesterification reaction. The KOH catalyst was found to be suitable for the transesterification of mustard oil over the NaOH catalyst. Optimum conditions of the independent variables for the KOH catalyst transesterification of mustard oil were determined as; catalyst concentration 1.5 % by weight; reaction temperature, 60˚C; and methanol-to-oil molar ratio of 6:1. The maximum yield of 96% for mustard oil was obtained at these conditions. The model showed a good agreement with the experimental results, demonstrating that this methodology was useful for optimization. The model was successful in explaining the variation of response with respect to the three process parameters studied.

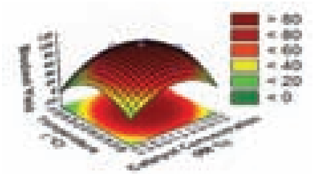

Fig.3. Response surface curve plot showing effect of catalyst concentration and temperature on FAME yield.

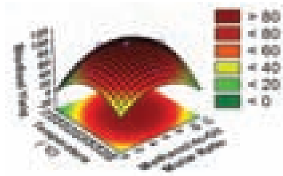

Fig.4. Response surface curve plot showing effect of reaction temperature and methanol-to-oil molar ratio on FAME yield.

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FTA-O-06

THERMAL CHARACTERISTICS OF SPINEL-TYPE COMPLEX OXIDES $Me_{1-x}Zn_xFe_2O_4$ (WITH Me= Cu OR Mg)

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Investigation of various properties of multicomponent oxides is the important scientific task for today in connection with intensive new materials development. Because of advanced properties, the oxide materials of different composition are widely applied in many fields of high technology. The thorough study of isomorphic series of multicomponent oxides gives an opportunity to analyses the effect of compositional variable on useful properties of compounds and to reveal the relationships between composition, structure and physical-chemical parameters. These data are important for elaboration the optimal conditions of technological processes.

The present work is devoted to study of thermodynamic properties of two most important series of complex oxides - $Cu_{1-x}Zn_xFe_2O_4$ and $Mg_{1-x}Zn_xFe_2O_4$, having spinel-type crystal structure. The following results are reported and discussed:

- Heat capacity (*Cp)* of the members (x=0; 0.2; 0.4; 0.6; 0.8; 1.0) of the series are experimentally measured in the temperature domain 300-900K using differential-scanning calorimeter DSC-111 ("Setaram" production). The mean experimental accuracy is
- On the base of experimental temperature function of heat capacity the main thermodynamic functions: entropy -S_T, enthalpy – *(T)*, Gibbs energy - *(T)* are calculated and tabulated as reference data for the temperature range 298-900K.
- Both isostructural series of ferrites have the similar type of compositional dependences of heat capacity at standard temperature with maximum at intermediate compositions. This coincides with the type of alteration of magnetic moments in relevant complex oxide systems. At the same time in both systems the Curie temperature (T_C) progressively decreases linearly with increasing a fraction of diamagnetic zinc ferrite.Top of Form

Bottom of Form

- Phase transitions in investigated systems are of following origins: the compositions, rich in copper and magnesium (x=0; 0.2; O 4) have the λ-type heat capacity curves, which are associated with the process of magnetic disordering in the ferromagnetic complex oxides and are realized as the second order phase transition. With increasing of zinc content, the ferromagnetic increment of heat capacity gradually decreases, that leads to unusual shapes of heat capacity functions for the compositions with x=0.6-0.8.
- In the compositions with high content of copper the special type of heat capacity anomalies are detected, which occurs because of effect of Yan-Teller. The temperature domains, compositional limits and the behavior of heat capacity functions of this transformation are discussed.
- The conditions of thermal treatment of compounds, especially quenching, significantly affects the thermodynamic properties of spinel-type compounds. This process is connected with redistribution of cations over vacancy of crystal sub-lattices. To obtain the equilibrium distribution of cations in sublattices of spinel crystal structure, the conditions of annealing and the required parameters of heat treatment were investigated, such as: enthalpy of stabilization, temperatures of annealing and quenching, and the correct temperature regimes of synthesis.

ASCERTAINMENT OF THE MECHANISM OF FORMING OF ZONAL CONCENTRIC “AGATE STRUCTURES”

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More than 100 years genesis of zonal concentric “agate structures” was topic for debates between famous scientists – geologists and chemists. On the basis of successively carried out scientific innovations the author could ascertain the mechanism of their forming: for the first time the attention was paid to hydrothermal metasomatic genesis of white opaline lining of agate geodes; for the first time were revealed zeolites in the composition of this lining; the lining consists of opal ($SiO_2 \cdot aq$) which was formed by transformation of chalcedony. But opal takes many times much volume than chalcedony that causes centripetal forces in jelly-like colloid solution. In their turn the centripetal forces, on the basis of autowave theory, generate rhythmic waves which form zonal concentric “agate structures” in the jel (analogous to the famous “Leisegang Rings”)

FTA-O-08

SHOCK WAVE ASSISTED CHEMICAL REACTIONS AND CONSOLIDATION OF Ta-Al INTERMETALLIC COMPOUNDS

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The main purpose of presented work is to combine hot explosive consolidation technology (HEC) with Self propagated High Temperature syntheses processes (SHS) to obtain Ta-Al based cylindrical billets with low porosity and improved physical and mechanical properties.

The first stage investigation were carried out for explosive consolidation of powders at room temperatures to obtain billets with increased density without cracks and activated surfaces of consolidated particles. The second stage experiments were carried out for same billets but consolidation were conducted in hot conditions above and under of combustion reaction temperatures. The intensity of loading was under 10GPA. The heating temperature was up to 950^{0}C. The time of heating billets before loading was under 30 minute.

The investigation showed that the initiation of CS process and the full SHS reaction in Ta-Al powder composites starts from 940^{0}C. In order to fabricate billets near to theoretical density with perfect structure and correct geometry it’s necessary to load billets before 940^{0}C. The consolidation of billets above the 940^{0}C temperature leads to cracking in whole volume of HEC billets. The application of B_4C additives and HEC of Ta-Al-B_4C composites leads to the dissolution of B_4C phase behind of shock wave front and formation of TaB, $AlCTa_2$ and $TaAl_3$ phases behind of shock wave front. The reducing of HEC temperature and consolidation of Ta-Al precursors near to 600^{0}C provides only partial reaction between the phases and formation of aluminates on the surrounding surfaces of Ta particles in whole volume of HEC billets are observed The type of obtained intermetalic compounds depends from percentage of separate phases in starting composition.

The above mentioned and other features of structure-property relationship of consolidated Ta-Al based composites depending on loading condition and set up of HEC device will be presented and discussed.

OXIDATION OF MANGANESE NITRATE SOLUTIONS BY OZONE - AIR MIXTURE

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Chemical method of obtaining of manganese dioxide, which considers the oxidation of manganese-containing solutions by ozone – air mixture with a formation of γ -MnO_2 is processed [1]. Simplicity, reliability, efficiency and the absence of ballast are those main features, which allows to create the waste-free production by means of ozone method.

Over many years our laboratory and the firm "Hydrogen Technologist" are connected by official friendly relations. In 1980s the ozonator construction was jointly elaborated, which is protected by author's certificate [2]. Ozonator worked under the action of photochemical, ultraviolet light and by "quiet" discharge. The disadvantage of ozonator involves a low efficiency. At now the firm "Hydrogen Technologist" made ozonators of new generation, which are introduced in various fields of Georgian industry.

The technology of the enrichment of Chiatura manganese-containing ores is tested, where the reduction-leaching process is realized in the reactor from the usual stainless steel by 40-45% nitric acid. Precipitation of admixture is carried out by ammonia. After filtration the silt is extracted from the system and ozone-air mixture is fed into manganese nitrate solution and formed γ-MnO_2.

Degree of ozone use was calculated in the terms of amount of obtained precipitate and its composition. Maximum degree of the use – 87%, and at acid addition (100g/l) reduces and comprises 52%, when the content of HNO_3 in the solution is equal to 320g/l. In neutral solutions the precipitate is fine dispersed - $MnO_{1,70-1,91}$ and in acid medium – $MnO_{1.92-1.99.}$

At the begining the precipitation of manganese dioxide intensively proceeds, but after 40 minutes the process become slower. The manganese oxidation degree from the nitrate solutions after 2 hours composes 1.94.

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FTA-O-10

COMPOSITES BASED ON POLYESTER LACQUER AND MINERAL FILLERS

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The work is devoted to the obtaining and investigation of some properties of composites based on polyester lacquer with quartz sand, andesite, trachite and clay. The composites were prepared with mechanical mixing of ingredients with following thermal treatment at 80^{0}C during 1 h. It is experimentally shown that the dependences of physical -mechanical parameters (strengthening on compression), thermal (thermal stability by method Vica) and water absorption on the filler concentration have an extreme character First two parameters have respective maximums at definite concentrations of the fillers and third- minimum.

The numerical data of obtained values are presented on Table 1.

#	Filler (wt%)	Density , kg/m3	Strengthening (compression), MPa	Water absorption, %
1	Trachite (80)	2300	125	5.3
2	“ (120)	2100	100	4.2
3	Andesite (80)	2305	160	4.0
4	“ (120)	2215	147	3.7
5	Clay (80)	2620	73	8.1
6	“ (120)	2425	45	7.3
7	Quartz sand (80)	3417	188	2.1
8	“ (120)	2908	164	2.9

In accordance with obtained results it may be made following conclusions:

1. With high mechanical strengthening are characterized the composites containing andesite and quartz sand. This result is due to high interactions between polymer matrix and filler particles;
2. The mechanical properties of composites with trachite and clay are relatively low because of low inter-phase interactions;
3. The water absorption data are agree with above conclusions -the higher is the inter-phase interactions, the lower is the water absorption.

RESEARCH OF INFLUENCE OF THE MODIFYING BaO AND SO_3 OXIDES ON PROPERTIES OF CEMENT CLINKER

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As a rule, P_2O_5, Cr_2O_3, SO_3, Na_2O, K_2O, BaO, SrO, CdO, MnO, TiO_2, FeO, MgO and other oxides are considered as mineralizers, modifying and alloying additives to cement charge in a small amount of which are present in clinker composition and the mechanism and character of their action often stay unknown. At the same time, simultaneous coexistence of several elements effects on the level of efficiency of each of them and makes more complicated the problem of investigation of the effect of micro additives.

Different researchers note positive effect of BaO on the growth of clinker strength which proves that barium is an effective “activator” of clinker hydration activity and mechanical strength. The role of BaO, as that of cement clinker minerals alloying and modifying oxide in the process of high temperature burning is known [1,2]. Ba^{2+} ions characterized with high activity expel Ca^{2+} from clinker minerals crystalline lattice, which, on its part, is used for saturation of two-calcium silicate (bellite) to tricalcium silicate (allite). Therefore, in barium containing cements the increased amount of tricalcium silicate is fixed compared to theoretical one. Allite is distinguished with higher hydraulic activity than bellite.

When studying barium containing clinkers the deficit material – viterite or barium ore with high barium content was, in most cases, used as mineralizer and alloying additive, which is economically ineffective.

At the same time the works have been carried out [3] when for receiving barium containing clinkers the wastes of the Kutaisi lithopone factory have been used, where $BaSO_4$ content achieves to about 60%.

In this respect our interest was attracted by quartz-adular metasomatites (QAM), the overlapping rocks of barite ore in David Gareji, South-East Georgia. Barium sulfate content changes in average from 5 to 20% which corresponds to 3-12% of BaO and 1.6-7% of SO_3 which, in its part, appears as mineralizing agent. In the content of other oxides these rocks in their chemical composition are close to the composition of clayey component used in cement industry. Because of this their usage in this direction is quite logical [4].

Clinkers were burned in laboratory high temperature furnace. The quality of burning process end was checked according the content of free CaO.

Clinkers were grinded in laboratory ball mill with addition of 5% natural gypsum up to achievement of 2700-3000 cm^2/g specific surface. The paste of normal consistency was prepared from the received cements and molded into 2x2x2 cm blocks which were hardened in water and testes on laboratory hydraulic press.

The conducted tests have shown that presence of BaO at clinker in amount from 0.3 to 0.7 and SO_3 from 0.4 – up to 0.6 masses. %, promote decrease the temperature of agglomeration on 50 - 70 ^0C, modify mineral composition of clinker and increase both the early, and branded durability of cement.

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FTA-O-12

OBTAINING LIGATURES FROM FINE GRAINED PARTICLES OF MANGANESE WASTE BY TECHNOLOGY -SHS METALLURGY

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The technical and technological parametres of synthesis for reception of ligatures from fine grained particles of manganese waste by SHS-Metallurgy is established. The technology of SHS – metallurgy is a new scientific area of research [1,2], which is based on the technologies of aluminothermy, magnithermy and progressive technologies of self-propagating high-temperature synthesis – SHS [3].

The analyses of obtained results are carried out. Economically, the most profitable technological direction depending on type of used wastes is proved. Optimum ways for decreasing the price of final product are determined.

The application of proposed technological solution allows to obtain products which is not threat for the ecology. It allows to return, in global scale, in an industrial cycle of ten billions tons of extracted and enriched wastes, manganese ores and to free million hectares of the land for rehabilitation which have been filled up with the waste.

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INFLUENCE OF DIFFERENT TEMPLATES AND SAC ON ZOL-GEL PROCESS OF SYNTHESIS OF NANODISPERSION SILICAS

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Sedimentary and colloidal slices are the voluble raw-materials having a large market and for its obtain waste of production of superphosphate are used. The main component of these waste is hexaftorsilicate of sodium (HFSS).

Some mass of powder was soluble in water with formation of HFSS which was filtrated for removal unsalable compounds. For obtaining of silica in solution of HFSS different quantities of Na_2CO_3 were added and at this following reaction was carried out:

$$Na_2SiF_6 + 2Na_2\,CO_2 = 6NaF + SiO_2 + 2CO_2$$

Forming particles of silica (SiO_2) depended on conditions of reaction have fall into sediment or have formed sol which than has turned into gel.

Investigation has shown that in result of HFSS hydrolysis amorphous porous silica was formed as gel which after drying was carried out in xerogel. Didecyldimethylammonium chloride (DDACA) (R)2-N+(CH_3)2Cl and chloride coco benzyl-dimethylammoniya (ChCBDA) R2-N+-(CH_3)2CH_2-C_6H_5Cl can be used both as stabilizators and templates.

The conclusion was made that addition of templates and SAS in solution of HFSS and Na_2CO_3 in their definite ratios has prevented participation of deposit and has allowed to obtain thick transparent gels from which by additional thermo-treatment or drying it is possible to obtain amorphous dispersion silica.

At primary addition of small quantities of abovementioned template and ethanol residue did not form but than during 3-5 twenty-four hours formation of gel was carried out. However subsequent increasing of quantity of templates and SAC at the same concentrations of initial compounds don’t render essential slowing effect on growing of particles of gel formation.

Influence of such additions as ethanol, DDASA and ChCBDA as templates on kinetics of gel-formation was determined. It was shown that addition of 0,1g ethanol to 20ml of HFSS has carried to formation of gel on second or third twenty-four hours also as at addition 0,03g of DDACh and ChCBDA. At addition of SAC 0,06g on 20ml of solution HFSS gel-formation has decreased what has carried out to falling out of deposit with further formation of gel.

It is possible to propose that templates and SAC have changed process of formation of particles SiO_2; have decreased process of polycondensation of silica, what can be explained by following reasons: sol-gel did not ended after formation of gel the most part of HFSS was hydrolysesed with formation nana-particles of silica and three-dimensional net of silica in solution presenting in net of silica also have carried out reactions of hydrolysis, polycondensation and aglomeration what has carried out to strengthening of silica frame in time. Also it is necessary to note that in process of drying syneresis was observed.

FTA-P-02

NATURAL ZEOLITES AS ADSORBENTS FOR CLEANING OF WATERS FROM ARSENIC IONS

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There is an intensive research worldwide to improve established techniques and to develop novel treatment technologies for removing arsenic from drinking water. The major technologies include precipitation-coagulation, membrane separation, ion exchange, lime softening and adsorption on iron oxides or activated alumina. Among these techniques proposed in the literatures, techniques involving immobilization of arsenic by adsorption have received much attention on natural geomaterials, including natural zeolites. The use of these sorbents is due to their relatively high capacity, selectivity, cation-exchange properties of some of them, comparatively low cost and availability (in Georgia as a local material). Enhancement of sorption on natural materials, modified with differentions is well known [1-3].

The problem of contamination of soil, surface and ground waters with arsenic compounds particularly acute in Georgia, where the hardrock mining began in 1932. Recently 100-110 thousands ton of arsenic-contained substances are on Uravi factory, that caused very high level of contamination. So, the question of cleaning the environment from arsenic is very important for our country.

The goal of submitting work was the study of natural zeolite clinoptilolite (CL) from deposit of Georgia in adsorption of As (III) in anionic and cationic forms. Arsenic used as adsorbate inform of arsenic trioxide (As_2O_3) (99.9%). The experiments were performed in a static-circulation mode with variation of ratio solid: solution, contact time, concentration of arsenic ion in model solution, temperature of pretreatment of sample. The analysis of arsenic ions in initial model and waste solutions was carried out by AA Spectroscopy. The adsorption value, coefficients of adsorption and distribution, the magnitude of ion leakage were calculated.

Study the dependence of adsorption value, coefficients of adsorption and distribution from modification type of initial CL showed that the more active adsorbents are cation-modificated CL, especially Cu- and Fe-contained samples. The introduction of copper and iron cations in the preliminary decationated zeolite twice increases adsorption value of AsO_3^{3-} and As^{3+} ions as compared to the initial zeolite, and 3-fold compared with decationated. It can be inferred that metal ions used for modification form a strong bond with CL and do not leach off the surface in aqueous phase. Acid treated CL showed the smallest adsorption ability in relation to AsO_3^{3-} and As^{3+} ions. The increasing of concentration from 0.5 mg/l till 50.0 mg/l causes growth of adsorption value, but the saturation wasn't reached in this limits.

It should be noted that CL from different Georgian deposits shows the different adsorption ability. May be this depends on different content of CL in tuffa and different chemical composition of zeolite.

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ELABORATION THE TECHNOLOGY FOR PRODUCTION FINE-GRAINED STRUCTURE POWDER COMPOSITES BN, B_4C AND $B_XC_YN_Z$ IN B-C-N SYSTEM BY SHS METHOD

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Modern scientific research main objective is to orientate industry onto development and realization of resource-saving, environmentally friendly technologies. For energy consumption and reduction of technological duration, Self-propagating High-temperature Synthesis (SHS) technology is one of the perspective one. The idea of SHS technology is realizing the process based on the exothermic reaction of components in combustion regime. The technology is characterized with high productivity, low power input, high quality of the obtained produce and ecological efficiency.

The main idea of the work is to study the possibility to fabricate radiation resistant and radiation protective ceramic materials from ^{10}B and ^{11}B containing row material (B_2O_3). [1]

At the first stage this leads to Elaboration the technology for production fine-grained structure powder composites BN, B_4C, and $B_xC_yN_z$ in B-C-N system by using effective SHS technologies. At the second stage on the base of fine-grained BN, B_4C, da $B_xC_yN_z$ composites, will be elaborated ceramic materials in Ti-B-C-N system, that will have high values of physical and mechanical properties such as hardness, compression stress, wear-resistance, resistant to scale formation in aggressive areas. [2]

These materials will work under high intensity dynamic loading/

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FTA-P-04

THE SYSTEM OF TECHNOLOGICAL CONTROL AND ACCOUNTING OF NATURAL URANIUM AT MINES IN KAZAKHSTAN AS A MODEL FOR MINERAL PROCESSING INDUSTRY

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Kazakhstan is the world's largest producer of natural uranium and, what is most noticeable, it is the most advanced country in terms of the uranium mining technology, a so-called in-situ leaching. While uranium mining was started in Kazakhstan in Soviet times, the present status of the leader was achieved in Kazakhstan in the last decade. Being a nuclear-weapons free country, Kazakhstan demonstrates a model of open cooperation in all spheres of economy, technology development, science, and education.

One of the elements of the technological leadership in the in-situ uranium mining is the system of accounting and control of natural uranium at all stages of its mining and technological processing developed in Kazakhstan in cooperation with IAEA and US DOE.

Being a very sensitive material, uranium requires the state-of-the-art technologies be used to assure safety and security, accounting, control and physical protection of the material and the facilities.

So, the technological aspects of natural uranium processing and the top-end experience gained in Kazakhstan with developed there system of accounting and control at uranium mining can be used in other related mineral mining industries, first of all, at mining of rare earth and precious metals. This system can potentially improve quality, safety, security and, finally, marketing competitiveness of the mining industry.

ELABORATION AND IMPLEMENTATION OF ELECTROLYTIC MANGANESE DIOXIDE RECEIPT TECHNOLOGY

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Technology of receipt of electrolytic manganese dioxide (EMD) was one of the most important engineering works, which was elaborated and put into production at the Institute of Inorganic Chemistry and Electrochemistry.

Works in the field of EMD receipt was begun in 60’s of the twentieth century in the Laboratory of current sources of Institute of Inorganic Chemistry and Electrochemistry under the direct leadership of Professor Levan Japaridze. A wide range of materials, first of all titanium alloys, was tested. The best results were obtained for anodes manufactured from commercial titanium and preliminary processed by corresponding methods, on which the manganese dioxide was precipitated.

As far back as in 1970 with the use of titanium anodes elaborated and manufactured in the Laboratory of current sources of Rustavi chemical plant (today – Joint-Stock Company “Azot”) were received pilot lots of EMD, which were delivered to leading USSR plants manufacturing current sources. Tests conducted on serial current sources showed the compliance of this product with best samples worldwide.

In 1975, for the first time in Soviet Union and Eastern Europe was put into operation EMD manufacturing workshop, which supplied up to 10 battery-manufacturing plants with high-quality EMD received on the basis of titanium anodes. Should be noted that EMD received under production conditions, was awarded two times with quality mark.

Titanium anodes manufactured according to our technology, when used under production conditions were characterized by high corrosion resistance and mechanical strength during product’s removal from anodes, low energy expenditures during conduction of electrolysis process under optimum conditions, high productivity (700-800 kg products were manufactured at one titanium anode within one cycle of electrolysis).

More than 30 author’s certificates and patents in EMD technology are issued for employees of laboratory of current sources, including up to 10 patents of USA, Germany, Spain and India.

It should be mentioned that we were among the first to implement titanium anodes on global scale, in particular right after Japan firms. In USA titan anodes were implemented only after 15 years compared with us.

At this moment the closed bath of new design for EMD manufacturing is developed in the L. Japaridze Laboratory of current sources and electrode materials of the R. Agladze Institute of Inorganic Chemistry and Electrochemistry, which has more than 10 advantages compared with available open bathes.

FTA-P-06

ELECTROCHEMICAL LEACHING OF MANGANESE OXIDE ORES

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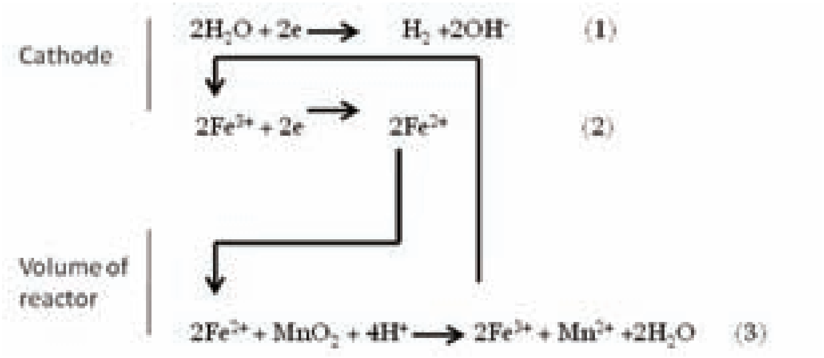
Manganese oxide ore processing which implies MnO_2 indirect electrochemical reduction in acidic media by Fe^{2+}/Fe^{3+} redox system is well known [1]. Under rigorous stirring of ore suspension in electrochemical reactor, MnO_2 reduction by Fe^{2+} ions, generated after electrochemical reduction of Fe^{3+} ions, takes place.



Limited current density of reaction (2) increases due to reaction (3) and so called limited catalytic current is achieved.

Electrode materials with developed surface was used in our research. Significant acceleration of leaching rate of manganese oxide ores was achieved due to following effects:

- It was possible to increase geometric cathodic current density due to development of cathodic surface area;
- MnO_2 direct electrochemical reduction proceeds in ore particles precipitated in pores of electrode:

$$MnO_2 + 4H^+ + 2e \longrightarrow Mn^{2+} + 2H_2O \qquad (4)$$

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DEVELOPMENT OF TECHNOLOGY OF GOLD EXTRACTION FROM MADNEULI'S GOLD-BEARING QUARTZITE DEPOSITS

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The real work is the first attempt in CIMR to development of technology of gold extraction from the Madneui's gold-bearing quartzite deposits, and also of the wastage extraction received from gold-bearing quartzite at gold extraction as raw materials for production of silicate wall materials and a glass container.

The first development stage of technology of gold extraction from secondary quartzite are devoted to check of technology of a sorption leaching of gold according to existing technology – in the country and abroad.

The geological and mineralogical-petrographic characteristic of secondary quartzite Madneuli's deposits was studied. For studying of real composition of ore and its technological properties were defined by carrying out a series of analyses: Several batches of parallel are established by the atomic absorption analysis the average content of gold in ore: the sample No 1 – Au–1,3 g/t; The sample No 2 – Au – 6,8 g/t.

The technology of gold extraction from ores was studied by a cyanation method. By using of sorption method for processing of gold-bearing ores and concentrates will reduce the leaching duration of gold by cyanide solution in 1,5-2 times.

In results of technological extraction by direct cyanidation of secondary quartzite Madneuli's deposits was established the optimal conditions for cyanidation.

Maximal extraction of gold of 96-97% at the content of gold in tails – 0,1 – 0,12 g/t.

Laboratory and technological research of processing waste of gold-bearing secondary quartzite as the main raw materials for production of silicate wall materials of autoclave concreting showed that they are suitable for manufacture of a silicate brick and products from heavy and honeycomb silicate concrete.

Preliminary results laboratory research give the chance to judge prospects and uses of tails of enrichment of secondary quartzite Madneuli's deposits in production of dark green glassware.

Development of waste-free technology of processing of quartzite will allow expand, on the one hand, a source of raw materials for separate branches of national economy, on the other hand to liquidate source pollution of environmental space; Besides, will give the chance to cut down non-productive costs, the bound to creation and operation of the tailings dam.

FTA-P-08

OBTAINING OF SUPERCONDUCTING MgB_2 COMPOSITES BY SHOCK WAVE CONSOLIDATION IN HOT CONDITION

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The rapid development of research of conductors based on superconducting compound MgB_2 makes them a very real prospect for technical applications of temperatures below 30 K.

The technology of development superconductive materials belongs to traditional powder metallurgy: preparing and densification Mg–B powder blends in static conditions with their further sintering processes. The application of shock wave consolidation technology to fabricate high dense MgB_2 billets with maximal critical temperature T_c=40K was also used but required a sintering to be applied after a shock wave compression to fabricate high dense MgB_2 billets.

We are going to apply the original hot shock-assisted consolidation method, combining the high temperature with a two-stage explosive process without any further sintering. The consolidation of MgB_2 billets will be made at temperatures above the melting point of Mg up to 1000^0C in partially liquid condition of Mg-B blend powders.

Structural studies will be conducted as well as the impact of the critical temperature and magnetic nanoparticles doping by carbon and superconductor properties.

THE IMPROVEMENT OF METHODS FOR PROCESSING OF GOLD-BEARING REFRACTORY SULFIDE ORES AND CONCENTRATES

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The problem of extraction of gold from refractory ores can be classified among the most important. The main method of extracting gold from ores and concentrates in the world of gold is the cyanide method. However, for all its merits, this method, applied to refractory gold sulfide ores, does not give economically and environmentally desirable (appropriate) indicators, which necessitates the search for alternative methods.

The problem of involvement of new methods in the processing of refractory gold sulfide ores and concentrates is also important for Georgia. At the present stage of requirements of ecology and economy the most appropriate methods for processing of such ores and concentrates is thiocarbamide method and the method of hydrochlorination.

For research we used the following gold-bearing refractory sulfide ores of Georgia: chalcopyrite, pyrite, barite-polymetallic, copper-zinc, antimonite.

The result of the study established the optimal conditions of the thiourea method of leaching gold from afore-named ores and concentrates with 85-90% gold extraction [1-3].

Also conducted research on the possibility of electrochemical leaching of resistant gold-bearing sulfide ores and concentrates. In this case, the used acid chloride electrolyte, containing as a selective complex-maker for precious metals is thiourea [4]. The leaching process proceeded in the conditions of “soft” oxidative mode without isolation of molecular chlorine and pollution of the environment by removing up to 90% of the gold from the ore.

It was developed technological scheme of leaching of these ores with making of zero-discharge technologies, satisfying modern ecological and economical requirements. The reactor was designed and tested for the electrochemical leaching of refractory ores and concentrates.

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FTA-P-10

SURFACE ELECTROCHEMICAL ALLOYING OF METALS

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The preparation of the plating of electronegative metals (Al, Y, Ti, Zr, Hf, V, Nb, Ta) is possible only from the molten electrolytes, but in this case such difficulties appear which are missed at the electrolysis of aqueous solutions. This is mainly caused by high temperatures of the process. It is of first importance that in this case the process is a highly advantageous. At high temperatures the plating is obtained at the cathode – at base metal. Along with it at surface layers of a base the diffusion – alloyed lager is also formed. Metal properties (hardness, corrosion-, heat- and wear-resistances) are determined by the composition of surface layers. For economy of alloying metal the variation of the composition of the metal surface layers is favorable instead of a total volume one. Hence the preparation of electroplating on base metals and surface alloying in the metals proceed simultaneously.

Titanium and steels: CT-3, CT-4, X18H10T were taken as the base metals in the form of the plates. The research was carried out at the temperatures of (973-1173) K; electrolyte background: equimolar melt: KCl-NaCl, depolarizer – Ma_2MoO_4. Electro reduction of molybdate occurs by the scheme:

$$MoO_{n/2+1}^{2-} \leftrightarrow MoO_{n/2} + O^{2-} \quad (I)$$

$$MoO_{n/2} + ne \leftrightarrow Mo + n/2O^{2-} \quad (II)$$

O^{2-} -ions, formed by acid-base reaction (I), suppress the reaction (II), autoinhibition of electrode process takes place. O^{2-} -ions are neutralized by PO_3^- -ions ($NaPO_3$), which capture O^{2-} -ions.
The electrolyte is: K, Na/Cl-Na_2MoO_4+ PO_3^- ($NaPO_3$) where [Na_2MoO_4]/[PO_3^-]=10:1

Thickness of molybdenum plating on titanium attains 85-110μm, current density 0.01-0.025A/cm^2, current efficiency: 90-94%, process duration 4-6 hours, thickness of diffusion layer 80μm (in the case of 6 hour electrolysis) base – steel CT-3 at 4-6 hour electrolysis. The surface is coated by molybdenum plating of 30-40μm thickness, and for alloyed layer thickness equals to 150-160μm. By increase of electrolysis duration to 12-15 hours the latter enhanced to 450-550μm. Nearly similar situation is in the case of other steels. It was established that corrosion – resistance is also increased.

THE POSSIBILITY OF OBTAINING GOLD FROM PYROMETALLURGIC WASTES

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Our aim was the elaboration of new method of extracting arsenic-containing compounds from pyrometallurgic wastes. As initial material the wastes mining-chemical factory of Racha, the “tails’ of the burning of the auripigment ore from the village Djvari taken from toms were used. Amyl-, iso-amy; and hexyl alcohols were chosen as extragents.

The main preventing factor for obtaining gold is high content of arsenic. If the mass portion of arsenic is more than 1%, gold can’t be extracted from such mixture – Bagrationi’s method can’t be used. Thus it is obligatory to separate arsenic from this mixture in the form of corresponding compound. On the basis of such approach other noble metals also can be extracted.

The wastes contain arsenic in the form of arsenic (III) and (V) oxides or the products of their transformation. We had established that under the action of amyl-, isoamyl- and hexyl alcohol, arsenic is quantitatively extracted, if water, formed during esterification is gradually separated by azeotropyc drying. Alcohol is used twice as much as theoretically needed and the yield of the corresponding ester rises. The content of arsenic in the raffinate becomes about 0,6%, so they can be used for separating gold. All this will have high economic and ecologic effect and can promote the budget of Georgia.

FTA-P-12

HIGH-TEMPERATURE ELECTROCHEMICAL SYNTHESIS OF COMPOSITE COMPOUNDS

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Preparation of intermetallides, polymetallic powders, metals borides and silicides are possible by electrochemical synthesis at 873-1073 K temperatures from the compounds of aluminum, manganese, high-melting and rare metals (Y, Ti, Zr, Hf, V, Nb, Ta, Mo, W) as well as from non-metals (B and Si). For this purpose the provision of co-deposition of the end product at the cathode in equilibrium regime is necessary. To do this, the values of the potential of the elements separation must be close to each other, in the range of 0.2Volt. At separation, the elements interact with each other at “atomic” level to form the composite materials.

In the Laboratory of fused electrolysis more than 30 composite materials (intermetallides, polymetallic powders, borides and silicides, including double ones were synthesized: YAl_3; YAlV; $MoCo_3$; MoNi3; WNi3; AlMoMn; MoTaCo; MoTaNi; MoYMn; MoCoSi; MoNiSi; TaB_2; NbB_2; NbMoB2; MoSi2WSi2; Ta_5Si_3; TaCoSi; TaNiSi; NbCoSi; NbNiSi; TaMoSi; MoAlSi; $Al_5(MnSi)_2$; YMnSi.

The scientific foundations for realization of elaborated technologies were established. The area of their use is wide and prospective.

FTA-P-13

OBTAINING OF MAGNESIUM – AMMONIUM ARSENATE (V) FROM FACTORY WASTE DISPOSALS

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The quantity of wastes from the production of non-ferrous and noble metals, which contain arsenous anhydride increase in the whole world and it is the reason of the pollution of environments. Naturally, the utilization of As_2O_3 for the preparation on arsenic-containing compound can solve this problem.

The most of the methods of preparation of magnesium-ammonium arsenate (V) are based on the ionic reaction:

$$Mg^{2+} + NH_4^{+} + AsO_4^{3-} \rightarrow MgNH_4AsO_4\downarrow$$

More rational method also exists, which is based on two successive reactions:

a) $As_2O_3 + 2H_2O_2 + H_2O \rightarrow 2H_3AsO_4$
b) $2H_3AsO_4 + 2MgCO_3 + (NH_4)_2CO_3 \rightarrow 2MgNH_4AsO_4 + 3CO_2 + 3H_2O$

The reaction is carried out at 35-80^0 C, at pH of the solution 7-9.
The main deficiency of this method is that the aim product can’t be obtained in pure form.

Our aim was to create the new method, which can solve this problem. For this purpose, we have used (as initial compound) triallylarsenites, which are obtained from the wastes of “Tsani” mining-chemical factory by interaction of amyl- or isoamyl alcohols. The products of interaction were oxidized by chlorine, than by magnesium oxide and concentrated ammonium hydroxide (pH≈9). The aim-product is obtained according the scheme:

$$\frac{1}{2}\,As_2O_3 \xrightarrow[-1{,}5H_2O]{3ROH} (RO)_3As \xrightarrow{Cl_2} (RO)_3AsCl_2 \longrightarrow$$

$$\xrightarrow[-2NH_4Cl\ -\ 3ROH]{MgO\ +\ 6H_2O\ +\ 3NH_4OH} MgNH_4AsO_4 \cdot 6H_2O$$

where: R= C_5H_{11} or iso-C_5H_{11}.

The process is cyclic and continuous.

Thus, we have elaborated new method of the preparation of magnesium-ammonium arsenate(V). The main advantage of this method is that initial compounds are 3-5 times cheaper (Cl_2, MgO, NH_4OH) than described in literature. Moreover, the aim product – magnesium-ammonium arsenate (V) is of high purity and satisfies the modern strict requirements.

Magnesium-ammonium arsenate is widely used for the production of special glasses. The requirement on these compounds grows, so this new method of its preparation has high practical importance.

FTA-P-14

INDIUM PHOSPHIDE QUANTUM DOTS ON GALLIUM PHOSPHIDE

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The indium phosphide (InP) quantum dots (QD) are an excellent system for optical application, communication and solar cells [1, 2]. In this work the band diagram and electronic structure of InP QDs embedded in GaP is theoretically studied.

The original method electrochemical deposition of metals indium (In), gallium (Ga) and alloys (In_x Ga_{1-x}) on the III-V semiconductor surface is used for fabrication of near-ideal In/GaP Schottky diodes. This method allows metal deposition on electrochemically etched semiconductor surface. The chlorides of metals are used for In and Ga deposition as was described in [3]. After metallization, In/GaP contacts were annealed in hydrogen during 3-10 min at the various temperature for formation InP nanocrystals on GaP surface [4, 5]. The action of annealing temperature on the electro-physical characteristics of In/GaP system is investigated, and the possible interactions between metal and semiconductor during formation InP nanocrystals are presented, here. It is discussed, also, the colloidal synthesis method of InP QDs and applications in medicine.

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EXTRACTION OF GOLD, SILVER AND COPPER FROM ENRICHMENT TAILS OF REBELLIOUS SULFIDE ORES BY BACTERIAL-CHEMICAL METHOD

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The optimization problem of use of mineral resources, which increased in recent years, and environment protection against pollution caused development in mining-geological production the new direction designed to solve both technological and natural-security tasks. One of approaches to the solution of these questions is widespread introduction of biotechnology methods, part of which, is bacterial leaching of metals.

Processing of ore deposits particular in case of open developments lead to accumulation of huge mass of a wastage and tails.

Madneuli Mining-plant are processing of copper, Barite-polymetallic, copper-zinc, barite-gold-bearing ores and gold-bearing quartzite by mine way. From the extracted ore primary processing, i.e. enrichment affects only the copper-pyrite and barite-gold ores derived from copper and barite concentrate. As a result, in Madneuli Mining-plant are large quantities of waste from production and enrichment of ore containing non-ferrous, noble rare and metals. For example, the flotation tailings of copper-pyrite, weighing 40 million tons containing 0.22-0.24 % of copper, 0,61-0,65 g/t of gold, 2,16-33,8 g/t of silver and others elements.

We are interested in additional recoveries of secondary Cu, Au, Ag, copper pyrite flotation tailings.

For the conduct the research was used a scheme based on the known methods of physical-chemical enrichment and biometallurgy.

Flotation tails, except the basic aluminosilicate are contain 0,29% of Cu, 0,6 g/t of Au, 8,0 g/t of Ag, 4,2% of S.

The copper-containing collective sulfide flotation concentrate was received, which contained 1,2% of Cu, 1,9g/t Au, 17,22 g/t of Ag.

The solution of a technological problem of receiving, both of non-ferrous metals, and gold and silver from sulfide concentrates is the destruction of a crystal lattice of sulfide minerals providing transfer of non-ferrous metals to solution or opening of gold for its subsequent extraction with a traditional hydrometallurgy way of cyanation. This destruction is most efficiently carried out by means of technology of biooxidation.

The studies were conducted in laboratory conditions in percolation mode. During bacterial leaching process used autotrophic thiobacteria A. Thiobaccilus ferrooxidans and A. Thiobaccilu sthiooxidans allocate from water of Madneuli's deposits mine. In the laboratory, it reached 96.1% leaching copper and subsequent cyanidation of bio-tails 85.5% gold and 81.7% silver.

FTA-P-16

STUDY OF THE MECHANICAL AND ELECTRICAL PROPERTIES OF HOT EXPLOSIVELY CONSOLIDATED NANOSTRUCTURED Cu-W COMPOSITES

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Copper–*(10-40) wt.%* tungsten powder blends were consolidated into cylindrical rods using hot explosive consolidation (HEC) process. Different types of Cu–W precursor compositions with a nanometer-scale W were consolidated to near theoretical density at 1000°C. The shock wave loading intensity was about 10 GPa;

The investigations showed that the combination of high temperatures (around 1000 °C) and the use of a two-stage shock wave processing method were found to be beneficial to the consolidation of the Cu–(10-40)%W composites, resulting in high densities, good integrity, and good electrical properties. The structure, mechanical and electric properties study of the samples depending on the distribution and amount of the precursor nano-W particles was carried out.

The acoustic spectrometry method was used to study the mechanical properties of consolidated composites (internal friction and Young modulus).

The measurements of specific electrical resistance of Cu-W composites with different nano-W content were carried out using the four-contact potentiometric method in the temperature range 77 - 410 K. The correlation of mechanical and electric properties of investigated Cu-W nanocomposites was established.

The resistance value increases with increase of tungsten component at given measurement temperature. The dependence of specific electrical resistance for all ratios of components remains linear. The temperature factor of resistance nonlinearly increases with the increase of tungsten concentration.

The value of annealing temperature, its duration and cooling conditions of sample influence the mechanical properties of composites revealing after their rolling. The failure at choosing the proper annealing mode could result in full destruction of sample.

COMPOSITES ON THE BASIS OF STRAW AND VARIOUS BINDERS

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Novel composites on the basis of dry hay and different organic and inorganic binders have been obtained in the spatial molds. Polyethoxisilane of two types (PhES-50 and PhES-80), polyethylene, colophony, wood glue and liquid glass were used as binders, concentrations of which varied in region 3-15 wt%. Spectroscopical investigations by method FTIR have shown a presence of some chemical bonds between components of the composites in result of reactions between active groups of the ingredients. These bonds may be the main reason of improving of physical mechanical and thermal properties of composites and their water resistance. Composite microstructure of the samples was studied by NMM-800RF/TRF type of optical microscope. It was shown that the composites are a multiplicity component systems, but does not show a pronounced binder in the form of insertion, which indicates that the optimum temperature of sintering is selected. In composites the gaps and cracks do not observe.

For composite materials made on the basis of powdery bamboo and different hardeners and additives scanning electron microscopic (SEM) investigations are provided. Besides of energy dispersive X-ray examinations have been carried out in parallel with the micro-spectral (EDS) examinations. From SEM investigation one can see outside the epidermis of the composites on the basis of straw, which is well organized partial corrugated structure. By energy-dispersive X- ray micro-chemical spectral analysis it was shown that the composites contain primarily C, O, Si, Ca, and aluminum.

It is established that these properties in general depend on the concentration of the binders. It is shown that the maximal values of the noted parameters for the composites appearance at relatively low concentrations of binders. Especially in case of PhES-50 and PhES-80 improved properties of composites are reached already at their 3-5 wt%. With rather high values of these parameters are characterized the composites, containing polyethylene and colophony due to their good wettability and composites containing 2-4 binders simultaneously. The experimental results show that at right selection of the used ingredients and their concentrations the materials with rather high exploitation properties may be riched.

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FTA-P-18

STUDY OF TEMPERATURE DEPENDENCE OF SOME PHYSICAL CHARACTERISTICS OF THERMOSTABLE NICKEL COATINGS ON ALUMINIUM ALLOYS

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The structure of the electrolytic coatings may be changed purposefully by thermal treatment and consequently exploitation properties of coatings may be improved.

Study of some electrical and mechanical characteristics (specific resistance, Young modulus, internal friction) and structure of electrolytic nickel coatings, obtained from nickel plating persulphate solution on the aluminum basis before and after thermal treatment (400-600^{0}C) is presented in the work.

Standard four-point contact method was used for measurement of electric resistance. Mechanical properties (Young modulus, internal friction) of the sample under test were studied by use of acoustic spectrometer. The structure of the sample was studied on scanning electron microscope. For coating obtained in nickelling solution under study the specific electrical resistance of heated (600^{0}C) and then cooled up to room temperature sample decreases in comparison to specific resistance of initial sample coated by nickel and approaches specific resistance of aluminum alloy.

The numerical value of the Young modulus lies in the range 40-65 GPa and approximately coincides with Young modulus for aluminum alloys (65.5-70.4 GPa). The change of the Young modulus in the measured temperature range is about 4%. The level of internalfriction decreases after thermal treatment at temperature about 100^{0}C.

It is determined, that after thermal treatment the structure of the sample improves, the distance of intergranular limits decreases, a diffusion zone between coating and basis increases and correspondingly the adhesion improves.

Obtained coatings may be used for functional aims in different technologies.

THE STUDY OF MINERAL COMPOSITION OF SULPHIDE SILT PELOIDS SPREAD IN ADJARA REGION BY USING X-RAY PHASE METHOD OF ANALYSIS

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The use of the natural healing factors for the treatment and prevention of various diseases presents the one of the current tasks for the modern medicine. The healing muds, so called peloids, have a special role in balneology and resort therapy due to their therapeutic action [1]. They belong to useful mineral resources and contain therapeutically active substances. The history of their use begins from the ancient times.

Adjara is one of the regions of Georgia, rich in peloids resources, which can be found on the seacoasts, as well as in the mountains [2, 3]. All these resources were known to the local population since the ancient times and were used for treatment of various diseases.

The aim of our research was to study the mineral composition of sulphide silt peloids of Adjara region by using X-ray phase method of analysis. The objects were the samples taken on various areas of Adjara region, the sulphide silt peloids of Chakhati, Kvirike, Niphy`s lake, Green lake, Gasaliani and Shratiani. The applied research method was X-ray phase analysis by using X-ray diffractometer DRON-3 [4]. As a result of the conducted studies there have been revealed, that the analysis samples mainly represent amorphous mass. In testing objects there have been determined the contents of the following minerals: Ca Na feldspar, K feldspar, Ca-montmorinollite, quartz, hematite, chlorite, magnetite, amphiboles, trace amounts of mica and chlorite [5].

By using the X-ray phase analysis there have been established the contents of important minerals in the study objects, it gives us the basis to continue further studies in order to determine their quantitative compositions.

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FTA-P-20

DEVELOPMENT OF TECHNOLOGY AND ANALYSIS OF LOTIONS CONTAINING INGREDIENTS OF BOTTOM MUD OF LAKE KUMISI (GEORGIA)

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Development of new lotion recipes requires formation of the systems, which are composed of a variety of components, each of which must perform its function in an optimal variant. Because there is no general theory for creation of lotions, selection of their components is performed empirically, based on centuries-old experience of their application, focusing on the research of the chemical composition of plants, mineral waters and a number of other objects. The biologically active compounds from plants should have light astringent and deodorizing action, which will help to open the skin oily contaminants, some antiseptic and tonic effect, they should feed the skin and give it purity and elasticity. Mineral biologically active substances are the donors of feeding mineral components for the skin. Therefore, the major task of developing lotion recipes is the correct selection of concentrations of the alcohol, fatty and mineral supplements, and biologically active substances for specific type of a lotion. Here are presented some variants of the developed recipes, using plants that grow in Georgia, and mineral supplements. Lotion for normal skin: Ethanol 95% - 15.0%, glycerin - 5,0%, aloe juice - 1,0%, hawthorn fruit in water - alcoholic tincture - 2.0%, therapeutic tannin - 0.5%, peppermint leaves in water - alcoholic tincture - 3.0%, probiotics - 0.3%, Kumisi Lake therapeutic mud in water –salty extract up to 100% . Lotion for oily skin. Ethanol 95% - 30.0%, glycerin - 3,0%, aloe juice - 4,0%, hawthorn fruit in water - alcoholic tincture - 4.0%, therapeutic tannin - 2,0%, peppermint leaves in water - water - alcoholic tincture - 3.0%, keratolytic - 0.3%, resorcine- 0.3%, probiotics - 0.3%, Kumisi Lake therapeutic mud in water - salty extract up to 100% . Lotion for dry skin. Ethanol 95% - 10.0%, glycerin - 15.0%, aloe juice - 4,0%, hawthorn fruit in water - alcoholic tincture - 3.0%, peppermint leaves in water - alcoholic tincture - 2.5%, probiotics - 0.3%, Kumisi Lake therapeutic mud in water - salty extract up to 100% . Lotion for problematic skin. Ethanol 95% - 25.0%, glycerin - 5,0%, aloe juice - 5,0%, hawthorn fruit in water - alcoholic tincture - 3.0%, therapeutic tannin - 3.0%, peppermint leaves in water - alcoholic tincture - 2.5%, keratolytic - 2,0%, resorcine - 1,0%, hydroquinone - 0.5%, boric acid - 0.5%, probiotics - 0.3%, Kumisi Lake therapeutic mud in water - salty extract up to 100% .

MODELING OF SMELTING OF FERROSILICOALUMINUM USING TKIBULI COAL TAILINGS AS RAW MATERIAL

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Present work aims the studying of the possibility of smelting of ferrosilicoaluminum using Tkibuli coal tailings as a raw material. Interest in these alloys is based on the possibility of their applications in different industries, e.g. as a reducing agent in metal-thermic reactions taking place during the production of low-carbon metals and alloys, as a complex deoxidizer in steelmaking, for preparing termites used in thermite-welding or production of explosives, for obtaining the foundry eutectic-alloy silumin, as well as production of aluminum by applying methods of selective dissolution or through the formation of an intermediate sub-compound.

Tkibuli coal deposit is characterized by the presence of large amounts of mineral impurities that determine their high ash content. In the ash-part, the dominating components are silicon dioxide and aluminum oxide (up to 50 and 35 %, respectively). Due to high contents of ash, alumina and silica in total, and the presence of a natural reductant, coal-waste is the extremely valuable resource for electro-thermic production of aluminum-silicon ferroalloys.

To assess the suitability of such raw materials for sore-smelting, the experiments were performed using charge-materials obtained from Tkibuli coal tailings. The missing amount of carbon in these raw materials was compensated by the ordinary Tkibuli coal. The crucible-melting tests were conducted in the ore-smelting laboratory furnace. Electrical characteristics of melting tests are as follows. For the transformer lower (secondary) side – U_1 = 30 – 40 V and I_1 = 1500 – 1800A. The tests were conducted at the operating voltage of U_1 = 30 V and current I_1 = 1600 A. The furnace power was 48 kW. It was used a bed-charge of following composition: waste of the Tkibuli coal enrichment – 54, Tkibuli ordinary-coal – 38, and quartzite – 8 %. Adding of the quartzite makes it possible to adjust the aluminum content in the smelted metal at the customer's request, as well as to avoid its disintegration.

The observed deviation from the stoichiometry is in the range of 0.9 – 1.0 %. Uptakes of silicon and aluminum by the alloy were 57 – 65 and 70 – 75 wt. %, respectively. Higher aluminum-uptake by the alloy in comparison with silicon-uptake is explained by lower evaporation / condensation temperature of SiO_2 than that of aluminum and Al_2O_3.

It was obtained alloy containing silicon 45 – 52, aluminum 20 – 25 %, and iron. The conducted experimental research indicates the principal possibility of receiving of ferrosilicoaluminum from the waste of coal-enrichment with addition of Tkibuli ordinary coal. To stabilize the technological mode and select ferrosilicoaluminum of rational compositions, as well as improve the technical and economic performance of this process, it is necessary to continue research and carry out a series of tests in big laboratory and semi-industrial furnaces at 200 kVA and 1000 kVA. Thus, we can conclude that the Tkibuli coal tailings can be a promising raw material for the steel industry development in Republic of Georgia.

FTA-P-22

ON THE ALKALI LEACHING BEHAVIOR OF URANIUM FROM ITS ORES

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The paper deals with formal thermodynamic modeling of uranium *in-situ leaching* (*ISL*) processes and the optimization of technological schemes. Presently, for the uranium extraction from ore, the *ISL* is used, i.e. its selective dissolution by a chemical reagent in the ore body, followed by subsequent removal of formed chemical compounds from the reaction zone by the moving stream of solvent. Pre-comminuted raw ore is leached with sulfuric acid (acid leaching) or carbonate solutions (saline leaching) in the presence of an oxidant for transferring uranium into the solution as sulfate or carbonate complexes of *U*(*VI*). In the case of *ISL*, carbonate solutions are mostly used 4- 3 without polluting the environment. Yet, carbonate leaching is more selective to uranium than acid one. As the oxidizing agent H_2O_2, oxygen, nitrate ions and alkali metal hypochlorite are mainly used. At the carbonate leaching of uranium from its ores, alkaline solutions are obtained, where uranium is in the form of complexes $UO_2(CO3)_3^{4-}$.For the extraction of uranium from carbonate solutions, its precipitation in the form of uranium peroxide $UO_4 \cdot H_2O$ is largely used. Since the pitchblende group, which constitutes the bulk of industrial uranium ores, is characterized by the general composition UO_{2+x}, where $0 \le x \le 1$, in which *U*(*IV*) is oxidized to *U*(*VI*) up to various degrees, for the thermodynamic modeling of *ISL* processes the dissolution of minerals of the composition UO_2 has been studied. The process of UO_2 dissolution in the carbonate medium is usually described by the equation: $UO_{2(S)} + [O] + CO_3^{2-} + 2HCO_3^- = UO_2\bigl(CO_3{}_3^{4-} + H_2O$ (1), where $[O]$ is an oxidant. The precipitation of uranium by acidification of carbonate solutions with H_2O_2 can be represented as follows: $UO_2^{2+} + H_2O_2 + nH_2O = UO_4 \cdot nH_2O_{(S)} + 2H^+$ (2)

However, equations (1) and (2) do not sufficiently describe various chemical processes in these systems. Indeed, by varying the experimental conditions (pH, total concentrations of reagents et al.), the composition and the stability of particles present in the system are changing. Thus, the composition and stability of the carbonate complexes $UO_2(CO_3)_i$ strongly dependent on pH and the total carbonate concentration in the solution. By increasing the pH, a significant role is played by the hydrolysis of uranyl ion. Furthermore, in the presence of H_20_2 the UO_2^{2+} ions form sufficiently stable $UO_2(O_2)_j$ complexes. Finally, the possibility of the reaction (1) depends on the nature of the oxidant. For full describing of the dissolution of the mineral (solid phase), the generalized equation (*GE*) of interaction of all the particles present in solution has been used [1]. Within the approach based on *GEs* of reactions, the thermodynamic calculation of the optimal conditions of underground leaching of uranium ores, based on the model $UO_{2(S)}$, has been carried out. The thermodynamic stability area of the mineral has been determined by the value of the Gibbs energy of the overall process [1-4], described by the *GEs*. The solid-phase is stable if $\Delta G_{S,tot} > 0$. The condition $\Delta G_{S,tot} = 0$ corresponds to the beginning of its dissolution and (or) sedimentation. It is shown that the most optimal oxidants from the thermodynamic point of view, there are hydrogen peroxide and alkali metal hypochlorite. The obtained results of modeling within the formal chemical thermodynamics are in good agreement with the existing experimental data and technological schemes for the *ISL* of uranium ores.

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FTA-P-23

X- RAY PHASE AND THERMOCHEMICAL RESEARCH OF MANGANESE CARBONATE ORE AND OBTAINED MANGANESE DIOXIDE

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For research of the processes of preparation of fine-dispersed electrolytical manganese dioxide the determination of manganese-containing minerals and non-ore minerals is of a great importance [1]. By means of X-ray, thermogravimetric, spectrophotometric and chemical analysis the phase and chemical composition of carbonate ore of Chiatura manganese deposit has been studied [2,3].

By X-ray and thermogravimetric methods the phase composition of fine dispersed manganese dioxide, obtained at the electrolysis of nitric solution of manganese (II) nitrate was studied. The data of X-ray phase analysis have shown that the main phase of the samples is the γ -modification MnO_2 which contains manganese (IV) hydroxide – $Mn(OH)_4$ as an impurity.

Thermogravimetric analysis has shown the first endoeffect at the temperature maximum in the range from 110 °C to 120 °C. This endoeffect belongs to the moisture evaporation from the sample under study and to dehydration of existing manganese (IV) hydroxide by the following reaction:

$$Mn(OH)_4 \quad MnO_2 + 2H_2O \qquad (1)$$

The second endothermal effect with a temperature maximum at 500 °C corresponds to the decomposition of MnO_2 with a formation of Mn_2O_3 and O_2 by the reaction:

$$4MnO_2 \quad 2Mn_2O_3 + O_2 \qquad (2)$$

The third endothermal effect corresponds to the decomposition of Mn_2O_3 with a formation of Mn_3O_4 and O_2 by the reaction:

$$6Mn_2O_3 \quad 4Mn_3O_4 + O_2 \qquad (3)$$

Obtained results were compared with each other. Thus, the data of MnO_2 phase composition determined by thermogravimetric analysis correspond to the results of X-ray phase analysis.

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FTA-P-24

RESEARCH OF THE ELECTRODE PROCESSES AT SIMULTANEOUS PREPARATION OF MANGANESE DIOXIDE AND HYDROGEN

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The electrode processes of the preparation of the fine-dispersed manganese dioxide in the course of the electrolysis of manganese nitrate solution have been studied.

The overall reaction for preparation of MnO_2 by electrolysis of manganese nitric acid solutions may be expressed by the following manner:

$$Mn(NO_3)_2 + 2\,H_2O = MnO_2 + 2\,HNO_3 + H_2$$

Two competitive processes at the anode - oxygen separation and oxidation of manganese bivalent ions may be expressed by the reactions:

$$2\,H_2O - 4e = 4\,H^+ + O_2$$

$$Mn^{2+} + 2\,H_2O - 2e = MnO_2 + 4H^+$$

At the cathode the hydrogen is produced:

$$2H^+ + 2e = 2H$$

$$2H = H_2$$

Probable competitive process at the cathode is a reduction of manganese ion:

$$Mn^{2+} + 2e = Mn$$

Initially, we studied in harsh condition, dependence of anodic potential on current density in various concentration of nitric acid (25, 50, 100, 150, 200 g/L). It was shown that starting point for separation of gaseous oxygen is sharply defined for given concentration of nitric acid corresponding to the potential of 1. 4. V.

Afterwards, was studied seperation of manganese dioxide at the platinum anode in manganese nitrate solution (200g/L) in the presence of various concentration of nitric acid. In the range of current density from 0.7 to 3.0 mA/cm^2, the potential of MnO_2 separation was 0.7-0.76 V at various acidity, respectively. In the range of current density from 3 to 40 mA/cm^2, performed experiments have shown that along with the increase of current density the simultaneous separation of MnO_2 and oxygen at the anode takes place at the potential 1.3-1.5 V. At the current density from 50 to 150 mA/cm2 occurs separation of MnO_2 near the anode and / or in solution volume at the potential 1.5 - 1.72 V.

In the case of cathode processes at graphite electrode, in manganese nitrate solution (200g/L) with the various concentration (25, 50, 75, 100 g/L) of nitric acid, the hydrogen separation begins at current density $i_k < 0.5$ mA/cm^2 in the potential range from 0.7 to 0.74 V. Cathode potential is slightly increasing by further increase of current density and after attaining of the potential – 0.8 V, it is independent from its growth.

PHYSICAL REASON FOR THE FORMATION OF ELECTRICALLY CONDUCTIVE PHASES IN SIDERITE

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Physico-chemical processes occurring in the earth's formations usually are studied in terms of the action of temperature and pressure, but the potential role of magnetic and electric fields in those processes are not taken into account. Perhaps this is due to the traditional physical representations that significant changes in condensed phases occur only in high fields, not typical for the earth's crust. Such representations largely retard development of the Earth sciences, interpreting the main features of natural processes, mainly as a result of the action of the thermal field and pressure with the gas-liquid fluid. For example, mechanisms of iron ore formation during the decomposition of siderite, graphite formation from carbon of calcite (calcite, siderite – rock-forming carbonate minerals – crystals with ionic bonds) are still not disclosed.

The purpose is to explore the mechanism of transformation in the rock-forming carbonates during heating with simultaneous impact of a weak electric field.

The paper establishes that new phases are formed in siderite and calcite at a temperature of the beginning the dissociation by simply heating, wherein there is an abrupt increase in conductivity, Fig. 1. Graphite, magnetite, and hematite were identified in siderite; graphite and probably grafan was detected in calcite. The dependence of the temperature of the beginning of the abrupt increase in conductivity on the mass content of silicon was established when treatment a mixture of carbonate micropowder and silicon. An increase in the silicon content leads to a maximum reduction of the conductivity temperature jump for siderite about 200...300 K; for calcite is about 750 K, Fig. 2.

The physical mechanism of spontaneous formation of graphite (grafan) as a result of the dissociation of carbonates in the electrothermal impact, based on the theory of nucleation of a new phase, with the involvement of quantum-mechanical model of the chemical bond stability in the Coulomb field is suggested.

The paper studied a new physical effect: the phenomenon of abrupt increase in conductivity of dielectrics, in particular the class of ionic carbonate crystals. The effect is exerted only if dielectric heating is accompanied by the electric field influence (in the experiments used a weak field which is characteristic of the Earth's crust). Simple heating or field action does not give the expected result.

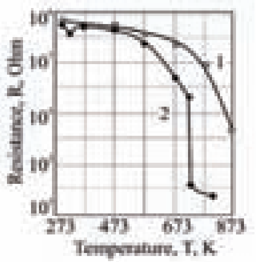

Figure 1. The dependence of the resistance reduction of siderite: 1 – heating; 2 – heating and action of electric field

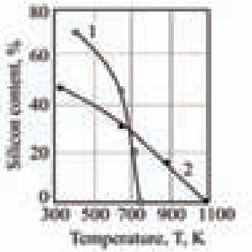

Figure 2. Pattern of temperature reduction of phase transition depending on the silicon content: 1 – in siderite; 2 – in calcite

The scientific controversy is in the fact that traditional representations of insignificant role of weak electric fields in the physical and chemical processes occurring in rocks, contrasted with fundamentally new experimental results showing the effect of weak electric fields as a powerful physical factors, in the event that their effect is directed to the destabilized microstructure of the condensed phase.

FTA-P-26

NATURAL GEORGIAN RAW VITAMIN COMPLEXES. DEVELOPMENT OF TECHNOLOGY

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People have been using natural raw materials of flora and fauna as food as well as medical purpose from immemorial time.

We focus mainly on selection of plant roughage materials with a high concentration of biologically active substances. We have characterized selected materials and pre-defined methods for production of functional products form them.

Plant roughage materials selected in Georgia were common following plants: cherries (Cerasus vulgaris Milli), elderberry (Sambucus ebulus L.), quince (Cydonia oblonga M.) and sea rocket (Bunias orientalis). If necessary, we will change plant roughage materials according situations.

Therapeutic and prophylactic efficacy are greatly influenced by variable factors such as exogenous and endogenous factors. A larger group variable factors are: 1) the physical condition of medicinal substances; 2) a simple chemical modification; 3) the nature of the ingredients; 4) forms of treatment, 5) as well as technological processes.

Production of final product from natural Georgian raw materials is performed at the final stage. The valuable product exists in biomass or liquids. We used different methods for separation of biomass and liquids:

Precipitation - gravitational force division;

Filtration – passing the suspension through the filtering material and retention of solid phase particles of biomass;

Microfiltration, ultrafiltration – passing the suspension through the fine pore membrane, retention of microbial cells and obtaining of pure solution.

During ultrafiltration not only cells are extracted but dissolved large molecules as well.

Coagulation – various reagents were added to suspension, resulting in a large cellular particles, which were separated from the fluid by sedimentation method;

After the operations listed above, extraction of valuable substances, common for intracellular and extracellular products, take place.

STUDY OF EXTRACTION OF ARSENIC AND GOLD FROM ARSENOPYRITE ORES BY HYDROMETALLURGICAL METHOD

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Possibility of extraction of Arsenic and Gold from arsenic containing sulfide raw materials has been investigated [1].

In order to extract gold, thermodynamic studies of preliminary alkaline leaching process of arsenic ores and residues from its calcination with addition of oxidant for extraction of gold bound with iron (II) and iron (III) arsenates has been conducted [2]. Izobaric-isothermal potentials of corresponding reactions (1,2,3,4) has been calculated and the possibility of their flow has been shown. The calculated values are shown in Table 1.

$$2FeAsS + 10NaOH + 7O_2 = 2Fe(OH)_3 \downarrow + 2Na_2SO_4 + 2Na_3AsO_4 + 2H_2O \quad (1)$$

$$2FeS_2 + 8NaOH + 7{,}5O_2 = 2Fe(OH)_3 \downarrow + 4Na_2SO_4 + H_2O \quad (2)$$

$$2Fe_3(AsO_4)_2 + 12NaOH + 3H_2O_2 = 6Fe(OH)_3 + 4Na_3AsO_4 \quad (3)$$

$$2FeAsS + 10NaOH + 4H_2O_2 + 4O_3 = 2Na_3AsO_4 + 2Fe(OH)_3 \downarrow + 2Na_2SO_4 + O_2 + 6H_2O \quad (4)$$

Table1. The values of the isobaric-isothermal potentials of the corresponding reactions

Reaction	ΔG^0Kcal / mol	ΔH^0Kcal / mol	ΔS^0Kcal / mol
1	-677,904	-791,8	-382,22
2	-694,029	-793,8	-334,8
3	-323,817	-301,11	76,2
4	-953,8	-10312,2	-259,8

The effect of hydroxide (NaOH) concentration, pH of the solution, temperature and addition of oxidants on the degree of alkaline leaching of arsenopyrite ore and residues from its calcination have been studied. Good agreement of experimental data with theoretical ones has been obtained.

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FTA-P-28

THE NOVEL HYDROELECTROMETALLURGICAL TECHNOLOGY OF JOINT PRODUCTION OF METALLIC MANGANESE AND ITS COMPOUNDS

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The novel technology refers to development of the hydroelectrometallurgical technology for the joint production of electrolytic manganese metal (EMM), active γ- modification macrocrystalline electrolytic manganese dioxide (EMD) and manganese sulfate monohydrate (MSM) from the Chiatura (Georgia) manganese ores. As a result, the currently worldwide existing independent technologies of production for each of these products will be unified in a single complex technological scheme.

The technology provides joint production of EMM and EMD in a single membrane electrochemical reactor [1]. Implementation of this innovative technology requires manganese sulfate solution autoclave processing after leaching of manganese ores and purification stage. As a result of the autoclave crystallization, one part of the obtained manganese sulfate monohydrate is supplied to the catholyte circulation independent technological contour for the production of the EMM, and the other part represents commercial product. The autoclave outlet hot manganese sulfate solution is used for the direct feeding of the anolyte to obtain EMD. Regime of significanly different temperatures in the cathodic (35^{0}C) and anodic chambers (94^{0}C) of the membrane electrochemical reactor could be maintained using the heat pump.

As a result of the carried out research, a cost-effective and energy-efficient, joint production technology of highly valued products from the manganese ores - EMM, EMD and MSM - will be created in Georgia; it has no analogues in the world and it will be attractive for investors to set up a new technology-based production in Georgia.

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COMBINED HYDROMETALLURGICAL TREATMENT OF JOINT CHALCOPYRITE AND MANGANESE OXIDIZED CONCENTRATES

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It is suggested to use the process of mechanochemical activation from chalcopyrite and manganese concentrates for obtaining the main components (Cu, Mn). In the process of mechanochemical activation, increase of the examined mixtures specific area takes place, which leads to the activity of the substances in the process of subsequent processing. Proposed process excludes the necessity for the usage of high temperatures and concentrated acids and guarantees the possibility of extraction of the main components (Cu, Mn) from initial raw material in the form of sulphates.

The optimal conditions of sulphuric acid extraction process of the former activated mixtures of chalcopyrite and manganese concentrates have been found: the process temperature – 90^0 C, liquid: solid ratio – 10:1, sulphuric acid concentration - 10%, grinding time -1h. The degree of copper extraction is -93.7%, manganese -99.8%.

Opposite of current, sulfuric acid extraction of jointly activated study of chalcopyrite and Manganese concentrates is provided. It is shown that the rise of the degree of copper extraction in solution is possible by opposite of current scheme. In the optimal conditions of extraction the degree of copper and manganese extraction is 99.7 and 99.8 % relatively. The obtained solutions, containing Cu-13; Fe^{2+} -10; Fe^{3+} -4.2; Mn^{2+}-80; H_2SO_4-33.5 g\l after purification from iron are valid for obtaining metallic copper and manganese compounds.

Substantiate the efficiency of combined recycling of copper-sulfide and oxidized manganese concentrates in ecological point of view. The sulfur-which exists in mixture – partially moves into the silt as elementary sulfur and also partly stays in the solution as sulfuric acid. Therefore, the emission of SO_2 into the atmosphere is not possible.

FTA-T-02

CHEMICAL-ENGINEERING PROCESSING OF GEORGIAN MANGANESE-CONTAINING RAW MATERIALS

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As it is known, manganese ores are the main metal-containing natural wealth of Georgia, and they are represented by Chiatura manganese deposit. It is one of the oldest among the world manganese deposits: duration of its operation counts more than 130 years. Basic amount of Chiatura ores after beneficiation is used for melting of manganese ferroalloys, while the remaining part is used by chemical, electrotechnical and other fields of industry.

Using the processing of manganese ores it is received a variety of chemical products with wide range of application, from which electrolytic manganese dioxide, electrolytic metal manganese, potassium permanganate were produced on industrial scale during last centuries in Georgia. Unfortunately, no one of them is produced anymore.

Chemical-engineering methods have the advantage that with their use it is possible to process not only rich, but also low-quality manganese-containing raw materials with the receipt of expensive production of high market demand.

All the abovementioned raises topicality and necessity of processing of manganese-containing raw materials of Georgia using chemical-engineering methods.

In last years we conducted works on processing of low-quality manganese-containing raw materials of Georgia by chemical-engineering methods, in particular by sulfurous leaching. First of all it refers to Chiatura carbonaceous ores and waste of former Rustavi large-scale production of electrolytic manganese dioxide – manganese-containing slime, in which the manganese content is 20-25% and 25-28%, respectively.

Laboratory tests and tests conducted on pilot plant showed the prospects of manganese sulfate and electrolytic manganese dioxide production from mentioned raw materials on industrial scale.

We offer number of novelties, which will substantially increase the efficiency of technology.

We schedule continuation of mentioned works on pilot-demonstration plant, assembling of which occurs in the building of pilot-plants of the Institute of Inorganic Chemistry and Electrochemistry.

THE THERMODINAMIC ANALYSIS OF PHYSICAL-CHEMICAL PROCESSES BEING IN THERMIC PROCESSING IN OF Na_2O-BaO-B_2O_3-SiO_2 SYSTEM

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Na_2O-BaO-B_2O_3-SiO_2 system has acquired recently the functions of starting system of receipt of materials (wares) obtained using more than one innovative technology. Without materials of various purposes obtained on the basis of this system it is impossible to get the composites, which simultaneously provide high strength, heat conductivity, resistance, heat-resistance, thermal stability and corrosion resistance. Many types of brand new materials – ceramics, glass ceramics, macro-, micro and nanocomposites, vitreous and vitro- crystalline materials of different purposes are obtained on the basis of this system. While investigating of Na_2O-BaO-B_2O_3-SiO_2 system thermodynamic parameters of reagents and products participating in more than 40 reactions of mentioned package turned out to be undefined. The investigation determined thermodynamic parameters of up to 20 undefined compounds have been established in total. On the basis of database of thermodynamic parameters of substances entering into reaction turns out to be close to 50. Three such compositions have been discovered which completely cover the area of receipt of amorphous materials according to their composition.

In my opinion as the author obtained results will promote physical-chemical analysis of Na_2O-BaO-B_2O_3-SiO_2 system and even more complicated systems and on this basis the creation of multifunctional borate, silicate and borosilicate composites without material-, labor and significant energy consumption.

FTA-T-04

THE PRODUCTION OF POTASSIUM PERMANGANATE IN THE FLOW ELECTROLYZER

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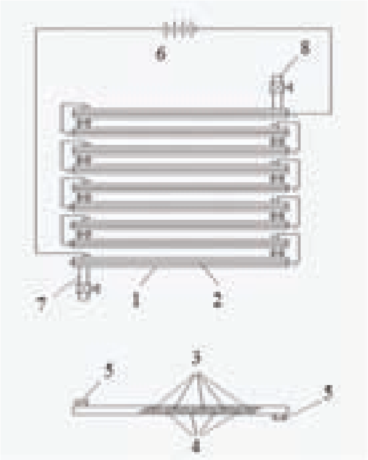
Potassium permanganate is a universal oxidizing agent. Today it is industrially obtained by combined semi-electrochemical two-step method: 1) production of potassium manganate from manganese ore; 2) electrochemical oxidation of manganate to potassium permanganate.

Polarization studies have shown that cathodic depolarization increases in the alkaline solution in the presence of permanganate and manganate ions due to their electrochemical reduction (up to MnO_2). MnO_2 current efficiency decreases with the increase of the cathode potential (reaching a minimum at about -1.6 ÷ -1.8 V) due to dominant hydrogen emission. To avoid cathodic reduction of MnO_4^- and MnO_4^{2-} ions the potentials of oxidation process K_2MnO_4 should be within the range of -1.6 -1.8 V (cathodic current density 6000÷15000 A / m^2).

It is known that the oxidation takes place under K_2MnO_4 diffusion control, so we have created a simple flow electrolyzer with an intense flow of the electrolyte at the anode surface. The electrolyzer consists of tubular cells with circular cross section inner surface of which serve as anodes (1). Conductive wires were coaxially mounted in stainless steel tubular cells (2), their surface was coated at regular intervals with a dielectric material (3); the uncovered part of the wire is the cathode (4). Thus, there is a ratio of the anode and the cathode surface areas equal to 1: 100, which minimizes the cathodic reduction portion of obtained product. The cells are interconnected by tubes (5) made of insulating material (these tubes are attached to the beginning and to the end of each cell). Cells in the electrochemical network are connected in parallel.



The principle of operation of the electrolyzer is: electrolyte is supplied through the tube (7) to the bottom of the electrolytic cell by a centrifugal pump. Redox reactions accompanied by release of gases occur at the anode and the cathode. The electrolyte and gases move in parallel and are pumped through the connecting tube (5) in the subsequent cell, etc. Electrolyte is separated at outlet (8), enters the crystallizer and centrifuge to obtain the final product. $KMnO_4$ current efficiency is more than 82%.

ADVANCED COMPOUNDS AND MATERIALS BASED ON NATURAL AND SECONDARY RESOURCES OF GEORGIAN REGION

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Georgia is rich in significant mineral resources – barite, bentonite clays, petroleum, natural gas, manganese, copper, mercury, arsenic, gold, medicinal mineral waters, Black Sea reserves of hydrogen sulfide, etc.

In spite of this fact, on the modern stage of society development, under conditions of ever-growing deficit of main strategic mineral and organic raw materials (metals, coal, natural gas, petroleum), the search for ways of targeted use of secondary resources [1] and accumulated wastes and creationof the base of cheap raw material resources becomes increasingly actual. These resources present additional technical-economical reserve for any inter-country and meanwhile give support for solving a number of ecological problems.

Two tendencies of our researches were ascertained:

- Use of natural resources and secondary raw materials in order to obtain various compounds and materials with specific properties;
- Development of advanced and economically feasible technologies based on these resources.

Our scientific teams created the various commodity forms:

- Isolation of pure manganese from poor ores and tailings by biometallurgic method (bacterial leaching) in the presence of strain *thiobacillus ferrooxidans* and pyrite. The final product - electrolytic metallic manganese was recovered with 99.83 %purityand 14 % yield. Obtainedresult were proved by the spectral analysis method;
- Obtaining compounds with specific properties based on arsenic isolated from industrial wastesand their use for preparation of ecologically safe antimicrobial hybrid polymer materials [2];
- Isolation of hydrogen sulfide from underwater layers (depth) of Black Sea and creation of advanced hydrogen fuel element (Prof. T. Marsagishvili, PhD E. Tskhakaia) which will replacepetroleum fuel in future.

Carried out researches are significant in terms of innovation, science, technology as well as economy, ecology and social. Such tendency of attitude towards natural and secondary raw materials sets a real perspective for developing of accessible, low stuff capacious and high-performance technologies that herewith considerably encourage economic progress in Georgian regionas well as will solve a number of ecological problems too.

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FTA-T-06

TECHNOLOGICAL PROCESS OF LIQUID-LIQUID EXTRACTION OF INDOLE GROUP ALKALOIDS

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The main property of alkaloids is an ability of salt formation. According to the technological classification, they are divided into strong, moderate and weak bases.

According to the extraction ability of alkaloids, organic solvents are distributed as follows: ether>benzene>chloroform>dichlorethane>petrol. The significant progress in alkaloids extraction of indole group has been marked since there was worked out methodologies of selective extractions and gradient pH techniques.

The concept of this methodology is defatting of raw material with petroleum ether (weak bases are removed), and further extraction with dilute solutions of organic acids, when acid solutions are alkalified pH 3-4, moderate bases are removed, at pH> 8.5 strong bases are extracted. Gradient pH technique supports the separation of alkaloids due to their basic properties and the usage of column chromatography –isolation of individual compounds.

The main producers of indole group alkaloids are: Apocynaceae, Loganiaceae and Rubiaceae families. Special attention deserve the plants of Vinca and Catharanthus genus of Apocynaceae family. Numerous researches have established, that alkaloids of these plants' belong to the certain chromophore systems of indoline, indole, oxindole and α-methylenindoline. Pharmacologists conclude, that α-methylenindolines are characterized with sedative, analgesic, hypotensive activities; indolines reveal cardiotonic and antiarrhythmic effects; indoles are sedative and hypotensive agents, while bis-indoles show oncolytic properties.

NMS

NEW METHODS FOR ECOLOGICAL AND RADIATION SAFETY, MEDICAL AND AGRARIAN RESEARCHES

INVESTIGATION OF POSSIBLE CHEMICAL WASTE DISPOSAL

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The problem of protecting the environment - one of the biggest challenges of our time. Industrial emissions, energy systems and transportation in air, water and mineral resources at the present stage of development reached such an extent that in some areas, especially in large industrial centers, pollution levels are much higher than acceptable health standards. Environmental pollution gaseous, liquid and solid wastes, causing degradation of the environment and harm to human health, recently left an environmental issue that has priority social and economic importance. The chemical industry is the fourth largest industry, essentially polluting after fuel energy, ferrous and non-ferrous metallurgy, automobile transport. At the same time, without the production of chemical plants currently it is impossible to implement conservation measures. That chemical industry manufactures various chemicals, coagulants, flotoagenty, sorbents, ion exchange resins, extractants and other materials, without which there are no wastewater or potable and process water, or the implementation of new technological schemes. For cleaning, gases produced various absorbing solution, sorbents and catalysts. The chemical industry consumes large quantities of raw materials, water and energy. Processes at chemical plants are complex and many-stage, and the range of products is vast. For the chemical industry it is characterized by extreme heterogeneity of waste. Industrial solid waste, hazardous waste water, gases, different in size and chemical composition of aerosols are released into the biosphere. Industrial solid wastes are chemically inert (refuse heaps, ash, etc.), reactive (rubber, plastic, etc.) and combined - industrial and construction waste. Solid waste management of various industries of Kazakhstan: phosphoric, rubber, textile, etc., and waste consumption is the solution to one of the most acute problems of pollution of the lithosphere. Of particular concern are the issues of waste products and technological marriage as an additive to create polymer composites. Modeling tradeoffs binders, ingredients, additives, fillers, hardeners predictive ability of composites with the necessary physical and chemical, sanitary and operating parameters to create a monolithic sports surfaces treadmills, volleyball and basketball courts, operating under alternating temperature changes. In this paper we explore the use of phosphate waste, rubber, light industry. As fillers were used phosphorous slag, crumb rubber, glass fiber, polyamide fiber, Nitron, polyvinyl chloride, down cellar, clay, kaolin, carbon black BS-120, etc. Curing agent compositions in some cases served as a departure of the oil industry – sulfur. In latex binders and liquid rubber additives stirred with a propeller stirrer at different speeds. The choice of fillers causes the nature of the polymer emulsion, depending on the binder. Curing monolithic coatings carried out in air for 24 hours. Sports and technical parameters of the coating are determined by the following parameters: tensile strength, elongation, Shore A hardness, elasticity, rebound, etc. The essential novelty of these compositions is the use of innovative methods of development of monolithic coatings based latex widely commercially available, and the use of waste as a filler of various industries: phosphate slag, rubber crumbs, lint basement, nitrone blue and green. Supplements of copper sulfate, polyvinyl chloride, stannous chloride dihydrate (DODFS) - dioksidifenilsulfona increase fire composition. Maleic acid contributes additional crosslinking compositions Clay improves mechanical properties of monolithic compositions.

Conclusions

1. Determined by the physical and mechanical properties of monolithic coatings based latex: P-136 (for the tire industry), (SBR) SCS-50-SE, liquid epoxidized rubber PEF-and copolymers FOR BA-DM with additives-waste various productions.
2. The possibility of obtaining monolithic sports surfaces using solid chemical waste RK.

NMS-O-02

OXIDE-MANGANESE CATALYSTS FOR SOLVING OF ECOLOGICAL PROBLEMS

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In the Laboratory of Catalysis of R. Agladze Institute of Inorganic Chemistry and Electrochemistry from the moment of its foundation (1961 year) the systematic researches are carried out for elaboration and study of physical-chemical properties of manganese catalysts for gas purification as well as for realization of other chemical- technological processes [1-4]. At present, the researches carried out elaboration of competitive oxide manganese catalysts for oxidation of CO of autotransport exhaust gases. The technology for deposition of the oxides of manganese and palladium on the fragments of alumosilicate blocks and on the stainless steel of “20 X 23H 18” mark is improved. The activity of the samples of Mn - Pd cataslysts was studied in the reaction of CO oxidation in blowing quartz reactor of 15 mm diameter; catalyst volume - 1 cm^3 , granule size 2.0 – 2.5 mm. Volume rate of gaseous mixture (1.0 volume % of CO + air), $W = 30 \cdot 10^3$ hour $^{-1}$. CO oxidation degree on the Mn - Pd catalyst, deposited on the steel, comprises 90 – 98 % in the temperature range from 130 ^{o}C to 160 ^{o}C . X – ray phase and thermal analyses of elaborated catalysts was performed. In the process of Mn - Pd catalyst formation the phase of manganese oxide, Mn_2O_3 is appeared on the carriers surface. By means of scanning electron microscope JSM - 65 10 LV the samples morphology, as well as the surface distribution of active components (Mn and Pd) was studied in the layer depth no more than 1 μm. The manganese oxides are the most deposited on the plates of alumosilicate blocks. Dispersity of manganese oxides on the plate surface comprises nearly 100 nm.

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NMR TECHNOLOGY FOR ASSESSMENT OF SOCIETAL, ENVIRONMENTAL AND CHEMICAL RISKS OF AMMONIUM NITRATE

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Ammonium Nitrate (NH_4NO_3) is agricultural fertilizer, which is produced in industrial quantities in Georgia. AN belongs to dual use chemical, as is potent explosive and detonator. There are risks associated with the use of AN. In airbags is used ammonium nitrate-based propellant. In 2014, it was announced about recall of cars with airbags manufactured by TAKADA with the defect that improperly inflate the airbags. There have been 10 deaths and more than 100 injuries due to this problem in the U.S. On 22 July 2011, in the Oslo bombing explosion AN explosive (ANFO) was used in front the building housing the Office of the Prime Minister and Ministry of Justice and the Police. In several European Countries use of AN is banned, e.g. Germany and Ireland. In 2008 Ammonium Nitrate Security Program was proposed by the USA Department of Homeland Security (DHS) in response to direction from Congress to “regulate the sale and transfer to prevent the misappropriation or use of ammonium nitrate in an act of terrorism” [1]. The fertilizer was banned in Afghanistan in 2010 because it’s an easy ingredient for Home Made Explosives (HME). In US Sandia National Laboratories in 2013 Kevin Fleming developed formula, which was not patented. Invention is the combination of iron sulfate with ammonium nitrate and resulted in an effective and cheap fertilizer which is useless as a component in an ANFO explosive; iron sulfate becomes iron nitrate and ammonium nitrate becomes ammonium sulfate. This metathesis reaction occurs if someone tries to alter the fertilizer to make it detonatable when mixed with a fuel [2].

In our study we are applying innovative method of NMR spectroscopy for the fast and reliable detection of nitrogen containing compounds. With this technique it is possible to study composition of synthesized compound at all stages of chemical synthesis and test final product as well. While ammonium molecule provides sharp peaks on spectrum, when ion is attached to larger molecule we observe broadening of the line-width, which is demonstrative for ammonium bound to other molecule [3].

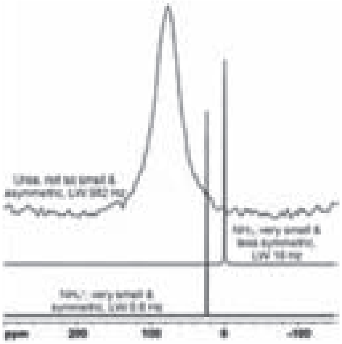

Figure 1. ^{14}N of NMR signals of NH_4^+ and NH_3.
Comparison of line-widths of ^{14}N signals.
The larger and less symmetric the molecule the wider the signal.

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NMS-O-04

INTEGRATED LIGNOCELLULOSE BIOREFINERY EXPLOITING WOOD-ROTTING FUNGI POTENTIAL

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Biorefinery is the continuous processing of biomass into a range of profitable products (food, feed, materials, and chemicals) and energy (fuels, power, and heat). Organic wastes are readily available in Georgia and are low-cost renewable resources for the production of various value-added products. In this presentation, the state of the art of lignocellulose bioconversion into value-added products by submerged and solid-substrate fermentation will be presented. It integrates the recent data on the physiology of wood-rotting basidiomycetes, focusing on the common characteristics and unique properties of individual fungi as well as on several approaches providing efficient expression of their biosynthetic and destructive potential. In particular, results of our extensive screening proved that mushroom submerged cultivation for the antioxidants, lectins, and extracellular polysaccharides (EPS) production with high yield is a promising approach. A common feature of white-rot basidiomycetes (WRB) is production of powerful extracellular hydrolytic and oxidative enzymes that effectively degrade biopolymers in plant biomass. To develop commercially significant technologies of lignocellulose-deconstructing enzymes production for their industrial and environmental applications, various approaches and strategies have been exploited in submerged and solid-state fermentation of lignocellulosic materials. The screening programs revealed a wide diversity of tested fungi and resulted in selection of new organisms with tremendous synthesis of cellulase and xylanase and lignin-modifying enzymes (LME). We established that several particular lignocellulosic growth substrates containing significant concentrations of soluble inducers play a crucial role in cellulases and ligninases production and determine the ratio of individual enzymes in final preparations. However, a fungus-specific lignocellulosic substrate should be elucidated. We showed that some microelements enhance LME synthesis although their effect is very specific depending on fungi physiological peculiarities. Special attention was paid to the regulation of LME production in the presence of aromatic compounds and synthetic dyes; some of them provide directed synthesis of LME. Moreover, our study underlines that the maximum expression of WRB biosynthetic potential depends on the additive effect of several factors. Furthermore, co-culture of the compatible fungi may be an appropriate approach to increase hydrolytic and LME production. Finally, we proved that the submerged and solid-state fermentation of agro-industrial residues by *Bacillus subtilis* 1933 and *B. amyloliquefaciens* 1895 is feasible for cost-effective poultry-beneficial probiotic formulations.

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CHEMICAL SECURITY AS A SYNTHESIS OF SCIENCES

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Chemical security is a relatively new domain belonging to a broader category: CBRN security. Its features distinguishing chemical from other i.e. biological, radiological and nuclear domain are due to the ubiquity of substances and variety of their distribution chain across the economy. Since security differs from safety in root cause - an intention in place of hazard itself, its nature is dynamic and multi-faceted. For that reason chemical security comprises various sciences in order to deal with. At its basics, safety likewise, it employs physics, thermodynamics and mass transport to describe hazard propagation. Security threat implies dynamic approach so traditional approach to a process as a “black box” has to be replaced by matrix analysis of possible vulnerable combinations of changeable process factors. Then, similarly to safety, security involves description and measuring of toxic effects on living organisms of the present substances, with the caveat that “present” is a result of the above mentioned matrix analysis and may differ from original process components. Ecology of closed environmental systems may be included as a part of the solution in mediation the effects of hazardous emission. Risk is not controllable in case of security because of unknown probability. Vulnerability is the controlled category in place of risk. Vulnerability depends on many factors, some of them technically determined like health and environment hazard, location, impact, but many of them non- technical like recognisability, availability of data, personnel quality, company security organisation and culture. The latter categories require employing tools from sciences like business management, sociology and psychology. The multifaceted nature of security makes measuring the effects a so called “wicked” problem. Yet another difficulty come with increasing role of integrated control systems (ICS) in chemical and related processes. Chemical cyber-security seems to share few only features with traditional security but since overall safety is an unity in the sense that every component leading to unsafe conditions for humans and environment is to be controlled, whether originating from pure hazard or intention, cyber- component is included into general security vulnerability reduction scheme.

NMS-O-06

TECHNOLOGY OF ECO-FRIENDLY HIGH TEMPERATURE HEAT-INSULATOR MATERIALS ON THE BASIS OF LIQUID GLASS AND FOAMED PERLITE

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With use of clinoptilolite, plastic clay and carbon black as modifiers on the basis of foamed perlite and liquid glass the eco-friendly and high temperature heat-insulators have been elaborated. It was shown that the addition of the modifiers to the composites improves their strength on compression by 1.8 - 2.3 times, density up to 250-450 kg/m^3 and coefficient of heat conductivity in the range of 0.06-0.08 wt/ (m · ^{o}C).

Modifier	Physical – mechanical properties	Pressure of sample production, MPa			
		0,3	0,5	0,8	1,0
Without modifier	Specific weight, kg/m^3	220	270	325	360
Carbon black		260	350	410	435
Clinoptilolite		310	368	420	485
Plastic clay		250	310	400	450
Without modifier	Compression strength, MPa	0,46	0,65	1,16	1,24
Carbon black		0,48	0,88	1,20	1,30
Clinoptilolite		0,68	1,12	1,46	2,42
Plastic clay		0,85	1,15	2,09	2,81

From the data of the table it is evident that the modifiers have a certain effect on physical-mechanical properties of obtained materials, in particular, on specific strength and on compression strength. Area of use: Drying ovens and thermostats, furnaces for the food industry, process furnaces (tempering, molding, etc.), furnaces for special purpose (vacuum, induction, etc.)[1-2].

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HYDROGENATION OF CARBON DIOXIDE OVER Fe-Zr/Al AND Fe-Ni/Al OXIDE CATALYSTS

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The increase in emissions of carbon dioxide in the atmosphere leads to the deterioration of the ecological state of the environment, climate change. One of the solution to this problem is to recycle of CO_2 into valuable chemical products. Among the methods catalytic hydrogenation of CO_2 recycling is one of the most appropriate [1, 2].

This paper presents the results of a study of Fe-Zr/Al and Fe-Ni/Al oxide systems as catalysts for the methanation of carbon dioxide. The first results of a systematic study of elemental composition of the catalyst surface, the distribution of the catalytically active component on the surface of the catalyst depending on the method of the catalysts preparation, the reaction conditions – mol. ratio CO_2/H_2, temperature and reaction time, the nature of the catalytically active composition are given. Elemental and phase composition of the catalyst before and after the reaction were studied by X-ray fluorescence microscopy and X-ray diffraction. The used XRF microscope combines optical visualization with elemental analysis and imaging. Two mono-capillary beams are used with 10 μm and a 100 μm diameters. The SmartMap imaging software of the XRF microscope allows to record a full EDXRF spectrum at each pixel of the element image and element distribution maps can be generated. Contents of Fe, Ni and Zr in the samples was determined by atomic absorption spectroscopy. Method of electron magnetic resonance of catalyst in conjunction with a chromatographic analysis of gas-phase products of reaction in-situ conditions used to identify the magnetic centers of the catalyst and determination of the dependence of gas-phase composition of the reaction products on the condition and concentration of the magnetic centers. Based on the obtained data the dependences of the target product yield on the content of the catalytically active component on the surface of the catalyst are determined. The nature of the catalytically active sites for methanation of carbon dioxide is discussed and mechanism of hydrogenation of carbon dioxide into hydrocarbons with the participation of these centers is given.

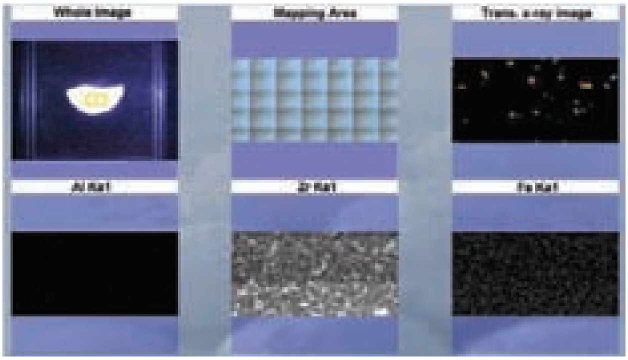

Figure . Element distribution maps for the sample of Fe-Zr/Al oxide catalyst

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NMS-O-08

ENANTIOSEPARATION OF CHIRAL ANTIMYCOTIC DRUGS IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY WITH POLYSACCHARIDE-BASED CHIRAL COLUMNS

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This work represents study of enantioseparation of some chiral antimicotic drugs using polysaccharide-based chiral selectors with polar-organic and reversed mobile phases in high-performance liquid chromatography.

The chiral compounds were diazole and triazole derivatives, which are used in medicine as antimicotic drugs for disease prevention and treatment as well. Was established effect of structure of chiral selector and mobile phase with different additives on value of enantioselectivity. Addition of ammonium acetate to mobile phase increased the enantioselectivity and generally caused dicrease of retention time. Addition of water in case of methanol as a mobile phase increased retention times, but with acetonitrile the trend was different, small concentrations of water decreased retention times firstly but after increasing the percentage of water in mobile phase, values of retention times were increased.

Changing of enantiomer elution order was occurred with Sulconazole by changing the chiral selector, from Cellulose tris(3,5-diclorphenylcarbamate) to Cellulose tris(2,4-diclorphenylcarbamate).

Effect of mobile phase composition and structure of chiral selector on enantioselectivity was studied. Some interesting trends were observed and described.

Terconazole completely separates enantiomericaly with Chiral selector tris (3,4-dimethylphenylcarbamate). With introducing an electron-donating substituent in benzyl moiety decreased the level of separation. Namely, terconazole does not separate with Cellulose tris (3,4-dichlophenylcarbamate) and partially separates with chiral columns Cellulose-2 and Cellulose-4.

Ornidazole partially separates on with chiral columns Cellulose-2 and Cellulose-4. But it does not separate at all with introducing an electron-donating or electron-withdrawing substituent in benzyl moiety.

Ketoconazole completely separates enantiomericaly with Chiral selectors Cellulose tris (3,4- dichlorophenylcarbamate), Cellulose-2 and Cellulose-4. In case of Cellulose tris (3,4- dimethylphenylcarbamate), addition of 5 % water in mobile phase caused coelution of peaks. In the case of 20 % of water in mobile phase, enantioseparation is ensured by hydrophilic interactions. With more quantities of water enantioseparation is analogous to reversed-phase chromatography. This can be explained by decreasing of hydrogen bonds between chiral selector and analyte. The same effect is observed with other drugs.

NMS-O-09

SEPARATION OF ENANTIOMERS WITH SUPERFICIALLY POROUS SILICA MODIFIED WITH POLYSACCHARIDE DERIVATIVES AS EFFECTIVE CHIRAL STATIONARY PHASES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

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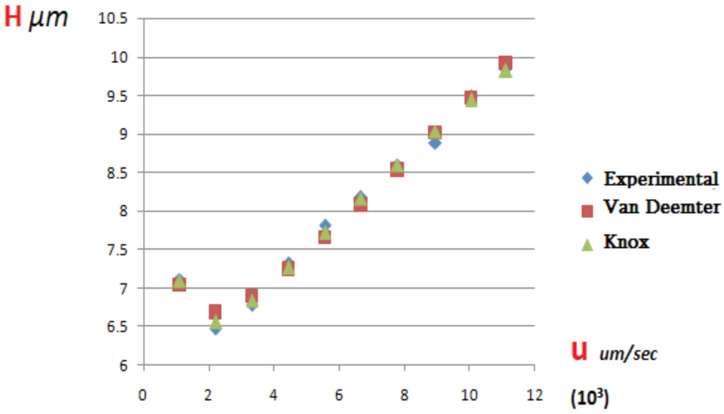
The first ever report on the preparation of chiral stationary phases (CSP) based on superficially porous silica (SPS) particles for the separation of enantiomers in HPLC demonstrated clear advantages of such materials. Higher enantioselectivity, limited dependence of plate height on the mobile phase flow rate and higher plate numbers and resolution calculated per unit time (i.e. higher speed of separation) were observed with columns made with superficially porous CSP in comparison to columns made with fully-porous silica-based CSP at comparable content of chiral selector (polysaccharide derivative) in the CSP [1]. In this report further evidences are described supporting the findings of our first study about the superior performance of polysaccharide-based chiral selectors in combination with SPS when compared to traditional CSPs based on fully porous silica (FPS) particles.



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NMS-O-10

PHOSPHATE SCAVENGERS FOR REMEDIATION OF GROUNDWATERS AND TREATMENT OF HYPERPHOSPHATAEMIA IN ANIMALS AND HUMANS: REVIEW AND COMPARISON

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Phosphates are not only the structural material of bone and teeth in biological systems; they play an indispensable role for life as a component of nucleic acids, adenosine triphosphate and phospholipids, and adding and removal of phosphates determines the way of storing and releasing energy within living cells. Phosphates enter biological systems with vegetable food, and phosphorus-containing fertilizers are used to replace the phosphorus consumed by plants from the soil.

However, redundant amounts of phosphates appear dangerous both to ecosystems and to animals and human beings. In agriculture, the excessive input of phosphate nutrients leads to over-fertilization. Moveable phosphate ions enter groundwaters, come to rivers, lakes and coastal marine systems and cause significant environment damage, especially algal bloom (eutrophication). Another source of phosphorus income to groundwaters, rivers, lakes and reservoirs is treated and untreated sewage containing detergents and water softeners. In animals and humans, an optimal amount of phosphates in blood is balanced by renal phosphate excretion. A massive acute phosphate load, as well as acute or chronic renal insufficiency elevate the level of phosphates in blood and cause the so-called hyperphosphataemia.

Precipitation of insoluble phosphates, adsorption and ion exchange are considered as major means for the mitigation of the phosphate level in solutions, and numerous materials are suggested so as to effectively bind this harmful anion. In this presentation, existing commercial and laboratory phosphate sorbents will be described, with special reference to lanthanum- and cerium-based ones, including our own works directed towards elaboration of sorbents where $La(OH)_3$ and $Ce(OH)_4$ serve as a coverage on proven non-toxic supports (TiO_2, Al_2O_3, SiO_2). Lanthanum compounds attract much attention being environmentally benign and non-harmful to animals and humans and showing one of the greatest affinities toward phosphate ions in sorption processes. Similarly, $Ce(OH)_4$ may be prospective in adsorption technologies due to its low toxicity and possible protective role in terms of human health.

Mixtures of $La(OH)_3$ and $Ce(OH)_4$ with TiO_2 and Al_2O_3 were synthesized by means of co-precipitation from acidic media. Since the precipitation of hydrous titania and alumina takes place at lower pH than lanthanum and cerium hydroxides, the rare-earth hydroxides form a coverage on supports. In order to obtain SiO_2 covered with $La(OH)_3$, a citric acid aided route elaborated in our works was employed. In adsorption studies, the ratio of the rare-earth hydroxide to support was varied so as to find scavengers of maximal efficiency and minimal cost. pH was adjusted in order to select materials with maximal affinity to phosphates in the gastrointestinal tract, either in stomach at pH~2-3 or in intestines at pH~8.5-9. It was found by means of IR studies that different affinity of adsorbents in acidic and basic media is caused by the formation of lanthanum and cerium carbonates. Specifically, at high pH, carbonates are more stable than phosphates and block the surface of sorbents. At low pH, carbonates dissolve and do not compete with phosphate ions for adsorption sites.

Another question to be discussed is the comparison of adsorption materials. The role of the so-called dimensionless constant separation factor is emphasized, and Langmuir adsorption isotherms are classified by their shape into unfavorable, linear, favorable and irreversible. It will be especially stressed that the constant separation factor is the only parameter including the properties of both the adsorbent (Langmuir equilibrium constant) and the adsorbate (the concentration of the stock solution) and enabling one to match adsorption data obtained under incomparable conditions. The history of its use will be revisited, and existing phosphate scavengers will be compared with its help. It would be shown, in particular, that the affinity of the materials obtained to phosphates is close to that of Phoslock®, the best commercial adsorbent for removal phosphates from soils comprising a lanthanum-substituted clay.

NMS-O-11

THE USE OF MODERN PHYSICAL-CHEMICAL METHODS OF SUBSTANCE ANALYSIS IN THE ANALYSIS OF GEORGIAN RED WINE

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Our aim is to study Georgian wines with LC/NMR/MS methods and prepare passports of their quality. In the work hereby we present LC/NMR/MS method research results of Georgian red wine “Khvantchkara”. ^{1}H and ^{13}C Chemical Shifts, Proton Multiplicity and J_{HH} for assigned compounds in Georgian Wine Khvanchkara are given:

acetic acid/acetates 2.06 (s, âCH3)/23.42 ; alanine 1.47 (d, 7.2, âCH3)/17.17; 3.80 (RCH)/54.79; γ-aminobutyric acid (GABA) 1.94 (âCH2); 2.48 (RCH2); 3.03 (γCH2) ; arginine 1.68 (m, γCH2); 1.90 (m, âCH2); 3.22 (t, δCH2) caffeic/ trans-caftaric acid 6.42 (d, 16.0, RCH); 6.91 (d, C5H); 7.12 (d, C6H); 7.67 (d, 16.0, âCH) citric acid 2.75 (d, 16.4, R,γCH)/46.54; 2.95 (d, 16.4, R′,γ′CH) p-coumaric/CCCC trans-coutaric acid 6.42 (d, 16.0, RCH); 6.91 (d, C3H/C5H); 7.56 (d, C2H/C6H); 7.67 (d,16.0, âCH) disaccharide 5.16 (d, 3.9, C1H)/97.02 ethanal 2.23 (d, 3.0, CH3); 9.67 (q, CH) ethanol 1.17 (t, 7.2, CH3)/19.56; 3.64 (q, 7.2, CH2)/60.19 ethyl acetateb 1.26 (t, 0.2, CH3); 4.12 (q, 7.2, CH2) formic acid 8.32(s, HCOOH)/169.8 R-fructose 4.09 (C3H)/84.68 â-fructose 4.09 (C3H, C4H)/77.56 gallic acid 7.12 (s, C2H, C6H, ring)/112.37 R-glucose 5.20 (d, 3.7, C1H)/95.15 â-glucose 4.61 (d, 8.0, C1H)/99.10; 3.25 (dd, C2H) p-hydroxybenzoic acidb 6.67 (d, 3.3, C3H, C5H, ring)/113.7; 7.54 (d, 3.3, C2H, C6H, ring)/129.9 isobutanol (2-methyl-1-propanol) 0.87 (d, 6.7, CH3); 1.73 (m, CH); 3.36 (d, CH2OH) isopentanol (3-methyl-1-butanol) 0.88 (d, 6.7, CH3); 1.43 (q, CH); 1.64 (CH2); 3.61 (t, 6.7, CH2OH) lactic acid 1.38 (d, 7.0, âCH3)/22.41; 4.31 (q, RCH) leucine 0.95 (t, δ,δ′ CH3); 1.72 (âCH2, γCH) malic acid 2.71 (dd, 6.0; 12.8, âCH)/39.48; 2.82 (dd, â′CH); 4.45 (RCH)/69.81 methanol 3.35 (s, CH3)/46.15 2-methyl-1-butanolb 0.87 (d, CH3); 0.88 (t, CH3); 1.10 (m, 1/2CH2); 1.38 (m, 1/2CH2); 1.53 (m, CH); 3.38 (dd, CH2OH); 3.47 (dd, CH2OH) niacin 8.0 (dd, C5H); 8.82 (dd, C4H, C6H); 9.11 (C2H) 2-phenylethanol 2.76 (CH2); 3.74 (CH2OH); 7.28 (m, ring); 7.34 (m, ring) proline 1.99 (m, γCH2)/26.40; 2.06 (â′CH)/31.57; 2.33 (m, âCH)/31.57; 3.32 (δ′CH)/49.07; 3.42 (δCH)/49.07; 4.11 (RCH)/63.76 1-propanol 0.88 (t, 7.5, CH3); 1.53 (m, CH2); 3.55 (t, 6.8, CH2OH) pyruvic acidb 2.35 (s, âCH3) succinic acid 2.62 (s, R, âCH2)/31.74 tartaric acidb 4.41 (s, RCH) threonineb 1.42 (γCH3); 4.42 (âCH) tyrosine/tyrosol 6.83 (d, C3H, C5H, ring)/118.13; 7.15 (d, C2H, C6H, ring)/133.30; 6.87 (d, C3H, C5H, ring)/118.46; 7.17 (d, C2H, C6H, ring)/133.80 uridine 4.17 (C4′H); 4.29 (C3′H); 5.87 (C5H ring, C1′H); 7.88 (C6H ring) a s) singlet; d) doublet; t) triplet; q) quartet; dd) doublet of doublets; m) multiplet.

NMS-O-12

DETERMINATION OF CONDITION OF COMPLETE SOLID SOLUBILITY IN THE SYSTEM OF $Li_{0,5}Fe_{2,5-x}Al_xO_4$ BY MEANS OF CALORIMETRIC INVESTIGATION OF EXCESS MIXING PARAMETERS H_{mix}^{ex} AND ΔS_{mix}^{ex}

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Generally for studying free energy of solid solutions' mixing ($\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$), it is necessary to determine excess thermodynamic parameters ΔH^{ex}_{mix} and ΔS^{ex}_{mix} at formation intermediate complex compositions from initial components.

The object of the given investigation is the system of the solid solutions $Li_{0.5}Fe_{2.5}O_4$ – $Li_{0.5}Al_{2.5}O_4$ with general formula $Li_{0.5}Fe_{2.5-x}Al_xO_4$. Two initial components and four intermediate complex solid solutions $Li_{0,5}Fe_{2,5-x}Al_xO_4$ (x=0; 0.5; 1.0; 1.5; 2.0; 2.5) were prepared by ceramic method, and identified by chemical and x-ray analyses. The samples were dissolved on Calve calorimeter at 973K in oxide melt 9PbO 3CdO $4B_2O_3$ in order to measure enthalpy of dissolution ΔH_{sol} (973K) and then calculate the excess enthalpy of mixing ΔH^{ex}_{mix} (973K). The results have been standardized ΔH^{ex}_{mix}(298K) using functions ΔH=f(T), obtained on high-temperature adiabatic drop calorimeter and heat of transformations ΔH_{trans} measured on scanning calorimeter. Differently from other similar investigated systems, we have the positive values ΔH^{ex}_{mix} (298K) with maximum 9.8kJ/mol for composition x=1.5.

The second necessary thermodynamic parameter ΔS^{ex}_{mix} have been determined by means of semiempirical calculation method using values of C_{p298} measured near standard temperature and taken from the known function C_p=f(T). This method allows us to determine ΔS^{ex}_{mix} avoiding special expensive law-temperature calorimetric experiment. The values ΔS^{ex}_{mix} J/K.mol are changed between 14 and 33.

The final result is the ΔG^{ex}_{mix} - Excess Free Energy of mixing and its concentration dependence which clearly informs us about character of the mixing mechanism of $Li_{0,5}Fe_{2,5}O_4$ and $Li_{0,5}Al_{2,5}O_4$. The results coincide with the known discontinuous mixing in this system.

Drawing the phase diagram of state, we have fixed the top of the "dome of decomposition" of solid solution in this system - 550K. This is the temperature above which the characteristic for the given complex solid solutions "order-disorder" transformation begins. These research of one system $Li_{0,5}Fe_{2,5}O_4$ – $Li_{0,5}Al_{2,5}O_4$ allows to use this approach to determine the condition of obtaining one-phased compositions in all extend of concentration for systems with a broken solid solubility.

QUANTITATIVE DETERMINATION OF TOTAL MANGANESE IN ZESTAFONI SOIL AND DRINKING WATER AND ABNORMALITIES CAUSED BY ITS ABUNDANCE

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According to the statistical indicators of the non-commercial legal entity “Municipal Public Health Center”, Zestafoni residents are plagued by nervous system diseases including the so called “manganese-induced parkinsonism” and musculoskeletal disorders.

We aimed to determine the total amount of manganese in Zestaponi soil and drinking water (springs, wells).

Methods: the research is carried out in the Chemistry Department scientific-research laboratory of Akaki Tsereteli State University and the physico-chemical analysis laboratory of R. Agladze Institute of

Inorganic Chemistry and Electrochemistry.

Soil analysis is carried out in full compliance with the procedure - 4 samples of soil are collected 15 km away from the ferroalloy plant in the following sequence: 3 km, 6 km, 10 km, and 15 km (Village Zeda Sakara). Samples of the water (springs, wells) were also respectively taken.

Methods: total amount of manganese in the soil is determined by Folgard’s and Potentiometric methods.

In arable land, total manganese, according to the maximum permissible concentration (MPC), is 1000 mg/kg. For low-acid soils with pH=6, MPC is 500 mg/kg. Total manganese in drinking water is determined by the persulphate-photocolorimetric method per photoelectric colorimeter. MPC of manganese in drinking water is 0,4mg/l.

Table 1. Total manganese in the soil

№	Distance from the ferroalloy plant	Folgard’s Method g / l	Potentiometric method g / l	The final result mg / kg
1	3 km	3,145	3,045	3045
2	6 km	2,320	2,30	2300
3	10 km	2,010	2,10	2100
4	15 km	2,560	2,400	2400

Table 2. Total manganese in the drinking water

№	Distance from the ferroalloy plant	Total manganese mg/l
1 Sample (spring)	3 km	1,25
2 Sample (spring)	6 km	2,3
3 Sample (well)	10 km	1,25
4 Sample (well)	15 km	3,05

As the survey shows, the total amount of manganese in the soil and drinking water is much higher than the standards adopted by our country (Order №297/NApproval of environmental quality standards. Valid - 20.09.2006 №70 –15 January,2014, Tbilisi).

The total amount of manganese in the soil ranges between2100 mg/kg and 3045 mg/kg, and in the water it is between 1.25 mg/l and 3.05 mg/l.

Because such number of manganese endangers human health, to get a full picture it is necessary to conduct the second phase of survey in order to determine total manganese in leaves and fruits of plants.

NMS-O-14

OILY WASTEWATER TREATMENT USING BLEND PSF-SPEEK HOLLOW FIBER MEMBRANE

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In the present work, a blend polymeric membrane was produced for oily wastewater treatment. Blend polysulfone (PSF) -sulfonated poly ether ether ketone (SPEEK) hollow fiber membrane was prepared via a phase inversion process. The prepared membranes were characterized in terms of morphology, N2 permeability, pure water flux, compaction test, contact angle measurements and oil-water separation. From SEM test, the blend membrane showed a more open structure with large finger-likes cavities compared to the plain PSF membrane. However, it seems that the blend membrane has a denser outer skin. This was confirmed by N2 permeability of the blend membrane which showed a significantly lower permeance. From contact angle results, hydrophilicity of the blend membrane significantly improved compared to the plain PSF membrane. Although the blend membrane has a dense skin, higher water flux of the membrane was related to the higher hydrophilicity. From oil-water separation test, a good rejection of 95% was achieved for the blend membrane. In addition, it seems that the rate of fouling was reduced for the blend membrane which can be related to high hydrophilicity of the membrane. Therefore, by controlling membrane structure a good water flux and rejection can be achieved for a long-term waste water separation system.

THE SIGNIFICANCE OF THE NEW PROPERTIES OF BEMIPARIN FOR APPLIED MEDICINE

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Coagulation and hemorheology play a significant role in blood circulation and ensure its trophic function. According to a modern concept it is impossible to develop physiological process if coagulation and blood rheology systems are not within the normal range. In the development of all pat-physiological processes coagulation and hemorheology play compensatory role, which is directed to adequacy and improvement of the tropic function. To study bemiparin we made research in vivo and in vitro systems. And found that bemiparin has a positive effect not only on the coagulation, but also on the rheological properties of blood. The study involved 10 rats of both sexes. Among them 10 rats (1:1) are in the control group. Rats' weight – 180±25g. We use a concentration of 0.01; 1 and 0.1 UI / ml, which covers the therapeutic range of doses used in clinical practice and selected from scientific papers. For the comparison of the action of bemiparin we will chose macromolecular heparin (the study will be blind and therefore successful brands, Trade Marks and accurate molecular weight cannot be anonymous). The anesthesia was performed with chloral hydrate (1 ml of a 4% solution per 100g body weight). Under anesthesia (0,02 ml a 2% solution of promedol per 100 g body weight). We will be surgery and isolated mesentery and post the mesentery on a warm table (37°C – approximate conditions in situ). We observed in the blood flow of rats' by microscope "Ortoplan, 170 / -Plapo (× 6.3)", special camera "Vario-Ortomat"«Leitz», Germany. In addition, we conducted a study in vitro. We determine the effect of bemiparin on blood rheology status (in vitro). Results of the microcirculation study showed that blood flow restores, when bemiparin (microdroplet) applique on the capillary with stasis (NaCl crystal did stasis). Similar results were obtained in vitro system. Despite the studies and information on bemiparin, bemiparin affects on blood flow is insufficiently described for clinicians. Makin bemiparin injections cause coagulation picture changes in animals. We show how the best parameters of coagulation may be reached and the number and the specific concentration of bemiparin. We statistically clarify certain coagulation parameters and the functional impact of bemiparins subcutaneous injection's frequency and quantity. This determine that the daily injections of bemiparin will be effective. This data help us to determine bemiparin's features for preventive measures based on the fundamental literature.

NMS-O-16

SYNTHESES OF NH_2/NH_2 CAPPED ANILINE OLIGOMERS AND THEIR DERIVATIVES

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Polyaniline and polymers obtained from aromatic amines have a special place among electroactive polymers due to their environmental stability and unique properties [1,2]. We have worked out a new and useful method for N,N-disubstituted quinonediimine synthesis using oxidative condensation of p-phenylenediamine (PPDA) in organic medium [3,4]. Particularly, NH_2/NH_2 capped aniline trimer and pentamer have been identified as a result of condensation of PPDA using molar ratio PPDA/potassium peroxydisulphate 4:1. It was found that with heating the terminal amino and quinone diimine groups of different molecules reacted. This is self condensation reaction, which proceeds according to scheme which leads to the formation of oligomers and polymers depending on the heating time. Obtained compound was oxidized by potassium persulphate with different molar ratio. Electric conductivities of both as synthesized and doped with iodine compounds were determined. Acetylation of obtained oligomers were carried out to obtain stable to heating compounds. It was shown, that the reaction of obtained oligomers with different nucleophiles provide opportunity for mono substituted aromatic amines synthesis. UV, PMR and IR spectral methods have been used to prove the structure of obtained compounds. Antibacterial and free radical scavenger properties of synthesized compounds were investigated and compaired with each other.

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ULTRASOUND IN MEDICINE, BIOLOGY, BIOTECHNOLOGY

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Ultrasound techniques have long found their place in medicine, and are widely used in the diagnosis, treatment, surgery. In recent years, medical ultrasound technology has become a routine in veterinary medicine, where it is in some cases even the used ultrasound wider than in medicine. However, abilities of ultrasound is far from exhausted. The development of electronics and acoustics, as well as the understanding of the mechanisms of biological and physico-chemical effects of ultrasound stimulates the development of new invasive and non-invasive methods. Focusing the ultrasound using phased arrays allow to destroy tumors in the body, without disturbing the covering tissues, and allow to quantify the sensitivity of nerve endings in the skin and in the depths of the body. The ability of ultrasound to increase the permeability of cell membranes forms the basis for a method for targeted delivery of drugs, in particular for cytotoxic drugs in tumor tissues. In biotechnology of microbial synthesis of antibiotics and other biologically active substances the low intensity ultrasound is used to stimulate the growth and development of microbial cultures. Using ultrasound is possible to receive a suspension of water-insoluble resins and other substances having potent therapeutic and prophylactic effect and applicable for children. Ultrasonic methods are introduced in the technology of producing special products for 3D printing bone grafts. Obtained by ultrasonic technics varnish from amber, which was not subjected to the biodegradation of the tens of millions of years, have been used to protect dentures and urological catheters against infectious and dangerous biofouling. Unfortunately, not all the advances in medical acoustics have been applied. It is well known ultrasonic prostheses for blinds, ultrasound prostheses of sound-conducting pathways for some diseases that cause deafness.

NMS-O-18

SOME CHARACTERISTICS OF THE SEPARATION OF ENANTIOMERS OF BETA-BLOCKER DRUGS USING POLYSACCHARIDE BASED CHIRAL COLUMNS IN HPLC

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This work presents a study of enantioseparation of some chiral β-blocker drugs on polysaccharide-based chiral stationary phases with different mobile phases. β-blockers are chiral compounds with basic nature, which are widely used in the medicine for treatment of some cardiac diseases. In many cases only one enantiomer of chiral β-blocker drug is responsible for its desired pharmacological effect, while the other one may be inactive, exhibit different activity or be even toxic. Therefore, enantiomeric purity determination of chiral β-blocker drugs is very important.
All HPLC experiments were performed with Agilent 1200 HPLC system (Agilent Technologies, Waldbronn, Germany). Lux series of chiral columns with 4.6x250 mm dimension and containing packing material with 5 micrometer particles were provided by Phenomenex Inc. (Torrance, CA, USA). Separation of enantiomers of chiral β-blockers was studied on polysaccharide-based chiral stationary phases by isopropanol and hexane-isopropanol eluents with different ratio in the presence of additives of diethylamine (DEA).

The emphasis was placed on some interesting examples of enantiomer eluent order reversal observed depending on the chemistry of the chiral selector, separation temperature, major component, as well as the minor additive to the mobile phase. The reversal of elution order of enantiomers was observed in some cases. For instance, the elution order of sotalol was opposite on Cellulose-2 and Amylose-2, Cellulose-4 and Amylose-2 columns (Fig. 1). The similar result was observed for penbutolol and timolol enantiomers on Cellulose-1 and Cellulose-2 columns, which differ from each other by the nature and position of substituents. The change of composition of the mobile phase also resulted in the reversal of the elution order.

Figure1. Reverse of elution order of sotalol enantiomers: A-Cellulose-1, B-Cellulose-2, C-Cellulose-4, D-Amylose-2.

Several interesting examples of enantiomer elution order reversal were observed for chiral b-blockers on polysaccharide-based chiral columns under polar organic-(isopropanol) and normal-phase HPLC conditions. Some cases of changing elution order and retention times of enantiomers were observed with addition of DEA / FA (Formic acid) to mobile phase.

Acknowledgment

The authors thank Shota Rustaveli National Science Foundation of Georgia (SRNSF) for providing financial support (Project N 31/90) and Phenomenex (Torrance, CA, USA) for donation of chiral columns.

TECHNOLOGY OF PURIFICATION OF IRRIGATION WATER WITH A HIGH SALT CONTENT IN ORDER TO PREVENT SECONDARY SALINIZATION OF ARARAT VALLEY

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Secondary salinization is an urgent problem that not only brings enormous material damage, but also spoils the nature of the world. And in this aspect questions of correct choice of areas under irrigation, prediction and prevention of secondary salinization and rational use of soil subjected to irrigation go beyond the purely scientific, and even national interests, acquiring, to a certain extent, international importance.

In Armenia we face with a similar problem in irrigation saline soils of the Ararat valley where highly mineralized water rivers Hrazdan and Sevjur are the main sources of irrigation.

Different methods of classification, allowing to determine the suitability of water for irrigation, based on the qualitative composition of salts in view of risks of salinity, alkalinity and carbonate alkalizing were applied to evaluate the properties of irrigational water from the rivers Hrazdan and Sevjur. Based on the assessment of the level of the total mineralization, the river waters require ***special approach and accounting for all conditions*** when used as irrigation water. Applying the method of Staebler it was identified that the river waters are characterized ***as poor***, there is an ***urgent need to prevent the gradual accumulation of alkalis for all kinds of soils.*** With regard to assessment of risk of potential salinization, according to the procedure of Antipov - Karataev, waters are ***unacceptable for irrigation***. Estimating the water quality on a scale of conductivity values and the level of salinity of the water of the rivers belongs to type 3, and are classified as the high salinity waters. Thus, a comprehensive evaluation showed that there is ***a need for measures to combat salinity.***

To protect soils under irrigation from alkalinization, soda salinization, it is necessary to bring in the soil or with the water periodically small doses of chemical ameliorators (gypsum, mineral acids), use physiological acidic nitrogen (ammonium sulfate, ammonium nitrate, sulfate, nitrate, ammonium, ammophos, diammonium phosphate) and calcium-containing (single and double superphosphate) fertilizers, introduce perennial broad bean grass into crop rotations. Restoring soil from soda salinity requires the simultaneous use of deep drainage as well.

The choice of method of the rivers Hrazdan and Sevjur waters desalting is determined with peculiarities of the quality of original and quality requirements to the quality of treated waters, capacity of the installation and the technical and economic indicators. Guided with the above mentioned, among the known methods of desalination by distillation, ion exchange, reverse osmosis and electrodialysis, the latter was chosen.

NMS-O-20

STRUCTURAL CHANGES OF POLYPHENYLENEOXIDES IN THE PROCESS OF FRICTION

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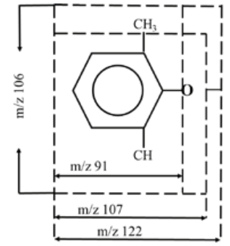
Aromatic polyether-polyphenylene oxide (PPO) with molecular mass 56000 and specific viscosity 0.47 dl/g seems most interesting among the known hetero chain polymers as a binding antifriction plastic mass. Investigation of thermal stability of the initial and pressed polyphenyleneoxide was carried out by the mass-spectrometry method [1, 2]. Specters were taken within the temperature range 25-500^0C, after every 50^0C. Energy of ionization electrons equaled to 70 e,v. The main thermal destruction of polyphenyleneoxide was observed at 450^0C; it was accompanied with emission of products with m/z 122, 1,7, 91, 135, 242.. Results of study of properties of industrial specimen of PPO polymers, showed that at the thermal impact (450^0C) the polymer undergoes destruction in the main chain (phenyl-o-phenyl bond is destructed) [3].



Alongside with it, at such conditions, Friss regrouping can take place (emission m/z 135). Low molecular admixes present in the polymer such as toluene, xylene, as well as insignificant number of dimmers, trimmers, reduce thermal stability of PPO to 200^0C and can lead to alteration of its structure at its treatment.

Study of tribochemical processes of polyphenyleneoxide samples was performed on a device installed in a chamber of mass-spectrometer, in close proximity to ionization zone, at the drum rotation velocity V=1m/sec and pressure P=0.1Mpa.

Investigations showed that maximum emission of volatile products was observed in the process of run-in during the first 5-10 minutes. At the increase of friction time amount of emitted product decreases. At the comparison of tribo- and thermal destruction processes of polyphenyleneoxide we can see that in the process of friction mainly the products are released which are inherent to low temperature thermal destruction of the initial PPO (m/z 106 and 91), which takes place, as it was shown earlier at 200^0C. On the base of the obtained data it was shown that under the terms of treatment at 300^0C, destructive-structuring processes take place in a polymer. Besides, Friss regrouping takes place that leads to branching of macromolecules and forming gel-fraction. Investigation of tribochemical processes during friction, showed that character of tribochemical processes in a polymer is conditioned by the formation of complex structure of pressed specimens containing branching, cross-linked polymer and low molecular fraction as a result of friction at the border of friction surface.

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DEVELOPMENT AND VALIDATION OF SAMPLING AND QUANTITATIVE DETERMINATION METHODS OF CARVEDILOL RESIDUES USING HIGH PERFORMANCE LIQUID CHROMATOGRAPHY FOR CLEANING VALIDATION

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Cleaning validation is a critical analytical responsibility of quality assurance system in pharmaceutical industry and ensures the efficiency of the cleaning routine procedure used in production which means that it effectively removes active pharmaceutical ingredient residues from the manufacturing equipment surfaces below a predetermined level and to prevent cross-contamination of next product.

The present study concerns to the development and validation of a simple, sensitive, rapid and effective HPLC method for quantitative determination of carvedilol residues in sample solutions obtained from pharmaceutical manufacturing equipment surfaces after manufacturing of finished product – Cardirate 25-Aversi (Carvedilol 25 mg) uncoated tablets. Cardirate 25-Aversi uncoated tablets were evaluated as „the worst case“ for cleaning procedure because active ingredient - carvedilol is practically insoluble water.

The surface was previously cleaned using disinfectant/ detergent and dried, and then it was successively wiped with one micro polyester swab moistened with selected diluent (sampling area 5 × 5 cm^2). The swab sampling procedure was developed in order to obtain a suitable recovery (> 90 %).

The HPLC method was developed using LC system “Ag 1260 Infinity” and Nucleosil C8 150 × 4.6 mm, 5 µm column with mobile phase - a mixture of phosphate buffer pH 2.5 and acetonitrile (50 : 50); The flow rate – 1.0 mL/min; The detector wavelength - 243 nm; The injection volume – 20 µL. The method was validated with respect to robustness, system suitability test, specificity, linearity-range, accuracy, precision (intra-day and inter day), limit of detection (LOD) and quantitation (LOQ).

The calibration curve is linear r^2=0.99996 over a concentration range 0.0075 – 60 µg/mL; LOD - 0.0015 µg/mL and LOQ - 0.0075 µg/mL; No interference from swab sample solution was observed and standard solution was stable within 21 days. The influence of swab material on determination of analyte was not observed; The main recovery of the method, the RSD of peak areas and retention times, the percentage difference, % between two different day determinations for precision study are within acceptable limits. The determined concentration of carvedilol residues in swab sample solutions varies 0.023 – 24.4 µg/mL which is below the calculated limit (62 µg/mL) of cross-contamination of next product.

Hence, the checked cleaning routine procedure provides sufficient removal of carvedilol residues and totally excludes the risk of cross-contamination of next product. The proposed developed and validated HPLC and swab sampling methods can be used to apply successfully for quantitative estimation of carvedilol residues for cleaning validation.

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NMS-O-22

REGARDING SOME STEPS OF E. FISCHER REACTION MECHANISM

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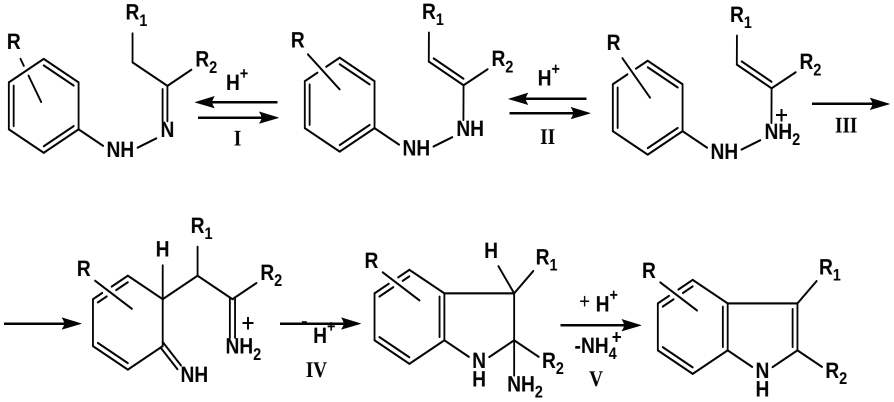
Among several known methods for synthesis of Indole rings, the most popular one is the classical reaction of E.Fischer Indolization reaction of Arylhydrazones in the presence of acid catalyst. Several articles regarding this mechanism are present, among them are synoptic articles. Nowadays accepted mechanism is the one shown on the scheme. For a while, one of the step in Fischer's reaction (III) – formation of new C-C bond was subject of discussion: To count it as [3,3'] sigmatropic rearrangement, as intermolecular nucleophilic reaction, as process where N-protonated N-hydrazine electrocyclic reaction goes through or as something else.



Authors of the article published in 2011, are confirming the argument regarding the importance of electric factors of this step. In particular, electron donors present in carbonyl fragment suspend the formation of indole ring [1]. Results of our observations are corresponding well with these data. Correspondence of optimal temperatures with the electronic nature of a substituent during the indolization of aryl hydrazones became clear. We conducted comparative analysis of these temperatures. We generalized literature and our experimental data [2, 3], as well as the results of quantum-chemical calculations.

In the report, obtained data, on an example of acetophenone derivatives ad some oxo compounds, is discussed. In particular, peculiarity of influence from groups R, R_1, and R_2.

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CHANGES OF LEARNING MOTIVATIONAL AND EMOTIONAL BEHAVIOR AND PASSIVE AVOIDANCE IN DEPRESSIVE RATS

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The aim of the paper is to study changes of motivational and emotional behavior and passive avoidance in depressive rats. It is well known that changes of some forms of motivational and emotional behaviour, learning and memory belong to disorders characteristic of depressive disease. In particular, this disease is characterized by depression of motivation and emotional processes and significant changes in declarative memory. However, existing results of observations in this regard are not unambiguous. This is why studying them in animals, which are considered models of the condition similar to depression, is of relevance and important.

The experiments were conducted on adult, white, wild rats (weight 200-250 g). The rats were chosen according to immobilization level using Porsolt test. Porsolt test implies the use of a special cylinder filled with water and the animal placed there cannot escape from the water. Each animal is placed twice into the cylinder. On the first day the observation lasts 15 minutes and on the second day, in 24 hours, 5 minutes. Healthy, so-called non-depressive animals while being in a Porsolt cylinder dedicate most of the time to swimming in the water and looking for a way to escape from the cylinder. Their immobilization level is low. Part of rats has a natural inclination to depression, which is evident when shortly after being placed in a Porsolt cylinder they give up because of a hopeless situation and spend most of the time hanging in the water. These rats have a high immobilization level and are called depressive rats. Our studies have been conducted on these two types of rats. The rats with a low immobilization level constituted a control group and the rats with high immobilization level, i.e. depressive rats, were an experimental group.

The changes of motivational and emotional behavior were studied with the use of an open field test. It was found out that there was a sharp depression of locomotion which manifested itself as significant decrease in the number of crossed squares. The quantitative indices of the parameters of vertical activity, standing up, lifting head, are also sharply decreased. Fear reaction in depressive rats is considerably increased, which manifests itself as decrease in entering in the open field centre and in grooming and sharp increase in defecation.

The changes of learning and memory were studied in the passive avoidance test, which is considered one of the focal points of declarative memory in animals.

It was shown that when placing the rats with a high immobilization level for the first time in the cylinder of passive avoidance, the latent period of entering from the light into dark section was sharply increased in them. It was found out that such animals have an impaired ability to evaluate a danger coming from the light area and this is why they do not hurry to escape from the dangerous area. The difference between depressive and non-depressive rats was maintained even after 24 hours from receiving a painful stimulation. In particular, the animals of control group remember that they have received a painful stimulation in a dark section and do not enter there, whereas the experimental animals still enter in the dark section, though with considerable delay, therefore, they do not learn passive avoidance.

The obtained results show that a horizontal and vertical locomotor activity and explorative behavior is impaired in so-called depressive rats with high immobilization level, fear emotion is increased in the open field, and learning and memory of one of the forms of the declarative memory, passive avoidance reaction, is impaired.

NMS-O-24

BIO BRIQUETTES POTENTIAL IN GERMANY

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Germany embraced a policy of de-carbonization in the late 90’s and has decided to establish itself as a role model for other countries. Additionally, Germany abolished nuclear energy in 2011 and will not allow for the replacement of existing plants - even though these two targets are hardly compatible. The country nevertheless started with an ambitious undertaking of firstly supplementing (and in the long run replacing) its energy production with renewable sources, and secondly reducing the energy consumption of heating, esp. in buildings. The total energy con-sumption for heating purposes in Germany amounts to appr. 5.000 PJ per year.

As in 2016, wood pellets are used in Germany as a minor source for renewable energy. Under the present circumstances, they are nearly exclusively used in private central heating systems, and (other than in the UK; Belgium or Netherlands) are not used for industrial purposes, esp. not for electricity production. This results in a yearly consumption of less than 2 million t, which are produced in Germany. However, the production potential is ten times as big.

There are two main reasons for wood pellets not being used more extensively: First, German consumers and legal regulation do not allow the use of binding agents in wood pellets intended for consumption in households. And second, this has led to wood pellets being produced in a very energy-intensive and therefore expensive way, using high temperatures and high pressure. The result are good-looking pellets that fall apart if they get into contact with water – nearly 20% are lost due to disintegration during transport.

NARALEX is a German Startup, using inventions made by Dr. Suren Nikoghosyan. The core is a binding agent, the NARALEX-polymeric that is made entirely from biological sources with no toxic or other negative impact on health or environment. The use of this binding agent allows for a pellet-production-process that needs much lower temperatures, lower pressure, no cooler, and therefore less energy. Additionally, the quality requirements regarding raw materials are lower and allow for cheaper material costs.

We expect to enter the German wood pellet market in the summer of 2017 and will act as a ma-chinery and polymeric provider for sawmills, who can produce at a much lower price with the NARALEX-system. Our aim is to significantly lower the price for wood pellets and allow for massive the use of wood pellets as a substitute for coal in electricity plants. This will be achieved by using Eastern European sawmill resources and Central European waste wood as raw materials. At this stage, NARALEX is the only method which can be used to produce wood pel-lets from waste wood.

The NARALEX-polymeric and the NARALEX-process can also be applied to other materials that need binding. We are investigating potentials in mining (coal dust) and building materials.

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NUMERICAL SIMULATION OF DISTRIBUTION OF ARSENIC DISCHARGED TO TSKHENISTSKALI AND LUKHUNI RIVERS FROM INDUSTRIAL WASTE

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Numerical simulation of distribution of arsenic discharged to Tskhenistskali and Lukhuni Rivers is elaborated using non–stationary linear three-dimensional equation of transition-diffusion of substances in continuous medium. Model is meant for study of distribution of polluting agents in mountain rivers in the first approximation. Tskhenistskali and Lukhuni Rivers are divided in eight and six conventionally uniform linear sections, respectively.

It is assumed that each of the river's section is a linear canal and river's hydrological parameters are constant along it. Therefore, in this sections the distribution of pollution may be described by transfer-diffusion equation according to [1]

$$\frac{\partial C_i}{\partial t} + u_i \frac{\partial C_i}{\partial x} + w_o \frac{\partial C_i}{\partial z} = \mu_x \frac{\partial^2 C_i}{\partial x^2} + \mu_y \frac{\partial^2 C_i}{\partial y^2} + \mu_z \frac{\partial^2 C_i}{\partial z^2}$$

where t is time; x, y, and z are the Cartesian coordinates; x axis is horizontally directed along the river flow; y is the horizontal axis directed perpendicularly to the canal; z axis is directed upward vertically from river bottom; u_i is the river's flow velocity at i section along x axis; river flow velocity is equal to zero along y axis; w_o is the velocity of sedimentation of polluting agent; μ_x , μ_y and μ_z are kinematic coefficients of turbulent viscosity along the x, y and z axes, respectively; C_i is the concentration of the contaminant in the i section of river. The river water velocity u_i in each river section is a known and constant value along the axis x, and changes along the y and z axes as follows: $u_i\,(x,y,z)=1.5U_{i,0} * \sin(\pi\, y/Y_i)\sin(0.5\pi\, z/H_i)$. $U_{i,0}$=const is the known value of the river water velocity in the i section. Y_i and H_i are the width and depth of the section i. $U_{i,0}$, Yi, Hi are taken from [2]. The initial concentration of the contaminant is obtained by the natural measurements. The numerical integration and solution of equation (1) is made using the split method and balance numerical scheme on the rectangle numerical grid.

Distribution of arsenic thrown to these rivers near the Uravi and Koruldashi villages is modeled using numerical experiments in case of stationary sources. Using the modeling there are determined the concentrations of arsenic in the rivers and mass amount of precipitated contaminant. It is shown that values of concentration received via mathematical modeling with permissible accuracy are coincided with data of field observations.

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NMS-O-26

THE MATHEMATICAL DESCRIPTION FOR RHENIUM ELECTRODEPOSITION OVER COMPLEX-FORMING CONDUCTING POLYMER

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Rhenium is one of the metals, used as the corrosion and thermically resistant material [1]. It is also used as a catalyst. Nevertheless, it is considered rare element with its unique natural mine disposed on the island of Iturup (also known as Etorofu, controlled by Russia and claimed by Japan), its compounds´ toxicity hasn´t been studied, so the development of electrochemical method of the remotion (recuperation) of rhenium is really actual task [2].

The development of the new metal remotion (recuperation) techniques involving electrodeposition may be difficulted by factors like

- Indefinite opinion in the deposition mechanism;
- Electrostatic, surface and(or) electrochemical effects, accompanying the synthesis;
- Electrochemical instabilities.

So, the aim of this work is to evaluate by mechanistic way the rhenium electrodeposition from the strongly acid solutions in the presence of complex-forming compounds.

It may be shown, that the behavior during rhenium electrodeposition from strongly acid solutions over the complex-forming compounds is more complicated, than in the case of their absence. The electrochemical instabilities may be caused not only by electrostatic repulsion between the anion and cathodes, but also by the interaction between the complex and the cathode and also will be dependent on the complex compound stability.

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UTILIZATION OF AGRO-INDUSTRIAL WASTE MATERIALS BY USING SEQUENTIAL SUPERCRITICAL FLUID AND ULTRASOUND EXTRACTION METHODS

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In recent years, there has been a growing interest in the so-called functional food additives. These ingredients are preferred by consumers to have a natural origin, being commonly extracted from natural sources such as plants or food by-product. Grape seeds and skin, orange and tangerine peel, tomato paste waste are the most abundant agro-industrial waste materials in Georgia. Extraction of natural food colorants and small scale high cost bioactive compounds from above mentioned waste materials is the main goal of our research.

The choice of the suitable technique for extraction of bioactive compounds from botanic matrix depends on: the desired class of compounds to be extracted, quality and yield required for extract; the process conditions and economic feasibility for scaling up the process.

Sequential supercritical Fluid extraction and ultrasound assisted extraction, the environmentally friendly separation techniques has been used for extraction of target products.

Supercritical fluid extraction is an advanced separation technique based on the enhanced solvating power of gases above their critical point. One of the most frequently used supercritical fluids is carbon dioxide. Besides the advantages of having a low critical temperature and being neither toxic nor flammable, carbon dioxide is also available at low cost and high purity; On account of these characteristics, the fluid is an ideal solvent for in the food dye, pharmaceutical and cosmetic industries, where it is essential to obtain final products of a high degree of purity.

Another modern technique we use is ultrasound-assisted extraction method. The application of ultrasound disrupts the cell wall structure and accelerates diffusion through membranes, allows cellular material release and improves mass transfer as well.

Ultrasound-assisted extraction is an upcoming extraction technique that can offer high reproducibility in shorter time, higher yields of bioactive compounds, simplified manipulation, decreased temperature during processing, reduced solvent consumption, and lower energy input.

Sequential, stepwise supercritical and ultrasound extraction methods makes available selective and quantitative extraction of oils, phenolics, carotenoids, lycopene, pentacyclic triterpenes and pectins from different botanic matrixes.

Selectivity, reproducibility was main challenge of our research. Thus, large range of pressure, temperature, extraction time and different solvent for sequential extraction of different class of compounds has been studded.

Essential oil, carotenoids, hesperidin and pectin has been extracted from tangerine and orange peel; quercetin and natural dyes from onion skin; lycopene and carotenoids from tomato peel, anthocyanins from “Saperavi” skin, phenolics and pentacyclic triterpenes from apple peel. Optimal extraction parameters and suitable extraction techniques have been selected for each target products. Main requirements were selectivity, reproducibility and feasibility for industrial means.

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NMS-O-28

ABOUT RADIOPROTECTIVE PROPERTIES OF SULFUR-ORGANIC COMPOUNDS

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Research of the protective effect of various compounds against the high-energy radiation is an important problem of the modern radiation chemistry and radiobiology. Regarded in that light the study of radiolytic behavior of sulfur compounds as potential radioprotectors is of a particular interest.

For this purpose in E. Nanobashvili Laboratory of Radiation Chemistry the systematic investigations are carried out to reveal the radioprotective properties of sulfur-organic compounds. In the presented paper the data of the study of the low-temperature radiolysis of various compounds – alkanethiols, alkylthiocyanates, dialkylsulfides and dialkyldisulfides in individual state and in binary mixtures with hydrocarbons and alcohols are presented. It was established that sulfur-containing functional group protects the hydrocarbon group of the molecule from radiation effect. In individual sulfur-organic compounds this effect is of intramolecular chatacter. In binary mixtures with alkanes and alcohols the efficient transfer of ionization and excitation energy from the solvent molecules to the molecules of sulfur acceptor takes place.

It has been shown that the effect of energy transfer depends on the nature of functional group as well as on the electron fraction of the acceptor.

The mechanism of the occurring processes is considered. The contribution of intra- and intermolecular ways of energy transfer in the processes of radiational-chemical transformation of above-mentioned systems is estimated.

OZONE IN AGRICULTURE

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Very powerful and strong oxidation capability of ozone has lately made it an element widely used in chemical, pharmaceutical and light industries as well as in medicine and agriculture – for the purposes of product storage and product disinfection during storage.

Various chemical agents are widely used to make seeds free from internal and external phytopathogenous micro flora before their sowing, to activate their natural processes and to protect plants during the process of their vegetation. However the positive effects of chemical agents have some negative impacts as well: environmental pollution caused by toxic chemicals and their accumulation in the soil and subsequently in the plants and their products.

Especially noteworthy is the fact that development of technologies that are based on using ozone is largely owed to ozone being environmentally friendly. Unlike other oxidants, reactions cause ozone to decompose into oxygen molecules and oxygen atoms. All these products are known as the agents neither participating in pollution nor producing the carcinogenic substances that are produced in the process of oxidation by chlorine or fluoride. Ozone only remains in the air for several minutes and in water - for 1.5-2 hours.

The purpose of the research was to study the influence of ozone on certain agricultural crops, in particular on cucumber and tomato seeds, for the purpose of accelerating their germination and achieving an increase in yields.

The influence of ozone on certain agricultural crops, in particular on cucumber and tomato seeds, has been studied for the purpose of accelerating their germination and achieving an increase in yields. Prospects for ozone treatment of seeds using ozonised water and ozone-air mixture have been established.

It was shown that the treatment of the seeds of some crops (cucumbers and tomatoes) causes an intensification of their germinability as expressed by the large area of plant leaves as well as by the great height.

Many countries throughout the world face the problem of and are in search of the ways for extension of storage life for food products, in particular, for perishable fruit and vegetables. Ozone is a particularly effective disinfectant which fights molds, bacteria, viruses, toxins and other contaminators in air and in water and helps to remove them from surfaces. Georgia faces the similar problem of treatment and extension of storage life for citrus fruit, especially for tangerines. The harvest season in Georgia lasts for 1-1.5 months.

The influence of ozone-air mixture on perishable fruit, in particular, on tangerines for the prupose of increase of their storage was studied. On each stage of experiment the time of exposure varied.

It was found that daily treatment of tangerines with ozone-air mixture flow for 60 minutes per day can extend their storage life to three months, and after ceasing the process of ozonation, the product maintains its quality for 3 weeks.

NMS-O-30

ABOUT ALGAE SPIRULINA'S ECOLOGICAL POTENTIAL FOR THEIR APPLICATION IN REMEDIATION TECHNOLOGIES

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Nowadays global chemical pollution of the biosphere tops the hazardous level.Succesfullyandecologicallyfriendlymethodofcleansingof environment is a phytoremediation – selectionandpurposefulplantingofthose plants, which roots provideto uptake andenzymestotransformthemoleculesof toxicants from environment.The establishment of possibilities of using algae in phytoremediation technologies for cleaning of chemically polluted water is very important in development of modern remediation technologies. The research interest to Spirulina as to potential phytoremediator is caused by following factors: During the aging the vacuoles of Spirulina cells are inflated with air bubbles and as a result they colonies are floated onto the water surface. Therefore, after remediation, Spirulina biomass will be easily separated (mechanically) from cleared water body.Spirulina is characterized by reproduction and fast biomass formation in extreme conditions (alkali area, high mineralization of medium, etc.) that are unfavorable for growing of most microorganisms.

The aim of presented work is estimation of remediation potential of blue-green algae Spirulina *(Spirulina platensis*) to different ecotoxicants: pesticide – DDT, 2,4,6-trinitrotoluene (TNT) and heavy metals – Cs and Cu.

The dynamics of organic pollutants and heavy metals assimilation by Spirulina have been studied. For this aim, alga was cultivated in toxicant-containing incubation medium and pollutant content was measured after various time intervals. According to the obtained results, the fastest uptake of DDT and TNT by Spirulina during first 5 minutes takes place. Thereafter, the rate of toxicant assimilation was suppressed. After 20 minutes from start of incubation, the intensity of uptake again was enhanced.

To study the ultrastructural distribution of toxicant was used TNT with labelled carbons[1-^{14}C] TNT.After 1 h of incubation, the radioactive carbon on internal membranes, vacuole membranes and in vacuoles was found. Also the enlargement of lamella cisterns takes place. After 2 hour expositionlabeled[1-^{14}C] TNT mainly in vacuoles, and particular in cellular matrix have been detected.According to the obtained results, penetration of TNT in Spirulina cells take place after 30 min, and thereafter the localization of toxicant on lamella membranes, vacuole membranes and in vacuoles take place. The uptake of TNT and/or its metabolites by Spirulina carried out via adsorption on surface of cellular hydrocarbons coat and then by moving into vacuoles and lamella cisterns.

It has been established that Spirulina has high ability to uptake and transform organic pollutants, also to absorb heavy metals. Thus, ecological potential of Spirulina will be the base of development of a new biotechnology for cleanup of waters polluted with organic pollutants and heavy metals.

Acknowledgements
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FUNDAMENTAL RESEARCH OF CHEMICAL COMPONENTS OF VEGETATION OF GEORGIAN FLORA

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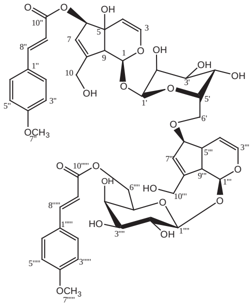
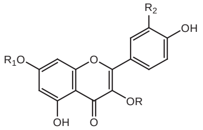
Vegetation of Georgia is known for its healing properties since ancient times. At present, special attention is given to the study of some species of the families: *Leguminosae*, *Scrophulariaceae*, *Urticaceae*, *Asteraceae* and *Geraniaceae*. 56 compounds were isolated by carrying out the basic researches on the chemical composition of species. 17 substances among them were structurally novel: 6′′′′-O-[6-O-(4′′-trans-p-methoxy-cinnamoyl-5-hydroxi-aucubigenin - (1→1′)-O-β-D-galactopyranosyl]-6′′′′-O-trans-p-methoxy -cinnamoyl-aucubin (laxoside) (*Verbascum laxum* Filar. et Jav.) [1]; flagalosides C, D (*Astragalus galegiformis* L.) [2]; falcosides C, D (*Astragalus falcatus* Lam.) [3]; pelargonidin-3-O-gluco-di-galactoside; pelargonidin – 3 – O - [(ξ-vanilyl-xylopyranosyl] - ξ - O -xylopyranoside; pelargonidin-3-O-xylopyranoside (*Urtica dioica* L.) [4]; micranthoside (+) 2*R*:3*R* and neomicranthoside (-) 2*S*:3*S* (*Eupatorium micranthum*) [5]; kaempferol-3-O-β-D-di-galacto-xyloside (pusilaside); 1-O-galloyl-3,6-hexahydroxidiphenyl-β-D-galactopyranoside (pusilagin I) (*Geranium pusillum* L.) [6].





Falcoside C - R = [β-Glcp-(1→ 3)-α–Rhap-(1→ 6)-β–Galp
R_1= Glcp
R_2= OH
Falcoside D - R = [β-Xylp-(1→ 3)-Rhap-(1→ 6)]-Galp
R_1= Rhap
R_2 = OCH_3
Flagaloside C - R= β-Galp-(6→ 1)-α-Rhap-(2→ 1)-Xylp
R_1= H
R_2= OCH_3
Flagaloside D- R= β-Xylp-(2→ 1)-β-Xylp
Pusilaside - R= β–Galp-ξ-β-Galp-ξ-β-Xylp
R_1= R_2= H

Laxoside

Structures of isolated compounds were established based on their physical, chemical and physical-chemical properties and spectral (^{1}H and ^{13}C NMR, HSQC, HMBC, COSY, DEPT, mass-spectroscopy) data.

The extracts containing above-mentioned compounds show interesting biological activities and have perspective for the use in medicine.

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NMS-P-02

SYNTHESIS, CHARACTERIZATION, PHOTOPHYSICAL AND ELECTROCHEMICAL PROPERTIES OF 4,4-DIFLUORO-8-(4′-BROMOPHENYL)-3,5-DIMETHYL-4-BORA-3A,4A-DIAZA-S-INDACENE (BODIPY)*

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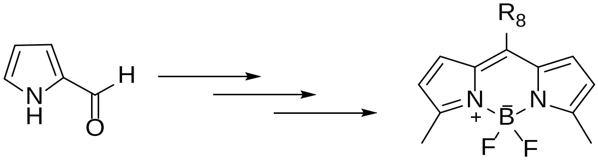
4,4-Difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY) dyes have attracted much attention due to the excellent applications in many areas such as fluorescent switches, supramolecular polymers, labelling reagents, chemosensors, photodynamic therapy, choromogenic probes, laser dyes, and sensitizers for solar cell applications. BODIPY dyes tend to be strongly UV-absorbing small molecules that emit relatively sharp fluorescence peaks with high quantum yields. These dyes are widely used to label proteins and DNA [1,2].

The meso position is the most sensitive to substituent effects because, upon excitation, an important variation in the electron density takes place at that site. From a strategic point of view, the meso position is arguably the most important because in the majority of the applications that have been devised for BODIPYs it is the position of choice for the attachment of the substrate to study [3].



In this study, 2-methyl-1H-pyrrole was prepared from the reaction of pyrrole-2-carboxaldehyde, hydrazine hydrate and KOH in ethylene glycol at 100 °C.

Different substituated 3,5-dimethyl BODIPY at mezo position was obtained from the reaction of 2-methyl-1H-pyrrole with different acyl clorides. Structures of these compounds were done by ^{1}H NMR, ^{13}C NMR, IR spectroscopies.

**This study was supported by TUBITAK (Scientific and Technological Research Council of Turkey) with project no 114Z176*

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NMS-P-03

SYNTHESIS AND RADIOPROTECTIVE PROPERTIES OF SOME 3,17-AMINOANDROSTALONES

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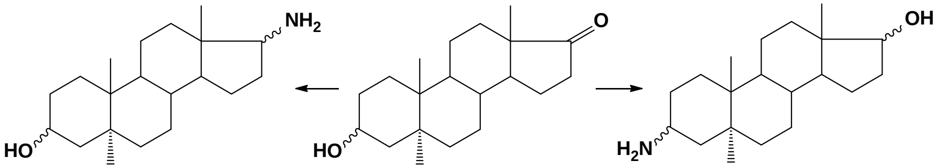
On the basis of epiandrosterone **1** and androsterone **2** several of 5α-aminoandrostanolones **3-10** epimeric at C-3 and C-17 have been synthesized and evaluated for radioprotective activity. Investigation of radioprotective properties of synthesized aminosteroids **3-10** showed that all epimers of 17-Amino-5α-androstan-3-ols 3-6 are inactive. Whereas, from the isomeric 3-amino-5α -androstan-17-ols 7-10, 3α, 17α-epimer **9** possesses a pronounced and 3α,17β-epimer **7** negligible activity.



3 - 6

1 - 2

7 - 10

3˙ 3β’17β
4˙ 3β’17α
5˙ 3α’17β
6˙ 3α’17α

1˙ 3β_OH
2˙ 3α OH

7˙ 3α’17β
8˙ 3β’17β
9˙ 3α’17α
10˙ 3β’17α

Radioprotective activity of compounds was evaluated on white not purebred mice males weighing 18-20 g, by a standard technique: sharp γ-radiation ^{137}Cs, power 171 rad/ min, a radiation dose – 875 rad (reference *drug is* Mexamine). The investigated compounds were entered in the form of 1% solution i.p. before 20 min to radiation. Efficiency of the compounds was determined by percent of animals survivors in a month after the influences of those. The results of radioprotective activity investigation of more active aminosteroids are summarized in Table.

Table. **Radioprotective activity of aminosteroids 7, 9**

Compound	Dose mg/kg (1/10 from LD_{50})	survival %**
Control*		0
7	14.4	0
9	18.1	25 ± 5^{a}
Mexamine	50	95 ± 2^{b}

* 0,9% NaCl; ** survival 30 hours after radiation; $^{a}p<0.05$, $^{b}p<0.001$

NMS-P-04

THE USE OF POLYCARBONATE FOR DRYING AGRICULTURAL PRODUCTS

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In agriculture, the widely used chemical materials are: a variety of glass, including polycarbonates, for drying agricultural products: fruit, vegetables, mushrooms, herbs, etc. By using these materials, the dried products are of better quality - the composition of biologically active substances and the organoleptic properties are better than the same product dried with natural drying in the open air.

Many of the properties possessed by polycarbonate, have been used in the agricultural and agrarian complex: high mechanical strength, frost and heat resistance (Polycarbonate can withstand extremes of temperature range from -50-60 C to + 100-120 C), strong wind, high degree of fire resistance and chemical resistance.

The proposed plants can dry different agricultural products as under direct sunlight, and without them. To this end, several options are available in the design. In solar dryer the air temperature is higher than in normal environment (in the sun) from about 10 to 35 degrees Celsius.

Fig. 1. The Convective solar dryer apparatus.

Conclusions

For the efficiency of the drying process of agricultural products is recommended to dry products in solar dryer with a polycarbonate coating. Studies have shown that the use of these systems are reducing the drying time, improves the preservation of flavor, nutrients and palatability, ensures the sterility of the product and facilitates storage of the dried product (it does not spoils and lasts longer than usual). Note that during storage the products that have been dried in solar dryer are more resistant to the mold and lasts longer than products that are dried naturally in the open air.

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ARTIFICIAL NEURAL NETWORK MODELING OF A NITRITE ENZYME-BASED ELECTROCHEMICAL BIOSENSOR

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During recent decades, environmental issues and public health concerns about the increasing concentration of nitrite in groundwater [1], rivers [2], and agricultural products [3] because of the overuse of nitrate fertilizers has led to numerous researches about nitrite sensing devices. Analytical biosensing techniques as of efficient and precise solution have been developed especially in measurement of ion concentrations in environmental and agricultural problems [4, 5]. In this study, the performance of an artificial intelligence modelling was evaluated in prediction of the nitrite concentration of samples having the cyclic voltammograms obtained by a nitrite enzyme-based electrochemical biosensor. To do this, artificial neural network (ANN) with Levenberg-Marquardt back propagation learning algorithm was used to learn electrochemical response of a nitrite biosensor developed by Quan and Shin [6]. According to them, an electrochemical nitrite biosensor was implemented based on co-immobilization of copper-containing nitrite reductase and viologen-modified chitosan on a glassy carbon electrode which the co-immobilized viologen-modified chitosan was used as a mediator in electron transfer between the working electrode and immobilized Cu-enzyme. To evaluate the performance of ANN machine learning method in proper and accurate prediction of nitrite concentration, electrochemical data of cyclic voltammograms of the biosensor in a potential range between -0.25 to -0.80 V (vs. Ag/AgCl) with 0.05 V/s sweep rate for different nitrite concentrations between 0 to 5 mM was used to train the ANNs with different architectures. The normalized mean squared error (MSE) values obtained for different ANN architectures is sown in Table 1. As shown in this table, the error parameter of train and test procedures was acceptable in general. The most proper performance belonged to 22-11-1 architecture with train and test normalized MSE values equal to 0.018 and 0.029, respectively. Results of this study show that machine learning methods can be used for prediction of nitrite concentrations of unknown samples by having their cyclic voltammograms with appropriate performance.

Table 1. Performance evaluation of different ANN architectures in prediction of nitrite concentration

ANN architecture	Train Normalized MSE	Test Normalized MSE
22-5-1	0.039	0.055
22-7-1	0.029	0.048
22-9-1	0.028	0.043
22-11-1	0.018	0.029
22-13-1	0.024	0.041
22-15-1	0.031	0.058

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NMS-P-06

INVESTIGATION OF POLY-COMPONENT SYSTEMS IN AIMS FOR SYNTHESIS OF A NEW GROUP OF INORGANIC POLYMERS-CONDENSED PHOSPHATES

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Very significant development of condensed crystal chemistry was due to the rapid progress of innovative methods of analysis, as well as to the evolution and achievements in inorganic polymer's chemistry. Double condensed phosphates – in fact inorganic polymers of poly- and monovalent metals have a various interesting properties, which explain numerous areas of their application. Several oligo-, cyclo- and poly-phosphates with diverse formula were obtained and described in chemical literature [1-7].

The offered data are the records of our studies – synthesis, analysis, examination of the experiments and their evaluation in correlation with achievements in inorganic polymer's chemistry [1-3, 8-10]. Condensed phosphates of polyvalent metals, notably double phosphates containing monovalent metals are obtained by us during systematic investigation o*f* --- systems at temperature range 100_-550where M^{I}- monovalent and M^{III} – Ga, In, Sc and partially Al. Molar ratio was variable: 15/2,5/1; 15/3,5/1; 15/5,0/1; 15/6,0/1; 15/7,5/1; 15/10,0/1. Many compounds were wholly examined by chemical analysis and the structures are determined by X-ray structural techniques [1-3, 8-11,12-14]. Some oligo-, poly and cyclophosphates are primarily synthesized and examined by us [8-12, 14-15]. These achievements are cited/examined in significant monographs of Prof. DURIF and Dr. Averbuch-Pouchot [2,4]. During our fundamental studies numerous (67) new formerly unknown condensed phosphates have been obtained. Dependency of compounds composition VS the temperature and the molar ratio, reliance of structure from duration of synthesis process are revealed.

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NMS-P-07

EVALUATION OF FERTILIZERS ON SOIL PROPERTY

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Compaction damages the physical properties and decreases soil porosity, aeration and infiltration rate by soil biota suffers. It also limits root development and plant growth by reducing water and nutrient uptake which decreases the yield. This research aims to study the effects the amounts of extra applied mineral fertilizers more than the recommended amounts on soil compaction, soil quality and crop yields. Soil compaction and soil penetration resistance was measured with electronic Penetrologger in 12 wheat plots at depth 0-30 cm (each plot is a treatment with 3 replications), and applies a randomized complete block design. Results indicate that the bulk density changed from 1.34 to 1.80 Mg.m^{-3}, penetration resistance changed from 0.89 to 3.54 MPa and permeability changed from 71 to 12 mm.h^{-1} in un compacted and highly compacted soil, respectively. Soil high compaction decreased permeability by 81.4%, the available water by 34% and crop yield by 40%.

Table.1 shows the variance analysis of soil compaction in order to compare the 12 plots on the basis of randomized complete block design. The results have been significant at ($P \leq 0.01$).

A result of soil analyses of physical properties (Table.1) shows bulk density of 1.34-1.80 Mg.m^{-3}and the mean aggregate diameter (M.W.D) changes from 1.43 mm in un-compacted soil (plot, P_2) to 0.28mm in highly compacted soil (plot, P_4). The aggregates diameter in un-compacted soil is 5 times greater than the highly compacted soil. The macro-aggregates are disintegrated into micro-aggregates, decreases the size and proportion. The total pore volume and porosity 17.4% is decreased which slows down water and air movement in soil. Previous studies revealed that the number of small pores decreases, and so does the amount of plant-available oxygen as a result, as soil density increases, total porosity decreased up to 17% in the severe compaction (Gupta, et al., 1989; Eden, et al., 2011; Rannik, 2009). These adverse effects may be due to restriction in root depth, where roots in compact soil are confined to macro pores, the rate at which they can extract water and nutrients from the soil between the macro pores may be considerably slowed (Jung, et al., 2008; Kaufmann et al., 2005), and reduction in nutrient uptake (Kuht and Reintam, 2004; Arvidsson, 1999). The latter may induce de-nitrification and slow nitrification (Lipec, et al., 1995; Elliot, 1986). Furthermore, the restriction may induce the roots to send hormonal signals that slow the growth of the shoot, even if they are able to take up adequate water and nutrients (Unger and Kaspar, 1994). The efficient management of soil proposes the correct utilization of agricultural practices to minimize the loss of structure, compaction, and nutrient losses in the soil, which are the main causes of its degradation.

Table.1 Results of the physical analysis of the studied soil in Pakdasht County (0-35cm depth)

Plot	Clay (%)	ρ_b (Mg.m^{-3})	M.W.D (mm)	Porosity (%)	Permeability (mm.h^{-1})	Available Water (%)
P_1	33	1.62	0.53	37.6	37	19
P_2	32	1.34	1.43	48.2	71	24
P_3	33	1.40	1.37	46.5	64	23
P_4	35	1.79	0.30	30.8	12	16
P_5	35	1.78	0.29	31.5	25	17
P_6	30	1.46	1.32	43.9	59	22
P_7	36	1.55	1.25	41.3	48	21
P_8	30	1.56	1.20	40.4	42	21
P_9	35	1.68	0.32	35.5	33	18
P_{10}	36	1.75	0.28	31.7	19	16
P_{11}	34	1.80	0.28	31.0	15	16
P_{12}	33	1.51	1.25	42.6	53	22

NMS-P-08

POPs MANAGEMENT ISSUES IN GEORGIA

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Environmental pollution is one of the major issues in Georgia. Among the problems, POPs pesticide is one of the important dangerous chemicals which cause acute risk on environment and human health.

Georgia has signed and ratified the Association Agreement with the EU. According to this Agreement, the parties shall develop and strengthen their cooperation on environmental issues, thereby contributing to the long-term objective of sustainable development. Policy objectives concerning management of chemicals, are included in the 2014 Association Agreement with the EU. Also, Georgia is a party to the Multilateral Environmental Agreements (MEAs) in the field of chemicals management.

The Ministry of Environment and Natural Resources Protection is responsible for the chemicals management planning. The responsibilities of the ministry include general chemicals management planning and elaboration of legislation. The Ministry of Environment and Natural Resources Protection is responsible to implement international obligations, mainly control and management of chemicals according to the Rotterdam Convention on the Prior Informed Consent Procedure for Certain Hazardous Chemicals and Pesticides in International Trade and Stockholm Convention on Persistent Organic Pollutants. Also, Georgia has signed The Minamata Convention on Mercury on October 10, 2013, but not ratified it yet.

In 1970, use of DDT was banned and to avoid further use of the chemicals, Soviet time government of Georgia decided to build a toxic waste polygon where DDT was taken. All other chlor-organic chemicals were banned in the later period. According the datas from Ministry of Agriculture, the owner of the Polygon at that time, the amount of the chemicals buried in Tranches and concrete pits where 2700t. Problem comes from the mismanagement and style of soviet planning system. In 2001 Georgia was one of the countries which signed the Stockholm convention on “Persistent Organic Pollutant” (POPs) and in 2007 it was ratified by Georgian Government.

In order to translate the Agreement into more specific actions, the Government adopted the 2014 National Action Plan for the Implementation of the Association Agreement. The National Action Plan for the Implementation of the Association Agreement presents a road map for development of legislation that is necessary for the implementation of EU directives that are relevant for chemicals management.

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CONTROL SYSTEMS ENGINEERING FOR ISOTOPE SEPARATION PROCESSES

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Georgia Holds a leading position in the world in production of high-tech products - stable isotopes of light elements, which are widely used in medicine, nuclear energy, microelectronics, chemical, and biological studies. Some may think it's a joke, but it's reality. Now National High technology Centre and partner companies produce isotope products as follows:
- Oxygen-18, enriched to 99% , 99.9% reached (the natural content is 0.204%), mainly in the form of water $H_2{}^{18}O$ and gaseous $^{18}O_2$.
- Oxygen-17 (the only manufacturer in the world of highly enriched product), enrichment of the 90 +%, reached 95%; (natural content is 0,037%), compounds: water $H_2{}^{17}O$, gaseous form $^{17}O_2$.
- Nitrogen-15 (practically the only manufacturer in the world), enrichment of 99% *, is achieved by 99.9% * (natural content is 0.365%), mainly compounds: ammonia $^{15}NH_3$, nitrogen oxides $^{15}NO_x$, ammonium $^{15}NH_4^+$ and nitrate $^{15}NO_3^-$ salts forms.
- Boron-10 (the only producer in the Post Soviet Countries), enriched to 98% * (natural content of 19.8%), in the forms of Boron trifluoride $^{10}BF_3$, boric acid $H_3{}^{10}BO_3$, Potassium tetrafluorborate $K^{10}BF_4$, elemental Boron ^{10}B - amorphous and crystalline various modifications, Boron carbide $^{10}B_4C$, Ferro Boron ^{10}FeB.
- Boron-11 (most of world production), enriched to 99.9% *, achieved 99.99% (80.2% natural content), e-purity Boron Trifluoride $^{11}BF_3$ form (available in the form of boron compounds mentioned above).
- Carbon-13, is currently being processed for the production of 99% isotopic enrichment (natural content of 1.07%) carbon monoxide ^{13}CO and carbamide $^{13}CO(NH_2)_2$.

Isotope separation high-tech processes require development and implementation of appropriate Control systems [1]. The computer control systems has been developed: Supervisory Control and Data Acquisition (SCADA) systems [2] based on Company GE Automation 90-30 Series programmable logic controllers (PLC) and PACSystemsTM Rx3i, Company Emerson Process Management / DeltaV controllers based Distributed control system (DCS) [3], Siemens Simatic PLC based control system. Some systems has been developed by cooperation of foreign companies, such as Swiss ENCO Engineering and CryoTec, but the major engineering company is the firm "semper" - the company's GE Automation (formerly GE Fanuc) service provider in the Caucasus region [4,5]. Control systems engineering based on GE Automation company hardware-software is characterized by a number of advantages compared with other firms, the company's policy is directed to engineering of open architecture control systems and to support of local forces engaging, for which provides the full support of the training of specialists, carrying out a full technical documentation and software needed.

Experience of control systems engineering for Isotope separation high-tech processes presents an important precedent for the development of modern control systems, even harder, than as isotope technologies. It is important that such a difficult engineering tasks to be solved by local specialists and the accumulated experience could be more widely used and extended to different sectors and scales of industry.

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QUANTITAVE DETERMINATION OF PHENOLIC COMPOUNDS IN WINES AND PARTS OF AUTOCHTHONOUS GEORGIAN RED GRAPES BY HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

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Grape and wine includes several hundreds of compounds identified from plants of *Vitis* family. These compounds belong to three general classes of natural compounds: phenols, isoprenoids and alkaloids. These compounds play an important role in pharmaceutical and food industry.

Phenols contribute to the characteristics of grape and wine. Color, taste, fragrance and antimicrobial activity of wine depend on the content of phenolic and allied compounds. The fruits (skin and seeds), stem and other parts of vine contain phenolic compounds.

The aim of the present work is to study qualitative and quantitative content of phenolic compounds in the grape bunch (stem, grape skin and seed) and wine of Georgian autochthonous vine variety Otskhanuri Safere by high-performance liquid chromatography.

A new reversed-phase high-performance liquid chromatography (HPLC) method was developed for separationand quantitative determination of phenolic compound sinvarious parts of red grapes and wines. Studied wines were produced based on traditional Georgian (Kakhuri) and European technologies. The phenolic compounds: gallic acid, protocatechuic acid, (+)-catechin, vanillic acid, coffeic acid, syringic acid, (-)-epicatechin, dihydroquercetin, rutin, o-coumaric acid, resveratrol, quercetin are determined quantitatively (mg/l) invarious parts of red grapes and wines. Seperationwas performed on a new ZORBAX Eclipse XDB-C18 reversed-phase column and water-acetonitrile gradient. The detection was performed by using UV-VIS detector.

Table 1. . Phenolic compounds in grape bunch and wine of vine variety Otskhanuri Safere

№	Phenolic compounds	Retention time (min)	Parts of grape bunch (mg/g dry weight)			Wine, Mg/L
			Stem	Skin	Seeds	
1	Gallic acid	5.057	0.259	0.0587	0.4753	12.53
2	Protocatechuic acid	8.855	nd	0.0725	0.0578	5.56
3	(+)-Catechin	12.965	0.2601	0.1370	0.1155	26.58
4	Vannilic acid	16.82	nd	nd	0.3265	nd
5	Caffeic acid	15.750	nd	0.2418	nd	1.29
6	Syringic acid	17.514	0.1092	1.9307	0.1503	3.02
7	(-)-Epicatechin	19.454	nd	1.362	nd	0.56
9	Dihydroquercetin	29.285	nd	0.0488	nd	0.76
10	Rutin	36.433	nd	nd	nd	nd
11	*o*-Coumaric acid	39.474	nd	0.0280	nd	nd
12	Resveratrol	47.683	0.0347	0.0432	nd	0.5
13	Quercetin	52.653	0.1169	0.8642	nd	5.67

Abbreviation: nd, not detected

ARSENIC-CONTAINING ORE PRODUCTION WASTE MONITORING IN SVANETI REGION OF GEORGIA

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Protection of the environment is one of the main indicators of the quality of life. Arsenic is found in nature as a chalcophile element –in the form of sulfides, thiosulfates, oxides, oxothiosalts, arsenides and arsenates [1]. The problem is the arsenic-containing wastes and the adjoining arable soils in Svaneti. Arsenic and its compounds are very toxic substances. Particularly urgent is this issue for such land-poor country as Georgia.

Ecotoxicology has its clearly defined task – to reveal the mechanisms of toxic impact of man-made factors on the environment and living organisms.

Arsenopyrite

Arsenopyrite “tails”

To study the wastes toxicity, the modern, international test methods – Toxicity Characteristic Leaching Procedure (TCLP) and Waste Extraction Test (WET) were used. According to the international standards, we can study arsenic solubility, form and toxicity level and spread has been established during 24 and 48 hours [2].

Arsenic and its compounds (arsenits and arsenates) are highly toxic substances and their carcinogenic properties are confirmed. In Georgia, Svaneti-Tsana arsenic deposit is in form of arsenopyrite. The implemented work represents a significant report for safety of Svaneti.

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NMS-P-12

INTEGRATED SYSTEM FOR DETECTION OF ACCIDENTAL EXPLOSIONS AND FIRES IN CHEMICAL PLANTS

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The development of contemporary detection systems is oriented to the creation of integrated systems ensuring monitoring of all possible threats that may endanger facilities to be protected as well as respective measures for threat prevention. Detection system shall meet the requirements of the Directive 94/9/EC on equipment and protective systems intended for use in potentially explosive atmospheres (ATEX).

G.Tsulukidze Mining Institute and CIPPS of University of Florida has designed wireless system for detection accidental explosions and fire in manufacturing sites. The system contain the following elements: a module of sensors for the identification of explosions, fires, smoke and methane; a module for the generation of an emergency signal; an emergency signal transmission module; an emergency signal receiving module, a power supply module.

The system provides the following 2 activities:

a) Sending the information to the security service. This information includes: Emergency level (emergency or pre-emergency conditions), type of threat (explosion or fire), place and time of the threat/accident;
b) Activation of automatic protective device.

This paper describes results of experimental investigations to identify and process information signals from different sources. The described works are necessary for designing the device integrated module of identification which is based on the constant monitoring on potential threat that may take place in manufacturing sites. The potential threats discussed in the paper are:

- Explosion, which identification is based on the monitoring of overpressure and methane concentration control in the media;
- Fire, which identification is based on the monitoring of flame and smoke parameters.

Results of tests of system show that potentially it can be used for identification of danger in 2.4 ms after excitation of a sensor of the detector and activation of protection device in 11 ms after the blast moment.

This research is sponsored by NATO in the framework of “Science for Peace and Security Programme” and ISTC.

THIOSEMICARBAZIDE DERIVATIVES IN STRIPPING VOLTAMMETRY IN THE DETERMINATION OF THE TOXIC METALS

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The study is focused on the electrochemical behavior of the toxic metals Cu(II), Pb(II), and Cd(II) ions in the presence of the thiosemicarbazides derivatives. Important effects of adsorption of the organic reagents and their metal complexes on the mercury dropping electrode are shown. An original method for evaluation of the stability constant of the adsorpted species has been proposed. It was demonstrated that the monosubstituted potassium phthalate (KHPh) in the system Cd(II) - 4-phenylthiosemicarbazde (4-FTSC) plays an important role not only for stabilization of pH, but it is also favorable for the formation and stabilization of the electroactive species. Introduction of the phenyl radical in the thiosemicarbazide molecule increases the sensitivity of the analytical signal and makes possible the determination of the cadmium content up to the nanomolar concentration.

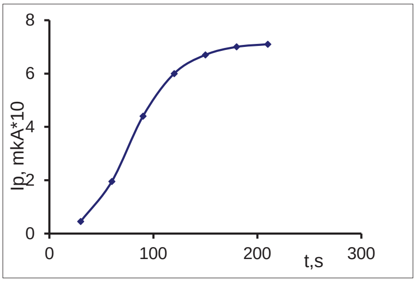

Fig.1. Dependence of peak current from the accumulation period of the complex on the electrode surface $4\cdot10^{-9}$ M Cd (II) + 0,04 M KHPh+$3\cdot10^{-3}$ M 4-FTSC , pH 4

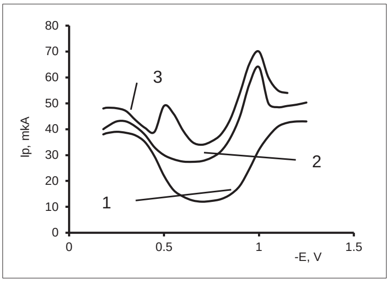

Fig.2. Voltammogramy complex in the presence of cadmium thiosemicarbazide diacetic acid :
1) 0,01M KCl + buffer pH 6
2) 1 + 5 • 10^{-5} M H_2TSCDAA 3) 2 + 6 • 10^{-6} M Cu (II)

Substitution of the sulfur atom by oxygen in the molecule of 8-quinolinaldehyde thiosemicarbazone changes the selectivity of the organic reagent. In the presence of 8-quinolinaldehyde semicarbazone, it is possible the selective determination of the lead, reducing 2-3 times the mass of the samples. Using the adsorptive accumulation on the electrode, a number of original methods for determination of the heavy metal in different systems have been developed. The 4-phenylthiosemicarbazide (4-FTSC) has been proposed for determination of the cadmium in river waters (fig.1), the thiosemicarbaziddiacetic acid (TSCDAA) and 8-quinolinaldehyde thiosemicarbazide – for copper determination in the river waters (fig.2), apple and tomato juices, 8-quinolinaldehyde semicarbazone - for determination of the lead in wheat flour and petrol. The metrological parameters of the proposed methods have been evaluated using standard additions, AAS spectrometry, and reference materials.

NMS-P-14

THE RESEARCH OF ECOLOGICAL STATE OF KAKHETI REGION PASTURES IN GEORGIA ON THE BASE OF ANIMAL HAIR STUDYING

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Contamination of environment with heavy metals is mainly caused by emissions of anthropogenic origin. High concentration of pollutants in the atmosphere, lithosphere is usually found in areas close to the pollution, but sometimes they move under the influence of wind and water through 100 and 1000 km, having impact on the biosphere and the global nature of the world [1]. Toxic heavy metals comprise a group of minerals having no known function in the body and are very harmful for plant, animal and human bodies. Our work is dedicated to the study of the heavy metals (copper, lead, zinc and cadmium) in animals hair of cow and sheep from mountain pastures located near the villages of the one of the regions in Eastern Georgia – Kakheti, namely in municipalities of Gurjaani, Akhmeta and Sagarejo. The hair can serve as good indicator for environmental pollution allowing simultaneous discussions on the concentration of toxic compounds in living organism as well as ecological quality of pastures. It should be noted that sample collection through cutting hair is absolutely harmless for animal and does not injure the animal, reducing the risk of possible contamination. Animal hair has undergone little studies, especially in Georgia. Animal hair samples were collected from approximately 20 sheep and 10 cows on pastures mentioned above. The investigations will be performed by differential-pulse polarographic method of analysis with a dropping mercury electrode by a three electrode cell system [2]. As revealed, each of the four investigated microelements reaches a sharp peak at certain very specific value of potential. The value of potential was taken towards the saturated calomel electrode potential. Polarographic curves show that of three investigated microelements (copper, lead and zinc) give a sharp peak at a certain very specific value of potential. As for cadmium, it has not been found in the sheep wool as well as of cow. On the basis of our investigations emerged in this region, toxic metal content in the hair of animals does not exceed the limits required by international standards, namely, content of thaws toxic metals are: lead – 0.00÷0.79 mg/kg, cadmium - 0.00÷0.03 mg/kg, cooper - 0.97÷5.44 mg/kg and zinc – 70.08÷297.43 mg/kg. As it appeared, the pastures are ecologically pure, consequently, in this region there is no need to plan of any works for cleaning of soil. The hair samples were collected in the period of pasturing in 2015-2016.

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NMS-P-15

THE STUDY OF THE IMMUNE CORRECTIVE PROPERTIES OF GREEK WALNUT (JUGLANS REGIA L.) SEPTA

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Today it is very actual searching of natural compounds including of plant origin with high immune correction capacity [1,2]. Special interest is directed to the walnut (Juglans regia L.) and its different parts, e.g. preparations prepared from plant's leaves and other parts have the ability to act against cancer. It should be noted that the positive therapeutic effects of extracts made from walnut septa are described in folk medicine for a wide range of diseases.

The goal of the presented work was study of the therapeutic properties of extract of walnut septa and investigation of its composition.

Materials and methods. Experiments were carried out on 120 white mice (25-27g). For the preparation of walnut septum extract, water is added on the walnut septa in a volume of 2/1 (water / walnut septa) and is boiled on a water bath until the evaporation of half the volume of water.

Liquid chromatographic (HPLC) analyses were carried out with a micro-column liquid chromatograph "Milichrom-4" (Nauchpribor, Oryiol, Russia) equipped with a UV absorption variable wavelength (190-360 nm) detector and syringe-type pump. The chromatographic column was a Silasorb C_{18}(5μm, Lachema, Brno, Czech Republic). Detection wavelengths were 240 and 280 nm. UV-vis absorption spectra were recorded in a UV-visible spectrophotometer Optizen POP using cells with 1 cm path length.

Results and discussion. An immune correcting property of aqueous extract from Greek walnut septa has been studied on experimental model of leukopenia in mice. It was determined that extract from Greek walnut has ability to correct the myelosuppression caused by cyclophosphamide injection in mice.

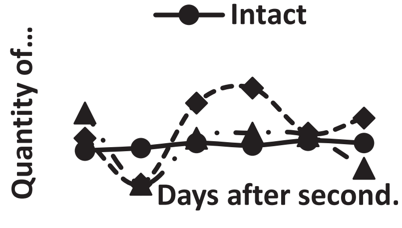

Fig.1 The Influence of walnut septa extract on quantitative changes of peripheral blood leukocytes after second injection of cyclophosphamide.

Comparative study of this feature was carried out after single and repeated injection of cyclophosphamide. Characterization of components of aqueous extract from Greek walnut septa was performed by cloud-point extraction and liquid chromatographic (HPLC) analyses.

Conclusions. It was found that walnut septum extract stimulates the division, differentiation and maturation of blast forms of myeloid as well as lymphoid lines in the bone marrow of mice with leukopenia. It was revealed that extract contain hydrophilic as well as the hydrophobic components.

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NMS-P-16

INFLUENCE OF ULTRASOUND ON SUPERCRITICAL FLUID EXTRACTION OF OILS FROM BOTANIC MATRIX

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In recent years, there has been an increasing interest in essential oils extracted from various herbs and agro-industrial waste materials. Over a long period of time essential oils were used as a food additives or fragrances. Newly discovered properties of essential oils include antibacterial, antifungal, antioxidant and anti-inflammatory activities. They are now widely used as natural insecticides, cosmceuticals, and aroma therapeutic agents.Essential oils have a complex composition, containing from a few dozen to several hundred constituents, especially hydrocarbons and oxygenated compounds. Different methods are used to separate these oils from the various plant materials. The composition of oil may vary to a large extent depending on the extraction method used. The steam distillation is a traditional technique for essential oils. Disadvantage of this method is thermal degradation, hydrolysis and solubility in water of some compounds that alter the flavor and fragrance profile of many essential oils extracted by this technique.

Supercritical fluid CO_2 extracts, are extremely pure plant extracts produced from a relatively new and highly efficient extraction process. CO_2 extraction produces superior herbal extracts that find wide use in the flavoring and herbal medicine industries. CO_2 extracts are oils similar to distilled essential oils that can be used in aromatherapy and natural perfumery to great benefit.

One of the main aspects that should be considered in SFE is the extraction optimization. The use of the optimum values for the different variables influencing the SFE extractions could significantly enhance the recovery of extraction yield of a target compound. On the one hand, the increasing of temperature results in the decrease of solvent density thus decreases the solubility and yield of oil. Increase of pressure increases density of CO_2, which induce complex extraction and difficult analysis. The ultrasound technique is based on the formation of ultrasonic waves of high frequency, which are capable of causing cavitations due to expansion and contraction cycles undergone by the material. Such cycles disrupt the cell walls of the vegetable matrix, favoring the penetration of the solvent and mass transfer, thus increasing the extract yield. Influence of ultrasound on supercritical fluid extractions of tea seed, grape seed, and orange and tangerine peel oil has been studded.

Based on the yield of extraction, the favorable conditions for supercritical fluid extraction grape and tea seed oils were: *T* at 60 °C, *P* at 250 atm. t at 4h. While ultrasound was applied as in USFE, the following parameters were preferred: *T* at 40 °C, *P* at 200 atm. t at 3.5 h. The results show that supercritical fluid extraction with the assistance of ultrasound could reduce the temperature, pressure, as well as time used in the process. Compared with SFE, USFE could give a 5% increase in the yield in case of grape seed and 7% for tea seeds. Ultrasound assisted subcritical fluid extraction method were applied as a first step in complex processing of tangerine and orange peel to recover essential oils. The yield of the oil increases up to 10%, but color becomes more intensive and composition more complex, which means that selectivity decreases.

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NMS-P-17

DEVELOPMENT OF RECIPE OF TOOTHPASTES CONTAINING MINERAL WATERS OF GEORGIA

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Nature of Georgia is rich in different resources – mineral waters, curative mud, some types of bentonite etc., which can be used in production of therapeutic and preventive cosmetic including recipes of toothpastes. Development on this topic using mineral waters “Lugela”, “Sairme” and mud “Akhtala” were held in Tbilisi State Medical University Iovel Kutateladze Institute of Pharmacochemistry.

Present report contains data on development of recipes of toothpastes with mineral waters “Plate” and “Zvare”. Because of its composition water “Plate” is the rarest among the mineral waters and has unique healing effect. The unique nature of water “Plate” is determined by its chemical and microbiological composition: 210 Ca^{2+}, 139,2 Mg^{2+}, 240 Na^{+}, 3,52 K^{+}, 0,13 Li^{+}, 1,2 Sr^{2+}, 0,5 Ba^{2+}, 1476 HCO_3^{-} ,236,8 Cl^{-}, 92 SO_4^{2-}; specific elements 68,57 SiO_2 (in sum), 5,837 H_3BO_3, 0,44 Mn^{2+} (in mg/l). Water “Zvare” is widely used with medical purposes due to its composition: 211,3 Ca^{2+}, 38,75 Mg^{2+}, 110,1 Na^{+}, 29,77 K^{+}, 0.115 Li^{+}, 10,35 Sr^{2+}, 0,11 Cu^{2+}, 1,41 Ba^{2+}, 880 Cl^{-} , 2482,7 HCO_3^{-}, 5,0 SO_4^{2-} , 5,1 NO_3^{-}; specific elements 0,63 I^{-}, 0,63 Fe^{2+}, 0,52 Mn^{2+} (in mg/l). Both waters when complementing each other have antibacterial, antifungal, anti-inflammatory effect; help to maintain stability of pH balance and oral flora.

The qualitative and quantitative composition of the pastes is chosen experimentally and is balanced on the basis of the following requirements: toothpaste has a preventative and healing effect on mouth organs and tissues, does not drip when applied to the surface of the tooth brush, makes good foam, has a soft texture and a pleasant taste and smell and is stable during storage. Let us consider the developed composition of the toothpaste.

Calcium carbonate produced by “Provençale” s.a. was used as an abrasive. Compared to the chalk, used earlier, precipitated chalk (size range of particles between 2-20 microns) reduces the volume of Radioactive Dentin Abrasion. Calcium carbonate is a natural product with a certain antiseptic activity and (in comparison with the gel toothpastes) a good cleaning capacity. Sodium carboxymethyl cellulose was used to stabilize the suspension (toothpaste). This made it possible to obtain thixotropic toothpaste with viscoplastic flow model. As a result it is possible to significantly vary the content of the abrasive filler in toothpaste. Sodium dodecyl sulfate is used as the foaming agent. During the experiments the content of the latter varied between 03-2,5% with the further determination of value of the foam number and stability of foam in order to find the optimal quantity.

According to international standards (ISO 11 609) the total number of microorganisms in a toothpaste will not exceed 10 colonies in a gram. Enterobacterias, pseudomonade, staphylococcus aurous, yeast fungus and molds are not allowed to be present in one gram of the toothpaste. The toothpaste will not contain microorganisms during two years from the release date and will not be a breeding ground for microorganisms. Given the above, sodium benzoate in a mixture with benzoic acid is used as preservative. Biologically active supplements imposed to the paste are comprised of a thick propolis extract and aloe dry extract. Such combination enables to achieve an antiseptic, antioxidant, antibacterial, antiviral effect, due to the presence of anthraquinones, flavonoids, coumarins, diterpenes, lignans, benzoic, caffeic and other acids.

Given data creates sufficient ground to conclude relatively high physicochemical, healing and consumer characteristics of the developed recipe of the toothpaste.

NMS-P-18

SOLVENT EFFECT ON COMPLEX FORMATION OF DIMETHYL SULFOXIDE

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With the quantum-chemical method AM1 are calculated the power, geometrical and structural features of dimethyl sulfoxide according to electronic structure, solvent effect on its complex formation ability with metals is established**.**

Coordination compounds of copper (II), cobalt (II) and nickel (II) with dimethyl sulfoxside. Copper (II), cobalt (II) and nickel (II) sulphates, nitrates, chlorides and bromides have been taken as initial salts. Synthesis has been carried out in ethanol solutions.

Synthesized coordination compounds are separated in solid form. Composition, individuality, solubility of obtained compounds in different solvents is established.

IR absorption spectra of synthesized coordination compounds are studied in order to establish the rule of coordination for dimethyl sulfoxide. Spectra are located in 400-4000 sm^{-1} range.

STUDYING THE CONTAMINATION WITH HEAVY METALS AND THE TOXICITY LEVEL OF ARABLE LANDS IN THE INDUSTRIAL REGION OF GEORGIA BOLNISI-KAZRETI USING MODERN TEST METHODS

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Our aim is to determine the contamination with heavy metals and the toxicity level, solubility, valence and acidity of Bolnisi-Kazreti arable lands, their forms and prevalence. The arable lands of Georgia's Kvemo Kartli industrial region Bolnisi-Kazreti (Madneuli Copper-Gold Mine), which are generally irrigated by the River Mashavera, have been studied. The waste water of the above-mentioned mine is discharged into the lands. In spite of the fact that the enterprise is engaged in the water treatment, an average level of contamination with heavy metals is still being observed. The copper tenfold exceeding the MCL is dominant. The constantly accumulating and soluble forms of heavy metals are fixed in soil by the TCLP and WET standard methods.

The soil non-irrigation (spring) and heavy irrigation (summer) periods have been studied and compared. The spectral and atomic absorption analysis methods have been used in the study. The currently established ecological monitoring system will, hopefully, further improve the existing situation. The content of heavy metals in the grass does not exceed the MCL, indicating that they are generally present in the soil in the insoluble form. An increased amount of calcium in soil leads to the accumulation of metals therein, resulting gradually in the contamination and infertility of soil. [1, 2].

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NMS-P-20

WASTEWATER TREATMENT FROM PHENOLIC COMPOUNDS BY MEANS OF AOPs

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Effective and environmentally safe advanced oxidation (AOPs) processes was used for removing toxic and stable in environmental conditions phenolic compounds from wastewaters. Oxidation and mineralization of phenol compounds existing in water solution were executed by influencing of hydroxyl ($^{\bullet}OH$) radicals which were obtained in electro-fenton (EF) and photo-electro-fenton (PEF) processes.

The electro-generation of necessary hydrogen peroxide was executed by means of oxygen (air) electro-reduction at cathode in the original filter-press type electrochemical reactor. Modern electrode materials were used, in particular as the cathode: carbon-containing gas-diffusion electrode - GDE (Black Pearls 2000, Vulcan XC-72 BASF, Co. USA), as a dimensionally stable anode -DSA (Ti-RuO_2-IrO_2, South Korea). To separate cathodic and anodic sections, cation-selective membranes (MK-40, Russia and Nafion 117, USA) were used. During photo-electro-fenton process as an ultraviolet light source, a lamp (UVC, $\lambda = 253$ nm, China) was used. Control of the process of mineralization of phenolic compounds was executed by analytical methods of determinations of values of chemical oxygen demand – COD.

The innovation of the work is the compact and easy in operation electrochemical cell for the on-site electro-generation of H_2O_2 and for treatment of the wastewater from the organic compounds by means of the AOP process [1].

By using special devices (fig.1) and EF, PEF methods, it was executed purification of model solutions of phenol (C_6H_5OH), p-nitrophenol ($C_6H_5NO_2$) and m-aminophenol ($C_6H_5NH_2$). It has been reached their highly effective decomposition according of COD.

Fig. 1. Devices used in EF and PEF processes

It was defined that on the gas-diffusion cathode there was electric generation of H_2O_2 current efficiency from 95% to 100%. It was ascertained that PEF processes were more advantageous than EF processes. According PEF method, during the processing, within 60 min the reduction degrees of COD of the 100 mg/l of starting content, were: for phenol - 97%, for p-nitrophenol - 95.7%, for m-aminophenol - 96.7%.

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NMS-P-21

THE STUDY OF SOME PROPERTIES OF PAPAIN CONTAINING GELS

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For the treatment of burn, necrotic and purulent wounds proteolytic enzymatic preparations of plant and microbial origin: caripazym, lekozym, iruksol and others are successfully used [1].

The present work belongs to development of new drug form of papain containing gels, to study of rheological properties of these gels, why such a basis to ensure optimal resorption and stability of the active substances were chosen.

For of the basis, glycerol, methylcellulose (MC-25) and mixture polyethylene glycols (PEG-1500 and PEG-3000) were selected [2].

It has been established the optimal ratio of content of the papain containing gels prepared on these high molecular basis and their rheological properties on different temperatures have been studied.

Results of researches showed, that the proteolytic activity of gels on the base of polyethylene glycol are stable within 6 months, but the same proteolytic activity of the gels based on methylcellulose are decreased in 15-20% during this period. Rheological researches also determined, that the gels on the base of polyethylene glycol are stable against technological procedures [3].

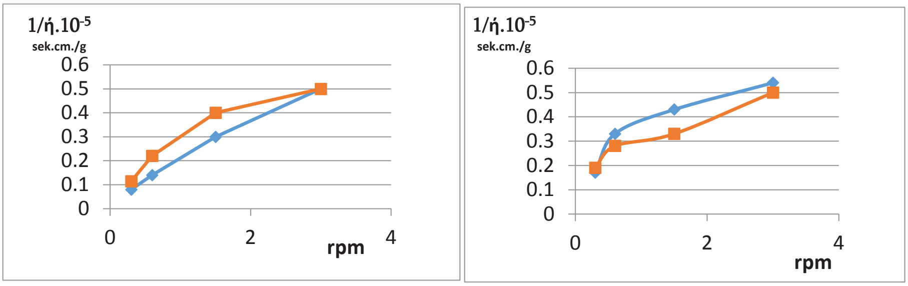

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Figure 1 and 2. The rheological curves of PEG-basis and PEG-papain at 22 ^{0}C.

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NMS-P-22

COMPARATIVE STUDY OF SOME PHYSICO-CHEMICAL PROPERTIES OF FRUIT BROMELAIN AND STEM BROMELAIN FROM ANANAS COMOSUS FOR DEVELOPMENT OF THE METHODS OF STANDARTIZATION

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In recent years, have been revealed anticancer chemotherapeutic drugs, the complexes of endo-proteases – bromelain from the stem and bromelain from the fruit, obtained from pineapple plant (*Ananas comusus*). The influence of the preparations on the tumor cells cultures *in vitro* and on the tumor formations *in vivo* are intensively studied [1] and their clinical researches are in progress. Lately, using the nanotechnology were studied anticancer effect in high concentrations of bromelain on tumor formations [2].

With development of effective drug form, the standardization of bromelain is also very important. The present work includes the initial studies of standardization of the fruit bromelain and stem bromelain and the comparative characterization of their physical-chemical properties.

An optimal concentration of cysteine at determination of proteolytic activity of fruit and stem bromelain is 0,01-0,02 mol/l. Speed of casein lysis by fruit and stem bromelain in its concentration from 0.5% to 2% is unchanged. From 5 to 20 minutes the speed of casein lysis is directly proportional to the time. The speed of casein lysis by fruit and stem bromelain was found to be directly proportional to the enzyme concentration within 0.05 g / L to 0.25 g / l (see. Fig. 1).

The pH- dependence in both cases is similar. Optimal pH for stem bromelain is at 7.5, for fruit bromelain- at 8.0 (see. Fig. 2). Optimal temperature in both cases ranges from 50^{0}C to 60^{0}C.

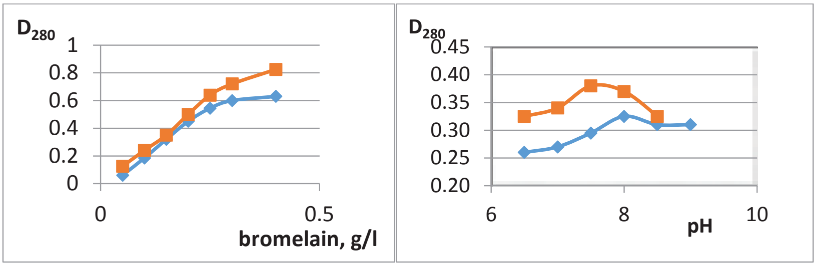

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Fig. 1 and 2. The effect of concentration of fruit bromelain and stem bromelain and pH on speed of casein lysis.

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INFLUENCE OF THE NATURE OF SOLVENT ON THE POLAROGRAPHIC BEHAVIOUR OF PIROMELLITIC ACID

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The aim of our investigation is piromellitic acid, which belongs to the class of organic compounds known as tetracarboxylic acids containing exactly four carboxyl groups in position of 1,2,4,5. Benzenepolicarboxylic acids are widely used in medicine and pharmacochemistry, namely, these are necessary components to synthesize bloodmaintenance substances for orthopedic and stomatological materials. Piromellitic acid is characterized by its anti-tumor activity [1]. Consequently, it is very interesting to study the adsorption of those acids in double electrical layer, especially for pharmacochemistry.

In our previous paper [2], it was investigated adsorption of piromellitic acid from 0.5M $NaClO_4$ aqueous solutions by measuring the differential capacity (C) as a function of electrode potential (E) by means of a.c. bridge.

Now, the aim of our investigation is study of kinetical behaviour of piromellitic acid by the polarographic method in wide ranges of concentrations ($10^{-5} \div 4.8x10^{-2}$ M) in water as well as in diatomic alcohol- ethylene glycol (EG). For polarographic study we selected the supporting electrolyte (0.5 M $NaClO_4$ in ethylene glycol), which makes possible the operation in wide potential region (0 ÷ -2 V). All potential values were measured with respect to saturated calomel electrode. The constant solution temperature (20^0C) was maintained by water thermostat.

As polarographic curves showed that in these two solvents the substance behaves differently: two waves of the curve is observed in aqueous solutions ($E_{1/2}$=-1,1V, $E_{1/2}$=-1,86 V), whereas it gives one wave in EG ($E_{1/2}$=-1,32 V). The process of discharge of piromellitic acid in EG is difficult due to the higher viscosity of EG as compared to the water. In both solvents the height of wave is directly proportional to the concentration of piromellitic acid.

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NMS-P-24

THE CLEANING SEWAGE OF MADNEULI BY SORPTION METHOD

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The study the possibility of cleaning the sewage of Madneuli mining and processing enterprise on sorbents with nonferrous metals' ions (Cu^{2+}, Zn^{2+}, Fe_{common}, Pb^{2+}) - natural diatomite, clinoptilolite, Askan-clay , coals (Georgia) and their modified forms was carried out. The chemical composition of wastewater was studied too.

The sorption properties of natural and modified sorbents with a different mineral composition, and the factors, influencing on the sorption of Cu^{2+} (S:F, pH, mixing time, concentration of Cu^{2+}) were researched.

It was estimated that the modification of natural diatomites and zeolites with calcium oxide significantly extend their cleaning degree of solutions from these ions.

A higher adsorption capacity with respect to the ions Cu^{2+}, Zn^{2+}, Fe_{common}, Pb^{2+}) are characterized for the modified forms of zeolite and diatomite. The purification degree of above-mentioned ions reaches 95-99%.

The optimal condition of wastewater treatment of Madneuli mining and processing plant is to use adsorbents – modified diatomite and clinoptilolite. The sorbent is in contact with the sewage due to intensive blending.

The study allowed establishing the optimal conditions for sorption and offers more effective sorbent for the extraction of copper ions from waste water Madneuli mining and processing plant.

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ADSORPTION OF TETRABUTYLAMMONIUM IODIDE AT THE MERCURY ELECTRODE FROM ETHYLENE GLYCOL SOLUTIONS

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The ionic liquids – melts of organic salts, being in the liquid state in a wide temperature range find extensive practical application at the present time. Ionic liquids are composed of bulky organic cations and inorganic anions. The most important characteristics determining the prospects of the use of ionic liquids in electrochemistry should be the ionic conductivity, the hydrophobicity and the width of the electrochemical "window". The width of electrochemical "window", the electrochemical stability of the ionic liquids (border "window" match the beginning and the end of the electrochemical decomposition of these ions) determine the potential range available for carrying out electrochemical transitions that do not affect the solvent. Ionic liquids have not only the catalytic activity but also in some cases are able to maintain and enhance the biological activity of biosensor. They are widely used in the field of electrochemical analysis in medicine, food industry, etc. All these make ionic liquids attractive to many areas of science and technology. Quaternary ammonium salts, in particular tetrabutylammonium iodide (TBA-I) also refer to ionic liquids. The data on adsorbability of TBA-I on mercury from ethylene glycol (EG) solutions is given in this paper. Tetrabutylammonium iodide - quaternary ammonium salt - $(C_4H_9)_4NI$ contains a volumetric organic cation of TBA-I and an inorganic iodide anion. TBA-I is slightly soluble in water (hydrophobic). TBA-I refers to ionic liquids by its structure and properties, this causes the interest of studying of its adsorbability from the EG solutions.

Based on experimental data of the dependence of the differential capacitance (C) on the electrode potential (E) C, E-curves have been constructed. C, E-curves have the shape characteristic for solutions containing small amounts of neutral organic compounds. Indeed, in minimum of C, E-curves, with increasing concentration of added TBA-I, capacitance decreases respectively reaching values 6 μFcm^{-2}, which indicates significant adsorptivity of TBA-I from EG solutions. Cathode desorption peaks appear when negative electrode polarization was increased. Comparing obtained results with the data of aqueous solutions, we conclude that the adsorbability of TBA-I from the EG is less than from water. It can be assumed that TBA-I is in ionic and molecular forms as in aqueous as well as in the EG solutions. At low concentrations, TBA-I is preferably in the ionic form. Attraction of these cations occurs in the electric double layer by specifically adsorbed anions of supporting electrolyte. After certain TBA-I concentrations, at very low electrode potentials (-1.6V) (those which with increasing concentration of added substance are shifted to the cathodic side), on C, E-curves appear characteristic for the adsorption of neutral organic substances cathodic desorption peaks, height of which increases with the concentration of organic substances.

On the basis of the experimentally obtained dependence of the differential capacitance on the electrode potential (C, E-curves) adsorption parameters (degree of coverage of the electrode by organic substance, the amount of interaction between the adsorbed molecules, the constant of adsorption equilibrium, adsorption energy, etc.) were calculated which show the strong adsorption ability of the studied compounds in this system.

NMS-P-26

BIOCHEMICAL STUDY OF LEAVES FROM GLEDITSCHIA (L.GLEDITSCHIA); A PLANT SPREAD IN GEORGIA

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The goal of our work is biochemical research of leaves and fruit parts of Gledichia (L. Gleditschia) spread in Georgia.

The height of Gledichia tree is 20m, sometimes it even reaches 40m. The stem bark of a tree is dark gray, (more black). Branches are dark gray. It is honey plant. Gledichia is spread naturally in the north of the United States. There are 7 cultivated species of Gledichia which are represented in many countries. North American conventional Gledichia with precious wood (Gleditsia triacanthos) is cultivated in gardens and parks of Crimea, the Caucasus (including Georgia) and Central Asia. Mostly, Gledichia is spread in the eastern part of Georgia. It is also found in Kakheti region.

According literature, there are sum of alkaloids in different parts of Gledichia: leaves, flowers, seeds. Therefore we tried to study the influence of environmental factors and seasonality on quantitative content of alkaloids in various parts of young Gleduchias from Tbilisi botanical garden and Chokhatauri.

Our previous studies suggest that alkaloids are distributed in various parts of young Gledichia from botanical garden and Chokhatauri as follows: in the month of May, the young leaves contain 0.89% alkaloids, while leaves collected in July, contain alkaloids only in trace quantities. As for the other parts of a plant, the flowers contain 0,32% and seeds contain 0,03% of total alkaloids.

Phyto-chemical studies of Gledichia (Gledischia triacanthos) growing in Georgia had been carried out for the first time by Prof. A. Gakhokidze in early 50’s of the last century. He extracted substances of flavonoid nature: akramerin and olmelin from the plant. He also was the first to obtain them by synthetic way.

3 glycoside, 1 epikatekin - olmelin $C_{21}H_{24}O_{11}$, fustin $C_{15}H_{12}O_6$, fizetin $C_{15}H_{10}O_6$; Saponins were found in the fruit of Gledichia, specifically in seeds liberated from husk. 2.6% anthraglycosides, 3.1% tannins are extracted form fruit husk. The existence of the vitamin K is confirmed. 26% sugars are in the meaty parts of fruits.

THE BIOSPHERE AND PLANT CHEMICAL POLLUTION

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Development of industry and transport and intensified chemicalization of agriculture is accompanied by systematic environmental pollution. Pollutants in the biosphere undergo various chemical conversions: they interact with each other, are photochemically oxidized, polymerized, etc. Incidentally, new highly toxic substances (the so-called "secondary pollutants") are often produced. The "longevity" of a chemical pollutant in the biosphere depends on the chemical nature of this substance, on its reactivity as well as on the conditions of the environment. Together with nutrients plants absorb compounds polluting the biosphere. The toxic gases contained in the air mainly absorbed through leaves.

In order to become incorporated into the total metabolism of the plant cell the foreign substance should be dissolved in water or fat, i.e. in the very medium in which biochemical reactions usual occur.

Detoxication of organic pollutants in plants may occur in three ways, one being the release of the organic substances absorbed by plants in an unaltered form. The substances absorbed by leaves is excreted by the root system and vice versa, the toxicant absorbed by roots is released through leaves. Binging of foreign organic substances with endogenous compounds of the cells in another pathway of detoxication in plants. To these processes belong e.g. reactions of glycosylation of foreign substances with the participation of the donors of hydrocarbon residues uridinediphoglucose or uridinediphogalactose, the reactions, of combination of organic xenobiotics with amino acids, peptides, proteins, etc. The resulting conjugates are localized in the vacuoles. The third pathway of detoxication of organic xenobiotics consists in their intense oxidation. Here, the molecule of xenobiotics undergoes hydroxylation, decarboxylation, deamination dealkylation, β-oxidation and other conversions, ultimately leading to total degradation. As a result the endogenous metabolites of the cell are produced from the molecule of xenobiotics.

Plants possess varied stability to exposure to the chemical pollutants of the biosphere. Their capacity to absorb and detoxicate foreign substances differs as well. Data on plant stability to various types of atmospheric pollution as well as a list of plants capable of absorbing hydrocarbons in larger quantities from the atmosphere are presented in the appendixes.

NMS-P-28

OBTAINING AND RESEARCH OF HERBAL BIOLOGICALLY ACTIVE COMPOUNDS

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Synthesized medical preparations together with efficiency displays a number of contraindications to the human health. Therefore, the number of preparations received from the natural plant materials in the nomenclature of the medical means is growing. The elaboration of extraction methods of biologically active compounds from the natural plant materials is important as well as research of chemical composition of medical compounds isolated from approved medicative herbs used in traditional medicine and extraction of selected biologically active compounds. In Georgia, there are a number of herbaceous medicinal plants approved in folk medicine. Extraction of therapeutic compounds by means of modern ecologically safe technologies from these plants is prospective. Some of them are intensively used in the manufacture of medicines [1,2].

Extraction of herbal compounds with antimicrobial activity is especially interesting for filling up the small nomenclature of medical means and for elaboration the new drugs. At the same time obtaining compounds with antiviral and other actions is interesting. Selection of local plants, which have a various biological activity (according preliminary data) will promote it. Obtaining of active compounds against pneumonia and malaria from herbs approved in traditional medicine will be carried out for the first time. Study of biologically active compounds of herbaceous plants with a high content of chlorophyll nettle *Urtica* and fern *Polypodiophyta* is also interesting. Chlorophyll as an antioxidant created by the nature affects not only on a specific organ, but also on the whole body, activates cellular respiration, gives strength and energy to the human body [3]. Chemical identification, determination of structure and, in case of necessity chemical modification for improvement of function of extracted and selected active principles will be carried out. The expected results are characterized by high reliability, as the chosen herbs within the years are successfully used in traditional medicine.

Application of various herbal plants for obtaining biologically active origins is planned: nettle *Urtica* and fern *Polypodiophyta* (chlorophyll containing), Common Knotgrass Polygonum *aviculare* (against pneumonia) and - Goldmoss Stonecrop Sedum *acre (*against malaria).

Extraction of active origins by original technology of stimulated natural sedimentation from grasses is widely used in folk medicine. Elaborated method ensures high yield and obtaining natural compounds in native forms. Tests of narrow fractions of received extracts for antimicrobial and antibacterial activity will be carried out. Chemical compositions of selected narrow fractions will be studied on modern GC/MS, also by means of other equipments. Importance of the work is remarkable for Georgia, and also for other developing countries. Thus, presented work will promote combined application of herbaceous plants for improving human health by safe medical means and is prospective for further commercial manufacture of safe biodegradable modern preparations.

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LOOKING FOR HIGHEST SELECTIVITY OF ENANTIOSEPARATIONS IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

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Separation selectivity makes the major contribution to the peak resolution in high-performance liquid chromatography [1, 2]. Therefore, it is preferable to operate with selectivity in order to improve the final result of chromatographic separation. At the same time improving enantioselectivity means to interfere with the thermodynamics of the separation process that is very challenging approach.

The separation of enantiomers of chiral sulphoxides was studied on 4 different polysaccharide-based chiral columns in high-performance liquid chromatography with 2-propanol and the mixture of n-hexane and 2-propanol as mobile phases.

In order to achieve the highest enantioselectivity one should optimize the structure of substance, chiral selector, mobile phase and the separation temperature. In the present study 2-(benzylsulfinyl) N-methyl benzamide, 3-(benzylsulfinyl) N-methyl benzamide, 4-(Benzylsulfinyl) N-methyl benzamide, 2-(4-nitrobenzylsulfinyl) N-methyl benzamide, 2-(4-trifluoromethylbenzylsulfinyl) N-methyl benzamide, 3-(benzylsulfinyl) benzamide and 2-(benzylsulfinyl) benzamide were used as chiral analytes. 4 cellulose-based chiral selectors, in particular, cellulose tris(3,4-dimethylphenylcarbamate), cellulose tris (3,4-dichlorophenylcarbamate), cellulose tris(3-chloro-4-methylphenylcarbamate) and cellulose tris(4-chloro-3-methylphenylcarbamate) were applied. As the mobile phase 2-propanol and the mixture of n-hexane and 2-propanol were used. The separations were performed at 25^0C, 15^0C and 5^0C.

The highest enantioselectivity ever reported in chiral HPLC (α=780) was obtained under following optimized conditions: Chiral analyte - 2-(benzylsulphinyl) benzamide, chiral selector - cellulose tris(4-chloro-3-methylphenylcarbamate), mobile phase – n-hexane/2-propanol-70/30 volume by volume and the separation temperature 5^oC.

Acknowledgments

Shota Rustaveli Georgian National Science Foundation (GNSF) and Georgian Research and Development Foundation (GRDF) are acknowledged for a partial financial support to this project.

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NMS-P-30

POSSIBILITY OF OBTAINING LUMINOPHOR FROM OIL-PIPELINE PRECIPITATE DEPOSITS

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Luminescence defectoscopy is based on the ability of a luminescent test solution – penetrant (solution of luminophore in the organic solvent) to penetrate unnoticeable surface defects (1µm) and then lighting in the UV radiation area to display their character and location.

Synthetic luminophores used in luminescent defectoscopy have high luminescent properties but at the same time are expensive and toxic.

The aim of the Project is to improve worked out by us simple technology to release high effective non-toxic luminophor from natural raw material and reduce it to the licensing condition.

Luminophore obtained by the offered technology has high operational properties. In particular, it has an ability to detect **microcracks less than 1** µm**;** luminescence intensity in relation to the standard - uranil nitrate is 450-500%, colour factor is greenish-yellow; the product is cheap, high adhesive and stable that corresponds to the International Standards.

The suggested technology is based on the use of local inexpensive raw material. In comparison with the prototypes it excludes two power-consuming steps, therefore the technological process becomes simple and the firs cost of the production lessens.

The use of the suggested luminophore is prospective in biology, medicine, analytical chemistry, criminalistics, poligraphy manufacture of luminescent dye and others.

Luminophore obtained by our technology is unique due to a simple way of its reception. This way is to combine chosen purposely some oil fractions and further express distillation in deep vacuum. At the same time it does not need additional cleaning.

The mentioned **luminophore is used to detect microcracks less than 1** µm in parts of a machine, metal constructions, concrete, glass, plastic, etc.

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IMPREGNATED NANO ZERO-VALENT IRON FOR DEGRADATION OF CHLORINATED ORGANIC

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The ecological situation requires effective wastewater treatment systems, especially in the mining and metal processing enterprises, tanneries, agriculture, household and other areas. It is particularly important to clean drinking water from organic pollutants. Known, that the chlorination of water causes obtaining of C-Cl bond-containing compounds, which eventually fall into the water-supply system.

It is estbalished, that on the intermediate stage of degradation of 2,5-dichloroaniline, phenol will be obtained, 1,4-dichlorobenzol is decomposed in a 3 h.

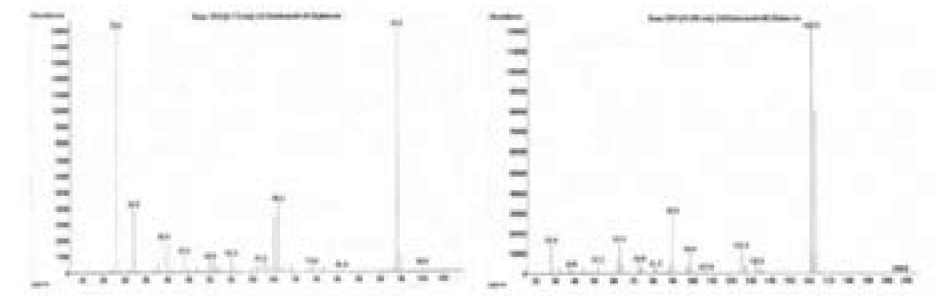

Fig. 1. GC/MS of initial 2,6 dichloranilin and after decomposition with Nano zero-valent iron.

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NMS-P-32

MIXED-LIGAND COORDINATION COMPOUNDS OF 3d-METALS WITH ORTO-AMINO-4,5-METHILPYRIDINE AND ISONYCOTINOILHIDRAZONE OF PARA-DIMETHILAMINOBENZALDEHIDE

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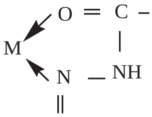
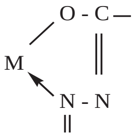
Calculation are made using quantum-chemical, semi-empirical AM1 method in different solutions in order to study the property of complex formation of para-dimethylaminobenzaldehyde isonicotinoil-hydrazone, as well as ortho-amino-4,5 methylpyridine molecules and to study their electronic structure. Water, acetone, methanol, ethanol, dimethyl sulfoxide, chloroform, hexane are selected as solvents. Molecule formation heat, value of total energy, dipole moment, ionization potential, valence angles between atoms and bond lengths, effective charges, atomic orbitals filling with electrons etc. are calculated in all cases. Oxygen atom of carbonyl group and nitrogen atom of azomethine group are manifested as donor atoms in hydrazone molecule. As to molecules of methyl derivatives of aminopyridine, according to calculation results a nitrogen atom of heterocycle is manifested as donor atom.





Manganese (II) cobalt (II), nickel (II) and copper (II) chlorides, nitrates and sulfates are taken as initial substances for synthesis of different-ligand coordination compounds with ortho-amino-4 and ortho-amino-5 methyl pyridines and with para-dimethylaminobenzaldehyde isonicotinoilhydrazones. 15 new coordination compounds are received in solid state. Their composition is determined using elemental analysis, while individuality is defined via determination of melting temperature. Some physical-chemical properties are studies, namely: solubility in different inorganic and organic solvents

Infrared spectra ($400\text{-}4000^{-1}$ cm range) of synthesized complex compounds absorption are studied. Rule of organic ligands, water molecules and acido ligands coordination in synthesized compounds is established. Study of infrared spectra of coordination compounds' absorption shows that hydrazone coordinates with complex-former metal via oxygen atom of carbonyl group and nitrogen atom of azomethine group, while methyl pyridine molecules coordinate via nitrogen atoms of heterocycle that testifies the data of quantum-chemical calculations.

Presumable structure of synthesized complex compounds are offered on the basis of quantum-chemical, absorption infrared spectroscopy and X-ray diffraction data.

INNOVATIVE APPROACH TO RECYCLING OF SHOCK-PROOFED TIRE-CASING

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Storage and burial of shock-proofed tires and all kind of rubber waste are economically ineffective and ecologically hazardous. During long-term storage the secondary wastes can emit toxic agents to atmosphere that will disturb the ecological balance. At the same time, shock-proofed tires experience insufficient changes in the moment of expiration of service life. That in its turn creates an opportunity of attainment of big economical effect during its secondary processing [1-3].

Scientific-engineering center "Utilization" of Georgian Technical University has developed the pyrolysis method of processing of shock-proofed tires, wherein tires under temperature influence decompose into solid, liquid and gaseous products that takes place at 300°C [4].

It is shown in the work that processing of shock-proofed tires is two-way profitable: first, it protects the nature from contamination and second, there are produced useful products, such as "stove" fuel, carbon as the component of mastic for bitumen production, and gas, which is used as heating agent for returning back to production [5].

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NMS-P-34

TRAVERTINE ART

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There are many specimens of cultural heritage carved in the mountains. The irreversible processes of nature make it difficult to maintain these unique cultural monuments – the combination of natural and human creativity. The mountains of any consistency are subject to damage and collapse, thus conserving the mountainous monuments is vital. It's necessary to provide constant supervision of monuments carved in the mountains and contributein their vitality via innovative conservative-restoration methods.

We studied effects of mineral-thermal waters on the environment. The waters are located within 10 km radius from the world cultural heritage monument of the XI-XII centuries carved in the mountains – Vardzia. Thermogravimetric and X-ray study of specimens from different bore deposits were conducted and their chemicalcompositions were obtained. The results revealed that 30—82% of deposits are calcium carbonates –major component of mineral travertine.

Table 1. X-ray fluorescence analysis on element content of several-micron thickness layer of samples collected at different distances from water bore, %

	Different locations from water outlet							
Elements	1	2	3	4	5	6	7	8
Al	0,299	0,132	0,421	0,192	0,00	0,258	0,14	0,158
Si	11,185	3,427	10,545	4,129	3,363	5,687	2,016	1,575
P	0,00	0,18	0,237	0,204	0,189	0,2	0,143	0,153
S	0,083	0,096	0,225	0,11	0,042	0,058	0,059	0,108
Cl	11,581	10,095	7,572	17,354	8,626	7,283	11,131	8,68
K	2,053	0,00	1,466	0,541	0,187	0,634	0,00	0,00
Ca	32,794	27,4	12,02	30,136	28,851	19,34	29,357	26,522
Fe	0,627	0,495	4,575	0,426	0,345	0,704	0,722	0,207
Zr	0,199	0,142	0,025	0,189	0,169	0,066	0,066	0,109
Cd	0,096	0,131	0,1	0,082	0,083	0,112	0,102	0,116
Sn	0,023	0,038	0,029	0,022	0,02	0,029	0,028	0,033
Sb	0,04	0,063	0,045	0,036	0,034	0,052	0,049	0,055
$CaCO_3$	81,73	68,20	29,35	75,00	72,00	48,20	73,20	66,00

The above mentioned research has contributed to the attempt of developing new, conservative-restoration methods of the monument carved in the mountains. The method intends to form rocks under natural conditions by accumulation of mineral water carbonates on weathered rocks serving as crystalization centers.

The presentation aims at introducing the research results to the public at large, stirring interest and fund raising to further continue research in this direction.

NMS-P-35

THE ELECTROLYTIC DISSOCIATION OF METHYL DERIVATIVES OF SUCCINIC ACID

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Succinic acid and its various derivatives are widely used in the organic synthesis and polymer industry, participate in the biologically important Krebs cycle. In this work an analysis of the regularities of the electrolytic dissociation of methylsuccinic, DL-1,2-dimethylsuccinic and meso-1,2-dimethylsuccinic acids in their dilute (0.0001-0.01M) solutions was carried out with the aid of a new method of determination the dissociation parameters of weak multibasic organic acids with the "overlapping" equilibria previously described by authors. Values of the usual and "partial" degrees of dissociation, the concentrations of all anions, hydrogen ions and undissociated acid molecules, the activity coefficients of all charged dissociation products were calculated. Together with the accurate equations were also suggested the simple empirical equations for fast approximate determination of the various dissociation parameters.

The law of dilution for both dissociation steps of these processes may be expressed as follows:

$$\mathrm{K}_1 = \frac{c(\alpha_1^2 - \alpha_2^2)}{1-\alpha_1} F_1 = \frac{c\alpha_1^2[1-(\alpha_2^{'})^2]}{1-\alpha_1} F_1 \qquad (1)$$

$$\mathrm{K}_2 = \frac{c\alpha_2(\alpha_1 + \alpha_2)}{\alpha_1 - \alpha_2} F_2 = \frac{c\alpha_1\alpha_2^{'}(1+\alpha_2^{'})}{1-\alpha_2^{'}} F_2 \qquad (2)$$

where α_1 and α_2 are the usual degrees of dissociation of first and second steps, $\alpha_2^{'}$ is the "partial" degree of dissociation of second step, c is the total concentration of acid, K_1 and K_2 are the thermodynamic dissociation constants of both steps, F_1 and F_2 are the quotients of the activity coefficients. The values of the latters were approximated by the Debye-Huckel equation.

The degrees of dissociation α_1, α_2 and $\alpha_2^{'}$ were evaluated successively by iterative solution of following quadratic equations:

$$\alpha_1 = \frac{1}{2}\left[-\frac{K_1}{cF_1} + \sqrt{\left(\frac{K_1}{cF_1}\right)^2 + 4\left(\alpha_2^2 + \frac{K_1}{cF_1}\right)}\right] \qquad (3)$$

$$\alpha_2 = \frac{1}{2}\left[-\left(\frac{K_2}{cF_2} + \alpha_1\right) + \sqrt{\left(\frac{K_2}{cF_2} + \alpha_1\right)^2 + \frac{4K_2\alpha_1}{cF_2}}\right] \qquad (4)$$

$$\alpha_2^{'} = \frac{1}{2}\left[-\left(1 + \frac{K_2}{\alpha_1 cF_2}\right) + \sqrt{\left(1 + \frac{K_2}{\alpha_1 cF_2}\right)^2 + \frac{4K_2}{\alpha_1 cF_2}}\right] \qquad (5)$$

NMS-P-36

FATTY ACID COMPOSITION OF SEED OIL OF *EUONYMUS VERRUCOSUS* L. GROWING IN GEORGIA

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Eunymus verrucosus scop is a common plant of mountainous and forest regions of Georgia. In order to find the euonymus growth sites, it was conducted reconnaissance investigation of the Tsiv-Gomborsogo ridge in 2013-2015**.** The survey confirmed that euonymus is widespread plant with diverse blooming crown**.** However, its chemical composition is less studied and filling the gaps in this field is of certain interest.

The subject of study was oil samples of seeds air-dry of euonymus, growing at Tsiv-Gombori mountain. The oil was obtained by an exhaustive extraction method with hexane in Soxhlet extractor. The oil yield was in the range of 46.39 -58.80 % (seeds were absolutely dry). Physical and chemical parameters determined by standard methods are the following: density, g/cm^3 - 0.9689; refractive index - 1.465, an acid number, mg KOH/g - 25.89, iodine number, I_2 %- 29.97, peroxide value, % 0.1.

Fatty acid composition of oil was determined by the methodology of GOST 31 663-2012 [1,2], by interesterification of triglycerides of fatty acids to methyl esters of fatty acids with the follow-up analysis by a gas chromatograph Agilent 7890A.

Fatty acid composition of *Euonymus verrucosus* L. seed oil

Fatty acid name	Fatty acid index	Fatty acid content (% of total acids)
Lauric	12:0	0.02
Myristic	14:0	0.34
Palmitic	16:0	18.70
Hexadecanoic	16:1	0.68
Palmitoleic	16 :1 9 cis	1.21
Margaric	17: 0	0.12
Stearic	18 :0	3.66
Oleic	18 :1 9 cis	36.84
Iso-octadecadienic	18: 2 i	0.03
Linolic	18 :2	33.13
γ -linolenic	18:3 ω-6	0.08
α -linolenic	18:3 ω-3G	5.08
Gondoinic	20 :1	0.11

The results show that triglycerides of palmitic-, oleic-, linoleic-, linolenic- and stearic acids are the main components of seed oils of *Eunymus verrucosus* growing in Georgia. Triglycerides of lauric-, myristic-, hexadecenoic-, margarine-, iso-octadecadienic-, gondoinic- and palmitoleic acids present in seeds in insignificant amounts.

It is notable the high content of unsaturated fatty acids in the test subjects ensuring high stability and great value of oil.

References:

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OPTICAL SEMICONDUCTOR AMPLIFIER IN COMMUNICATION

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Information security and safe exchange of information is one of the major concerns of the current society. Secure information network is ensured with the use of quantum-mechanical systems and is expected to become the main means of ensuring information security in the near future.

As the optical signal is transferred over long distance through optical fiber, it weakens to the limit that photo detectors cannot detect it. That is why optical amplifiers are incorporated between the data source and receiver. 1.30 to 1.50 μm electromagnetic wavelength amplifiers are required to arrange optical communication, but there are no individual elements or binary connections that would be commercially justifiable and emitting light in the range of 1.30-1.50 μm.

Therefore, a need has evolved for the development of high technologies in order to produce Nano-materials. Nano-materials suitable for the named application are group III and IV semiconductors (InP, InGaAsP). This work covers technologies for the production of optical semiconductor amplifiers and also includes study of their properties.

INNOVATIVE FORMULATIONS OF MEANS OF PLANTS PROTECTION BY USE OF LOCAL RAW MATERIALS

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The new compositional formulations have been developed for integrated protect plants from pests. Compositions of preparations contain approved, tested and efficient components as formulations that are adapted to the local conditions.

The turpentine oil obtained from the pine pitch as an additive to the main active substance synthetic pyrethroid is used in the formulation of insecto-acaricidal preparation “Antisept”. On its basis in a new composition of the formulation together with acquired repellent properties the insecto-acaricidal activity had been increased. That was revealed in prolonged impact on the pests from 15-18 days up to 22-25 days. Prolonged activity of preparation is covering the duration of pests development cycle and the low concentration of active substance is sufficient for pests destruction. Consequently, the preparation “Antisept” with a small content of pyrethroid and a low ecological load has the same effectiveness as the expensive imported insecto-acaricidal means.

Fungicide preparation “Antifungal” was prepared based on hydro and zinc dihydrogen phosphate. It was developed due to strict ecological requirements to the food products for replacement the fungicides containing heavy metal - copper. Water soluble hydro- and dihydrogen phosphates are obtained by interaction of orthophosphoric acid (40-50 % Mass. on P_2O_5) with zinc oxide (10-15% mas.) at 25^0C. That hydro- and dihydrogen phosphates have no any acute and chronic toxicity, local irritant activities and cumulative properties. Prolonged action of preparation on the skin and mucous do not cause local and general allergic reaction has not any mutagenic activity. Preparation does not cause corrosion of metals. The fungicidal activity of the environmentally safe “Antifungal” according to the conducted field tests is almost the same as effectiveness of the Bordeaux mixture with the average level of the toxicity.

“Proinsect”, the preparation against winterers of pests is the concentrated water-oil emulsion with high content of oil phase (up to 80 %). Paraffinic oil is used as an oil phase. Obtaining of a stable suspension with water is guaranteed by the content of two Surface active agents - hydrophilic and organophilic. Preparation is dissolved in water (1:50 ratio) and obtained working fluid contains high content of oil that determines the reliable prolonged fixation of the preparation on the plants, even in case of rain. By the effectiveness of “Proinsect” has a best indicator of than it’s their foreign counterparts. For the originality of recipe preparation “Proinsect” we received a patent for an invention - P 5346.

Silicon-containing humic preparation “Si-humat” is prepared on the base of humic acids isolated from local brown coal (Akhaltsikhe) that were treated with potassium hydroxide. In the condition of mechanic and chemical interaction of humics and finely dispersed diatomites humic compound enriched by the active silicon is obtained. The preparation, on the basis of conducted field tests, increases the strength and sustainability of plant leaves and young shoots against various diseases and pests. High content of silicon in preparation determines important increase of plant stability towards the biotic stress (pests, fungal and viral diseases) as well as increases sustainability towards the abiotic stress (drought, high and low temperatures).

It should be noted that the developed compositions (together with the maintenance and improvement of efficiency) are significantly cheaper (20%) and are customized to the local market requirements. Preparations had been tested during 3 years in field conditions with the positive results for protection of vine, peach and other plant cultures from various pests (Lobenzia botrana, Grapholita molesta, mites, greenflies).

POLYMERIC COMPOSITIONS ON THE BASIS OF POLYMERIC ACID AND BENTONITE

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Polymeric hydro gels (PHs) are of practical interest because of the possibilities of their usage in many fields of science and industry to solve various problems. PHs can be used in medicine as medical compounds; for division and adsorption of ions of different metals; in ecology for purification of sewage from different organic and inorganic impurities; for obtaining of sensors. The base of PHs in most cases is synthetic polymers, distraction of which in natural conditions is difficult which is their weakness from the ecology point of view. By this reason, construction of absorbents on the base of biodegradated materials and decreasing in their composition the content of synthetic polymers is one of the important tasks. Obtaining of compositions on the basis of cross-linking polymers by introductions in their composition of different natural materials is one of possible ways to solve this problem. By this reason polymer - bentonite compositions are of special interest. The choice of bentonite clay (BC) as component for polymeric compositions is determined by its high hydrophility, low toxicity, ecological safety; good adsorption ability and also its accessibility and low cost. These properties of BC's have allowed to consider it as the most perspective materials for obtaining of composites. Authors of [1] have shown that BC particles have attached to gels some new physical-chemical properties and also improved their mechanical properties.

In these investigations, some peculiarities of obtaining of composition hydro gels (CHs) on the basis of cross-linked polyacrylic acid (PAAc) and bentonite clay (BC) were investigated. Methods of optical microscopy and rentgenography have shown that, in CHs, destruction of crystallic structure of montmorillonit occurs due to the penetration of polymeric macromolecules in between bundle layers as a result of which CHs have a uniform homogeneous structure. The kinetics of swelling of the obtained CHs in water was investigated and it was shown that they have a high sorption ability to water in wide interval of pH. Sorption of metilenic blue (MB) by gels from water solutions was investigated by static method. It was determined that sorption ability of CHs was higher than by hydro gels on the basis of PAAc. Sorption of MB has increased with increasing temperature of medium and consequently the bonding of MB by CHs has carried out owing to chemosorption.

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NMS-P-40

PHYSICAL-CHEMICAL PROPERTIES OF MACROMOLECULAR SUBSTANCES ISOLATED FROM NATURAL WATERS

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Macromolecular substances (humin and fulvic acids) are active participants of physicochemical processes proceeding in natural waters [1, 2]. Investigation of regularity of their spreading in hydrosphere is the actual matter of environment chemistry. Physical-chemical properties of humin and fulvic acids isolated from natural waters were studied by us.

For isolation of fulvic and humin acids, we concentrated the surface waters by the frozen method. Filtered water samples were acidified to pH 2 and was put for 2 hours on water bath at 60^0 C, for coagulation of humin acids. Then the solution was centrifuged for 10 min at 8000 rpm. For isolation of fulvic acids from centrifuge the adsorption-chromatographic method was used [2]. The charcoal was used as a sorbent. Desorption of amino acids and carbohydrates was performed by means of 0.1N HCl. For the desorption of polyphenols the 90% acetone water solution was used. The elution of fulvic acids fraction was performed with 0.1 N NaOH solution Obtained alkalic solution of fulvic acids for the purification were passed through a cation-exchanger and were dried under the vacuum until the constant masses were obtained.

For purification, isolated humin acids were dissolved in 0,1 M NaOH, then humin acids were reprecipated. The purification procedure was repeated four times. Purified humin acids were washed with bidistillated water until the negative reaction on the Cl^- ions, then humin acids were dried under the vacuum until the constant masses were obtained. Obtained humin and fulvic acids were used as standards for the photometric determination,elemental analyse and determination of acid-base pro The concentration of fulvic acids in surface waters of Georgia changes from 0.3 mg/l to 4.5mg/l and at the average it is ten times higher than the concentration of humin acids.

The elemental composition ranges of humin and fulvic acids are **C**: 50,4-52,8%; H: 3,8-5,9%; N:2,8-5,5%; O:37,0-42,7% and C:48,7-54,2%; H:4,3-5,2%; N:1,7-2,4%; O:38,8-45,1% respectively.

We have studied acid-base properties of humin and fulvic acids using potentiometric titration methods. It has been established that pK(COOH) at the average for humin acids equals to 4,12±0,10, for fulvic acids equals to 4,19 ±0,10. pK(phen.-OH) at the average for humin acids equals to 10,52±0,20 (for fulvic acids equals to 10,46±0,20. Obtained datas should be taken into consideration at different pH, during calculation stability constants of geopolymers with heavy metals.

The work was done by support of CRDF Global, Shota Rustaveli National Science Foundation (SRNSF) and Georgian Research and Development Foundation (GRDF)

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INVESTIGATION OF COMPLEX FORMATION PROCESS OF CADMIUM WITH GEOPOLYMERS (FULVIC ACIDS)

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Fulvic acids are one of the first geopolymers, which were found in natural waters. They have functional groups and that is why they take an active place in complex formation and sorption processes and stipulate migration forms of toxic metals.

In spite of researches, experimental datas on stability constants of complex compounds of fulvic acids are heterogeneous and they differ in several lines from each other [1,2]. This condition is stipulated by the ionization degree and also by the changes of the value of pH in complex formation process, by the ignoring of average molecular weights of their associates, which finally causes the wrong result.

Our objective was to obtain pure samples of fulvic acids, to study complex formation process between cadmium and fulvic acids of pH 9,0 ; 8,0; 6,0; 5,0 by the gel chromotographic method and calculation of the conditional stability constants.

Taking into consideration an average molecular weight of fulvic acids at various pH, for the optimal determination we used sephadex G-25(the limits of Fractionating100–5000).

The main solution of fulvic complexes were obtained by the solubility method. Cd(OH)2–FA-H_2O, pH=8, $\mu = 0.01(KNO_3)$. The obtained main solutions of fulvic complexes are devided into 4 parts,which differs from each other,only with the values of pH (9,02; 8,00; 6,03; 5,01) .The complex formation process of fulvic complexes were studied on various pH by the gel filtration method. We took 2-2ml aliquots of solutions with various pH,put it one the top of the gelchromotographic column,we did the eluation process with the bidilstilate which has the same pH as the solution.

If we take into consideration the datas of gelfiltration , we determined The quantity of metals connected with the fulvic acids,in such fractions which releasing volumes fits the substances with molecular weight 300≤ Mw>5000.

On the basis of experimental datas was calculated the stability constants of fulvic complexes by the (1) equation :

$$\beta = [\sum_{Me} - C`_{Me}]/\{[C`_{Me}][FA]\} = [C``_{Me}]/\{[C`_{Me}][FA^{2-}]\} \quad (1)$$

$$C`_{Me} = \sum_{Me} - C``_{Me} \quad (2)$$

$$[FA] = C_{FA} - C``_{Me} \quad (3)$$

where $C`_{Me}$ the quantity of metal which was not involved in the complex in mol/L, $\sum_{Me}$ – The total quantity of metal in main solution. mol/L $C``_{Me}$ – The amount of metal, connected with fulvic acids (determined fractions 300≤ Mw>500 mol/L [FA]–free ligand mol/L; C_{FA} –the total quantity in the system mol/L). pH=9: lgβ =4,17;pH=8 :lgβ= 3,77 pH 6: lg β= 3,66; pH 5: lgβ= 3,06

We can successfully use The obtained datas for evaluation the role of geopolymer in complex formation processess of all types, groups and class of natural waters.

The work was done by supporting the World Federation of Scientists and the World Laboratory.

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NMS-P-42

REFLECTION OF THE RESULTS OF RESEARCHES CARRIED OUT IN CHEMISTRY AND CHEMICAL TECHNOLOGIES IN SCIENTIFIC PERIODICALS OF GEORGIA

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As a result of bibliomertric analysis of the printed and electronic scientific periodicals reflected in the Georgian Abstracts Journal (GAJ), the publication activity of researchers according to sciences has been identified. In this respect, the sphere of chemistry and applied chemistry occupies one of the leading positions. Publications in chemistry and applied chemistry are placed in the columns of both pure chemical sciences as well as of the neighboring sectors and their share in the total number of scuientific papers published in 2012-2016 makes 13% (in 2007-2011, the percentage of world publications in the sector of chemistry was 11.62% [1]). Below given in the number of publications placed in the GAJ according to the spheres of knowledge (the first five):

##	Heading	Number of abstracts	% from total
1.	Medicine	712	22,1
2.	Ahriculture	445	13,8
3.	**Chemistry, Applied Chemistry**	**421**	**13,1**
4.	Economics	328	10,2
5.	Mathematics, Computer Sciences and Informatics, Physics	254	7,9

Analysis of the sources of authoritative international scientific databases demonstrated that Georgian publications are representeed in the same bases rather insignificantly. According to the 2015 data of SCImago Journal Rank (SJR indicator) [2], out of 239 world countries, Georgia according to the scientific publications holds the 88th place (Armenia – 79, Azerbaijan – 90).

Recommendations for enhancing the publication activity of researchers, raising the quality level of publications and accessibility of the outcomes of Georgian scientists' research [3]. An English-Georgian language publication of international scientific databases serves the same purpose [4], which is to assist the specialists of all the spheres of Georgian science, including those of chemistry and applied chemistry in placing the outcomes of the carried out research in the universally recognized scientific networks.

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HPLC SEPARATION OF ENANTIOMERS OF SOME CHIRAL CARBOXYLIC ACID DERIVATIVES USING POLYSACCHARIDE-BASED CHIRAL COLUMNS AND POLAR ORGANIC MOBILE PHASES

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In the present study the separation of enantiomers of chiral carboxylic acid derivatives was attempted on different polysaccharide-based chiral HPLC columns with polar organic eluents. Along with the successful separation of analyte enantiomers the emphasis of this study was on differences in enantiomer elution order between various columns and mobile phases. In addition, the effect of column temperature on the retention and separation of enantiomers was studied [1].

The separation of enantiomers of 14 chiral carboxylic acid derivatives was studied on 6 different polysaccharide-based chiral columns in high-performance liquid chromatography with methanol, ethanol and acetonitrile as mobile phases with emphasis on the elution order of enantiomers.

Some interesting examples of enantiomer elution order reversal were observed function of the nature and composition of chiral selector and mobile phase. For instance, the enantiomer elution order for carprofen, ketorolac, naproxen, proglumide and surprofen reversed with changing the chemical structure of the chiral selector. Also, the enantiomer elution order for carprofen, ketorolac and naproxen changed by varying the composition of the mobile phase. In addition, the interesting effect of column temperature on the retention and separation of some analytes was observed. For instance, the enantiomers of surprofen were only partially resolved at lower temperatures but baseline resolved at higher temperature.

As this study illustrates, the affinity of enantiomers of chiral carboxylic acid derivatives towards polysaccharide-based chiral stationary phases is dependent on the nature of the chiral selector and on the mobile phase composition. Sometimes only subtle changes in the structure of a chiral selector or mobile phase composition may lead to a reversal in the affinity for a particular pair of enantiomers. Temperature can be considered as a very useful parameter for improving the separation. Further studies of these phenomena may provide useful information for understanding the chiral recognition mechanisms with polysaccharide-based chiral stationary phases.

Acknowledgments
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NMS-P-44

SEPARATION OF ENANTIOMERS OF CHIRAL WEAK ACIDS WITH POLYSACCHARIDE-BASED CHIRAL COLUMNS AND AQUEOUS MOBILE PHASES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY: TYPICAL REVERSED-PHASE BEHAVIOR?

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When polysaccharide-based chiral columns are used in combination with aqueous mobile phase for separation of enantiomers in high-performance liquid chromatography, the separation mode is commonly called “reversed-phase” in analogy to achiral separations. In several earlier and recent studies on neutral and basic chiral analytes it was shown by our group that due to multiple type of interactions involved in selector-selectand binding and enantioselective recognition with polysaccharide derivatives, the above mentioned separation system may not always behave like a reversed-phase system [1]. In the present study additional examples of non-reversed-phase behavior are described for the first time for weak acidic chiral analytes. In addition, the reversal of enantiomer elution order was observed again for the first time for several analytes based on water-content in the mobile phase.

All HPLC experiments were performed with an Agilent 1200 HPLC instrument (Agilent Technologies, Waldbronn, Germany) equipped with a G1367C HiP ALS-SL autosampler, G1316B TCC-SL temperature controller, G1311A quaternary pump and G1314D VWD variable wavelength detector. The Chemstation software (version B.03.02-SR2) was used for instrument control, data acquisition and data processing. HPLC separations were performed at 20 °C at 1 ml/min mobile phase flow rate if not mentioned otherwise. All mobile phases contained 0.1% formic acid (v/v). UV detection was performed at 240 nm. The absolute configuration or optical rotation sign of enantiomers were assigned based on spiking experiments with enantiomerically pure standards or correlation with earlier publications in which the authors have used optical rotation and circular dichroism detectors sequentially connected to a UV-detector.

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INNOVATIVE MODEL OF PROTECTION OF HOTHOUSE VEGETABLES AGAINST PESTS AND DISEASES

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Demand of the population for vegetable crops in Georgia is high during the whole year in Georgia, therefore satisfaction of demands in autumn-spring is realized at the expense of hothouse economies. For growing vegetable crops in closed ground conditions it is necessary to create optimal climatic conditions necessary for their growth-development, which is also favorable for vitality of plant pests and for spreading plant diseases. Proceeding from the above stated, specific care is attributed to protection of plants from harmful pests in hothouse conditions.

Among the vegetable pests are mainly spreader: the orangery white moth, louse (vegetable garden, peach, and tobacco), web ticks/mite and lately - *Tuta absoluta*. Mostly spread pests of potato are: hothouse white-fly, potato mite, web-ticks, louse, and nematodes. Lately in Georgia we observe spreading of American potato moth -*Tuta absoluta*. Among the diseases of vegetable crops of closed ground especially frequent are root dotes (white and grey). Alongside with it we often observe false mildew and powdery mildew, anthracnosis, bacteriosis, fusrosis, verticilliosis. In case of a potato, mostly spread diseases are: mildew, alternatiosis, askochitosis, stolbure, various type mosaic, crossporiosis, septoriosis, phytophtorosis, leaf dark spots, and apex dote.

Against the above stated pests and diseases costly imported foreign made biological preparations are used and their share in the self-cost of vegetables grown in hothouses is rather significant.

Desirable ecological and economic results can be achieved by application of ecologically friendly means such as pheromone sex-attractant/traps, color-traps, entomologic glue, nutrients obtained from natural raw material, as well as bio-pesticide preparation of prolonged action for small ecological charge. The system of protection of vegetable crops from pests and diseases developed on their basis will provide high reliability of harvest and quality in closed ground conditions, as well as ecological purity of obtained product.

Application of pheromones greatly reduces expenditures of chemical means, since number of coupling decreases, and respectively possibility of healthy egg laying capacity decreases too. Pheromone dispensaries emit active components within 6-8 weeks. Alongside with it, it is important that application of chemical insecticides against *Tuta absoluta* is inefficient, since this pest leads hidden life and it winters in ground. Therefore, currently the most efficient for the struggle against pests is considered sex-pheromones by corresponding traps, especially for *Tuta absoluta*, which leads hidden life and passes winter in soil.

NMS-P-46

SYNTHESIS OF POTENTIAL BIOACTIVE STEROIDAL OXIMES, SEMI- AND THIOSEMICARBAZONES

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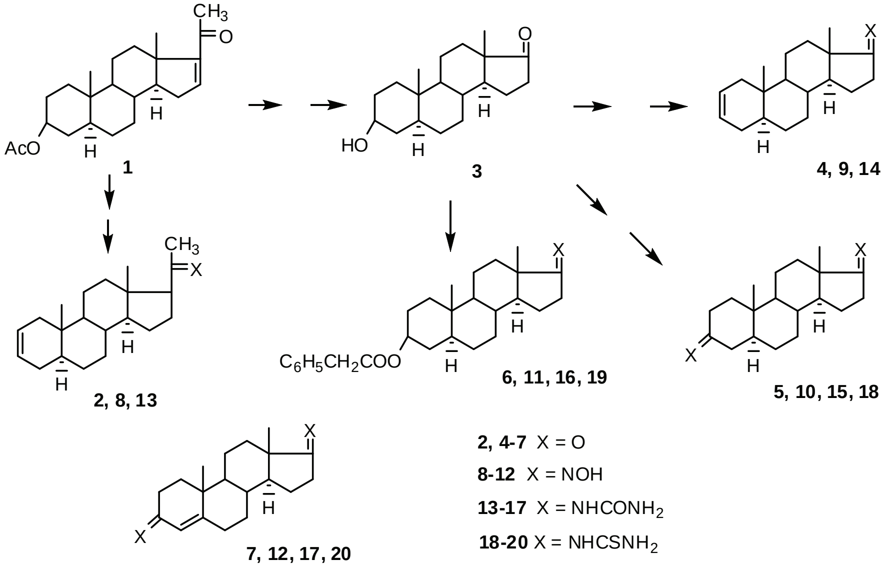
By TSMU Iovel Kutateladze Institute of Pharmacochemistry for the synthesis of 5α-steroids suitable raw material tigogenin is delivered. By the splitting of its 5α-pregn-16-en-3β-ol-20-one acetate 1 was received, from which by reduction and defunctionalization of a ring 5α-pregn-2-en-20-one 2 was synthesized. By the transformation of steroids 1 epiandrosterone 3 was received. By the defunctionalization of A-ring of the latest 5α-androst-2-en-17-one 4 was isolated. 5α-androstan-3,17-dione 5 and 3β-phenylacetoxy-5α-androstan-17-one 6 was synthesized by the oxidation by Jones reagent or by the modification with phenyl acetic acid chloranhydride of C-3 hydroxyl group of steroid 3.

In order to synthesize potential biologically active steroidal compounds by the interaction of ketones 2, 4-6 and androst-4-en-3,17-dione 7 with hydroxylamine in pyridine corresponding oximes 8-12 have been received. By the condensation of steroids 2, 4-7 with semicarbazide hydrochloride in ethanol semicarbazones 13-17 have been isolated. By the condensation reactions catalyzed with acetic acid of ketones 5-7 with thiosemicarbazide thiosemicarbazones 18-20 have been synthesized.



2, 4-7 X = O
8-12 X = NOH
13-17 X = $NHCONH_2$
18-20 X = $NHCSNH_2$

The structures of synthesized steroids **8-20** established by IR-, NMR- and mass-spectral data.

NEW TECHNOLOGICAL LINE FOR PRODUCTION OF FUEL BRIQUETTES AND PALLETS

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Over the course of the past century humanity perceived the situation which formed in the field of production and consumption of energy carriers:

- Unprecedented consumption of natural energy carriers (wood, coal, oil, gas) gave rise to the problem of reclamation of carbon-containing waste (dust, formed as a result of coal mining and enriching, sludge, fragments, sawdust, chips, bark, collected at lumbering and wood-working manufactures and solid waste of other adjacent productions).
- The continuous increase of prices on energy carriers required the production of relatively inexpensive alternative raw material of thermal energy.

Fuel briquettes, which are made from solid carbon-containing (coal dust, sludge, pieces; sawdust, rasping, thinning of biomass, nut shell and other residual wood) waste, are relatively cheap kind of heat carriers.

Technologies and devices of fuel briquette production available at consumer's market are mainly based on material pressing using various hydraulic systems. Such devices are characterized by processing complexity: they have complicated hydraulic systems; by high self-cost: they contain energy-intensive electric actuation (gearing) mechanisms; use of special engineering materials is necessary for manufacturing of separate elements of devices.

We proposed the technological line with the use of which it is possible to arrange energy saving compact and simple instrumentation productions of fuel briquettes and pallets which meet with European standards by recycling of any carbon-containing solid waste (coal, biomass). Technological line involves: partition of material, drying, forming of briquettes and packing.

Innovetive aspects of technological line are:

- Forming of eco-safe fuel briquettes of high heating capacity from coal waste as well as from practically all types of biomass by the use up to 2 percents of organic binder- "Naralex" (trademark) in mass for briquettes [1];
- Device for briquetting design of which gives an opportunity to simultaneously carry out several operations in continuous, uninterrupted mode, in particular – delivery and dosing of basic materials, their mixing, formation into technological mass and briquette forming. Obtaining of targeted product (briquette, pallet) occurs in automatic mode by one-time passing of finely dispersed and powdered carbon-containing materials in it. Change of product form and size (length, diameter) is possible using calibers' changing [2];
- Device for efficient drying of raw materials [3, 4].

Technological line allows us to fabricate product, which meets with European standards, from carbon-containing waste of any origin. On the basis of this scheme it will be possible to arrange low-tonnage production in the regions and villages, where local accumulation of abovementioned waste takes place.

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NMS-P-48

UTILIZATION OF CERTAIN MINERAL RESOURCES IN GEORGIA TO MAKE TOOTH PASTES

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Important resources of vegetable as well as mineral raw materials are available in Georgia.

However, portion of its perfumes and cosmetics on the market is small. Lugela is the only factory-produced toothpaste. This article presents the data of developed recipe of a new toothpaste, containing some of the natural resources, available in Georgia. The basic requirements to toothpastes may be formed as follows: high-quality cleaning features, pleasant taste, deodorizing and refreshing action, absence of local irritant, allergy causing, and toxic agents, As well as stability during storage. The pastes contain: natural and synthetic, anti-microbial, anti-stomatitis action as well as various therapeutic agents.

In the present study qualitative and quantitative composition of the toothpaste is selected so that the toothpaste had an effective preventive and curative action. The effective cleaner - chemically precipitated chalk with the particle sizes within the range of 2 - 20 microns and with a specific antiseptic activity is used as an abrasive agent. Sodium carboxymethylcellulose is used to stabilize the toothpaste suspension. Foaming agent - sodium lauryl sulfate or sodium laurite sulfate, also having small emulsifying, superficial - cleaning and antibacterial action. Glycerin is used for obtaining a homogenous plastic mass. The characteristic feature of the designed composition is that the composition contains as the antimicrobial agents the complex of biologically active components, extracted from the plants which are found in Georgia – tannin containing extracts (Smoke-tree leaves, hazelnut leaves, oak bark), eucalyptus and rose hip oils, propolis extract. Mineral waters Chargali and Utsera are used for mineralization of the teeth enamel and improvement of the antiseptic activity. For example, a variety of Utsera wells have about 6.5 - 11 g / l mineralization, containing carbonic acid of pH 6,4 - 6,8 in the form of main components: HCO_3 - 4,2 - 7,9 g / l; Na + - 1,2 - 2,4 g / l; divalent iron content of 2 - 10 mg / l; K + 4,9 - 7,9 mg / l; also containing lithium, strontium, and others. Chargali mineral water has a similar mineralization. The obtained samples of the toothpaste are stable in storage, using of citrus oils as odorants gives them a pleasant smell and taste, as well as improved antiseptic qualities. Here are provided some of the indicators. Calcium carbonate mass share no more than 38,0%. Appearance and consistency - a homogeneous mass without grains. The color, smell, taste, microbiological purity - meets with the requirements of the state standards. Mass share of heavy metals no more than 0.002%, total content of the tannins (tannic substances) is 3.2 - 3.4 g / l. Qualitative tests for zineol, the carotinoids, metal ions, and potassium ions is positive, foam quantity (in sm) of not less than 6.0.

PREPARATION OF POLYMERIZED NITROGENOUS FERTILIZERS

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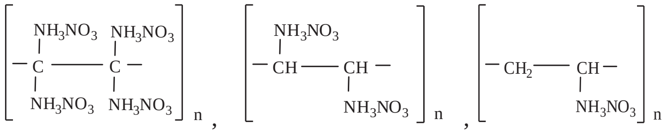
Intense growth of the population requires elevation of production of farm produce, by assimilation of new territories, but arable lands are gradually decreasing due to progressing urbanization and intensified industry. One of the ways to provide population with farm produce is intense introduction of new technologies in agriculture, namely application of nitrogenous fertilizers in increased doses. According to available information annually more than 200 million ton nitrogenous fertilizers are introduced globally in soil, but due to their very good solubility in water, significant part of fertilizers is lost as a result of bleaching and evaporation, which alongside with tremendous economic loss conditions global environment pollution.[1]

The most widely used among nitrogenous fertilizers is ammonium nitre, which is produced in great quantities. It is well soluble in water and easily washed off to soil. Therefore the goal of our research was synthesis of a polymer nitre, to be implemented in the pores of natural sorbent, which will gradually release nitrogen thanks to degradation effect of soil microorganisms. For this we used polymer acceptor – polyamine type nitrogen-containing oligomer with reactivity centers, which is inculcated in natural sorbent pores; it undergoes further structuring and on its base the polymer adduct (polymer nitre) is obtained. [2]

Thus, we can increase nitrogen concentration in the system up to 25-30%. Nitrogen concentration in the adduct can be regulated by alteration of a molar ratio of the initial acceptor and the second reactive acidic component. [3]

Structure of one of the forms of polymer nitre's iterated elemental ring, with respect to initial amine oligomer structure can be imagined in as follows:



$$\left[-\overset{NH_3NO_3}{\underset{NH_3NO_3}{C}}-\overset{NH_3NO_3}{\underset{NH_3NO_3}{C}}-\right]_n,\quad \left[-\overset{NH_3NO_3}{CH}-\underset{NH_3NO_3}{CH}-\right]_n,\quad \left[-CH_2-\underset{NH_3NO_3}{CH}-\right]_n$$

New generation polymer fertilizers synthesized by us – biodegradable polymer nitres, is not washed-off to soil. Thanks to biodegradation microorganisms present in soil it is gradually transformed into the form easily assimilated by plants. Plants are provided with dozed, controlled nutrition for the whole vegetation period, which guarantees obtaining of ecologically sound products. Application of a polymer nitre enable us to reduce fertilizers hectare norm up to 50%.

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NMS-P-50

TECHNOLOGY OF PREPARATIONS FOR STORING THE RESIDUAL RADIOACTIVE MACHINERY OIL

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As a result of exploiting the nuclear equipment, radioactively contaminated residual oils are produced that need proper utilization. For utilizing the radioactive waste, whole series of expensive technologies were created, which in the process of and storing increases the volume of radioactive waste three times, mass of the waste even more. As a result the space and funds needed to store the waste also increases.

After concreting and dismantling its main units, it was time to dismantle cryogenic plant and to safely dispose of the accumulated radioactively contaminated motor oil. With the financing from International Atomic Energy Agency a special project was developed and is being implemented at Andronikashvili Institute of Physics.

For the abovementioned reasons, current method for either solidifying or burning the oil was declined. In order to reduce the volume of the oil to be stored following decision was made – reduction of the flowability of oil by addition of porous supplements. Following cheap porous substances were chosen for the project: wood sawdust, activated or normal charcoal and tuff sand. Based on the research we received the following recommendations:

From studied four substances, priority was given to activated charcoal with 0-2 mm fraction, which is characterized by high porosity and ability to adsorb impurities (including radioactive impurities) from the oil into the pores, which reduces the volume increase of stored oil to 15-20% compared to 300% using traditional methods, purifies the oil and in case of the leak prevents large-scale radioactive contamination chance with high probability.

On this picture you can see the condition of used oil in the systems: a) contaminated oil – wood sawdust; b) contaminated oil – activated charcoal; (b) 2 months after the start of the experiment, where you can clearly see the change in oil's color on top of activated charcoal.

Identification of how well activated charcoal purifies contaminated oil of radioactive impurities is the prioritized subject of our future research.

MIGRATION OF CHLORINATED ORGANIC PESTICIDES AND THEIR IMPACT ON THE AQUATIC ENVIRONMENT

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Halogenated organic pesticides, being in large quantities and extremely dangerous for our population in the Republic of Moldova, become increasingly widespread in the environment due to the damage of old deposits from the Soviet period. Our study of the migration of chlorinated organic pesticides has shown their movement in the soil depth. For instance, hexachlorocyclohexane migrates during 10 months at a depth of 50 cm. The major amount of this substance is contained in the upper soil layer of 10 cm. The chlorinated organic pesticides washing could be also accompanied with the particles in suspension and humic substances. In order to establish the residues washing in time from agricultural lands, a number of pesticides have been determined in: (a) soils from the catchment area of the Bic River, which is the right tributary of the Nistru River, (b) fields treated by pesticides around the Gratiesti village as well in (c) unprocessed lands for a long time (8-10 years). Other chemical tests in the soils near pesticide deposits in the Draguseni village of the Hincesti district (the Prut River Basin) show the presence of POP traces, indicating that the actual impact of pesticide storage has been occurred through less than 8-10 years, or the effluent migrations have taken place until the present. Testing soil samples for a long time in the uncontaminated area shows that the full washing and decomposition of pesticides in soil under natural conditions take place in a period of about ten years. Lakes and ponds are able to cumulate as well certain amounts of pesticides. Negative effects of the secondary pollution by pesticides are found to be obvious in: (I) strongly silted lakes near to the Copaceanca River at its shedding in the Raut River (upstream the Balti city), (II) Cubolta River from the Plop until Putinesti villages, (III) Dubasari Lake dam, (IV) cascade of lakes of the Ialpug River, (V) upstream the Comrat and up to Congaz cities etc. Our laboratory simulations through the oxidation of reduced nitrogen forms highlight a clear braking effect of the self-purification and nitrification processes in siltation tanks. This phenomenon stimulates an additional eutrophication and pollution of surface waters. Homo- and heterogeneous catalysis using precipitated tetraphenylporphyrin ((TPP)Co) cobalt(II) at a graphite foil electrode is studying at present, which will allow the sensitive detection of a wide range of different organohalides, including a number of industrial pollutants such as 1,2,3,4,5,6-hexachlorocyclohexane (lindane) and carbon tetrachloride, a representative of haloalkane compounds, haloalkenes such as tetrachloroethylene, and aromatics such as 2,4-dichlorophenoxyacetic acid, pentachlorophenol, and the DDT insecticide. We intend also to investigate the electrochemical reduction of organohalides catalyzed by the dicobalt $[Co(II)L_2]$ catalysts, where by “L” a number of ligands are denoted. The combination of electrochemical and catalytic methods will be used in order to (a) amplify the neutralizing and mineralization effects of halogenated organic chemicals, (b) increase the rate of disposal of chemical waste and (c) minimize the cost of the disposal of halogenated chemical wastes in the Republic of Moldova.

NMS-P-52

REFINEMENT OF DRUGS IN ORDER TO REDUCE TOXIC IMPACTS AND INCREASE THE THERAPEUTIC EFFECTS

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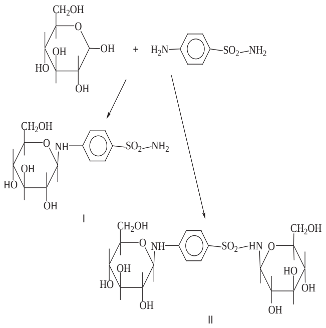
The glycosylation principle of medicinal remedies presented by the Professor, A. Gakhokidze [1] based on the carbohydrate fragments of active transport in cell membranes is considered as a new approach to creation problem of targeted action of effective medical preparations.

The transfer *of sylph amid* preparations in water-soluble forms (streptocide, sulfidinum, sulfazolum and others) has gained great importance especially in medicine as bacteriostatic agents towards to a number of pathogenic microorganisms. The purpose of our study was the theoretical confirmation of results and the fixation of recommendations for improving experiments. For full characterization of the reaction, the calculations have been carried out by means of semi-empirical quantum-chemical method - AM1 [2].



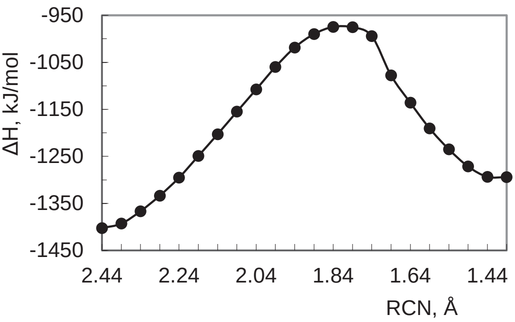


Figure 1. The dependence of energy system change (ΔH) between nitrogen and carbon atoms RC-N distance during interaction of streptocide glucose with a single molecule.

Mono-glucostreptocide is a water-insoluble drug which allows its use as an injection. In medicine, the only infusion solution used for detoxification is α,D-glucopyranose, whose specific motion is in the range of (+51,5°) – (+55,5°). The solution should be non-pyrogenic (i.e. it must not contain microorganisms), for this reason the solution is examined in advance, for, if it contains pyrogens, the temperature of human body rises up to 41°.

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[1] R. Gakhokidze, N. Sidamonidze, S. Mamulia, R. Vardiashvili, L. Tabatadze; Laboratory Practicum carbohydrate chemistry; 2006, Tbilisi, 33

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NMS-P-53

SOLVENT EFFECT ON COMPLEX FORMATION OF DIMETHYLACETAMIDE AND N,N-DIMETHYLFORMAMIDE

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Our task was determination of energetic, geometrical and structural characteristics of organic ligands, dimethylacetamide and dimethylformamide by computer quantum chemical calculation. We also studied the complex-forming ability of ligands with metals, in the gaseous phase, as well as variety of solvents, particularly in water, dimethylsulfoxide, methanol, ethanol, acetone, chloroform and hexane. It was determined that, the solvents increase the stability of both molecules. From the solvents that we studied, the highest value of this parameter attained in the water, the lowest value in the hexane. The study of electron density nitrogen and oxygen atomic orbitals, showed a high electron density of oxygen s-orbitals and nitrogen p_z-orbitals (Table 1). As so far it is known that, p_z-orbital is able to participate in the creation π −bonds but it cannot create a σ-bond with the complex-forming metal. This makes it possible to suppose the formation of monodentate bonding of oxygen atoms with complex-forming metals.

Table 1. Some of results of quantum chemical calculation

Ligand	Solvent	Formation heat kJ/mole	Atom	Charge	Atomic orbital electron populations			
					2S	$2P_x$	$2P_y$	$2P_z$
DMAA	Gaseous phase	-173.39	O	-0.370	1.917	1.692	1.287	1.473
			N	-0.343	1.470	1.067	1.055	1.752
	Water	-222.67	O	-0.575	1.915	1.731	1.322	1.607
			N	-0.307	1.469	1.078	1.064	1.696
	Hexane	-186.13	O	-0.428	1.916	1.699	1.303	1.509
			N	-0.340	1.468	1.070	1.058	1.743
DMFA	Gaseous phase	-154.60	O	-0.365	1.915	1.110	1.873	1.466
			N	-0.353	1.417	1.063	1.073	1.746
	Water	-208.52	O	-0.588	1.914	1.156	1.907	1.610
			N	-0.312	1.472	1.086	1.073	1.681
	Hexane	-170.37	O	-0.430	1.915	1.124	1.884	1.507
			N	-0.345	1.471	1.070	1.073	1.732

In dimetylacetamide molecule the calculated length of C–C bond is equal ≈1.5 Å. In dimethylacetamide molecule, as well as in N,N-dimethylformamide, calculated lenght of C–O and C–N bonds the average values are accordingly 1.3 and 1.4 Å. The calculated values of N–C–O angles in dimethylacetamide are within 119.5÷120.5°, in N,N-dimethylformamide – 122÷123°. The angles of C–N–C are within 119÷122° in both molecules. It should be noted, that the results of calculation are in accordance to $Ni(NCS)_2[CH_3CON(CH_3)_2]_4$ and $Me(NCS)_2[HCON(CH_3)_2]_4$ (*Me*=Mn(II); Co(II); Ni(II)), X-ray data.

NMS-P-54

SOLVENT EFFECT ON COMPLEX FORMATION OF UREA

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With the quantum-chemical method AM1 are calculated the power, geometrical and structural features of urea. Potential donor atom-complexing - oxygen atom O (1). According to electronic structure, solvent effect on its complex formation ability with metals is established**.**

Synthesized coordination compounds of d-elements with urea. Some d-elements sulphates, nitrates, chlorides and bromides have been taken as initial salts. Synthesis has been carried out in ethanol solutions.

Synthesized coordination compounds are separated in solid form. Composition, individuality, solubility of obtained compounds in different solvents is established.

IR absorption spectra of synthesized coordination compounds are studied in order to establish the rule of coordination for dimethyl sulfoxide. Spectra are located 400-4000 sm^{-1} range.

SYNTHESIS, CHARACTERIZATION, ELECTROCHEMICAL AND ELECTROPHYSICAL PROPERTIES OF 4,4-DIFLOR-8-(4′-BROMOPHENYL)- 1,3,5,7-TETRAMETHYL-4-BORA-3A,4A-DIAZA-S-INDACENE (BODIPY)*

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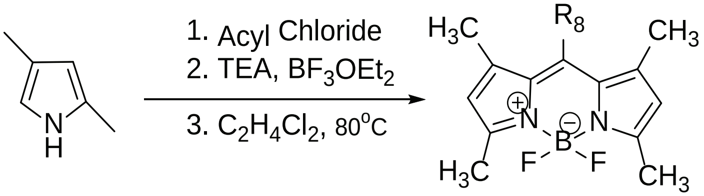
4,4-Difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY) dyes have attracted much attention due to the excellent applications in many areas such as fluorescent switches, supramolecular polymers, labelling reagents, chemosensors, photodynamic therapy, choromogenic probes, laser dyes, and sensitizers for solar cell applications. BODIPY dyes tend to be strongly UV-absorbing small molecules that emit relatively sharp fluorescence peaks with high quantum yields. These dyes are widely used to label proteins and DNA [1,2].

The meso position is the most sensitive to substituent effects because, upon excitation, an important variation in the electron density takes place at that site. From a strategic point of view, the meso position is arguably the most important because in the majority of the applications that have been devised for BODIPYs it is the position of choice for the attachment of the substrate to study [3].



In this study, 1,3,5,7-tetramethyl-4-bora-3a,4a-diaza-s-indacene (BODIPY) was synthesised starting from different acyl chlorides and 2,4-dimethyl-1*H*-pyrrol which is commercially availible. Structure of these BODIPYs were charecterized by ^{1}H NMR, ^{13}C NMR, IR spectroscopies and Their electrochemical and electrophysical properties were invastigated by using flouresence spectroscopy and cyclic voltametry methods respectively.

**This study was supported by TUBITAK (Scientific and Technological Research Council of Turkey) with project no 114Z176*

References:

[1] Goud, T.V., Tutar, A., Biellmann, J.F., *Tetrahedron*, 62, 5084-5091, 2006.
[2] Tutar, A., Erenler, R., Biellmann, J.F., *J. Chem. Soc. Pak.*, 35 (4), 1197-1201, 2013.
[3] Arbeloa, T., Banuelos J., *J. Org. Chem.*, 80, 5771−5782, 2015.

NMS-P-56

INCORPORATION AND NEUTRALIZATION OF RADIONUCLIDES IN MAGNETOCONTROLLABLE MINERAL-LIKE MATRICES BASED ON CENOSPHERES OF ENERGETICAL ASHES

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The article shows the promising applications of hollow aluminosilicate microspheres of volatile energy ashes, formed from aluminosilicate melt of the mineral part of coals when pulverized combustion and accessible renewable aluminosilicate raw materials with an annual production capacity of only in Russia 100 thousand tons.

As a raw material used a certain fraction of cenospheres particle size 20-250 mm, a bulk density of 350 g/cm^3 and a surface area of 12.5 m^2/g, which was isolated from the concentrate of cenospheres from fly ashes of burning coal of Ekibastuz field in Kazakhstan at the thermal power plant of Almaty city. The chemical composition of the initial cenospheres, mass. %: SiO_2 – 59.73; Al_2O_3 – 26.41; Fe_2O_3 – 5.51; CaO – 2.15; TiO_2 – 1.19; Na_2O – 0.82; S – 0.87; P – 0.539. According to quantitative XRD analysis the phase composition is represented mainly by quartz and mullite.

Mossbauer study of cenospheres showed that the cenospheres containing more than 7 mass. % Fe_2O_3 iron takes part in two phases – the defective magnetite (67 %) and the phase, the parameters are close to the disordered orthosilicate of monticellite $(Ca, Mg, Fe)_2SiO_4$ (33 %). Defective magnetite at room temperature is two equally populated magnetic states: ferromagnetic and superparamagnetic. Sublattice of magnetite diluted with diamagnetic substitution. The diamagnetic dilution and small size spinel formations leads to a superparamagnetic state and the destruction of the fast electronic exchange between Fe^{3+} and Fe^{2+} ions in the *B*-sublattice of magnetite.

Cenospheres with a lower concentration of Fe_2O_3 (3-4 mass. %) contain iron in spinel (47 %) and orthosilicate (53 %). Spinel is paramagnetic at room temperature. In the silicate the iron is in the divalent state occupies octahedral M2-type position.

For neutralization of liquid radioactive waste used the modified microspherical adsorbent. The results of elemental analysis of modified cenospheres after transmission through it of a productive solution of radioactive wastes summarized below: Mg – 0.018; Si – 18.21; P – 0.641; Cl – 3.151; K – 2.017; Ca – 3.725; Cr – 0.02; Mn – 0.206; Fe – 11.808; Cu – 0.04; Zn – 0.039; Sr – 0.215; Pd – 0.071; In – 0.545; Eu – 0.088; Yb – 0.006; Re – 0.005; Ir – 0.009; Pb – 0.042; U – 59.141. The obtained results indicate that the modified aluminosilicate microspheres extracted from fly ash of thermal power plant in Almaty, can be used for sorption of uranium.

Curing Cs(Na)-containing solutions to study the phase composition of the cured was performed using model solutions of nitrate of sodium and cesium as imitators of radioactive ^{137}Cs-containing solutions of high salt regenerators of reextract cesium or distillation residues of nuclear power plants. Curing was carried out in the mixing mode of cenospheres with a solution of $NaNO_3$/$CsNO_3$ at a predetermined ratio – drying at temperatures of 80-120 °C – heat treatment at selected temperatures.

With the use of cenospheres of the particular composition of the obtained chemically stable mineral-form immobilizing ^{137}Cs-containing solutions with the inclusion of the ^{137}Cs radionuclide in the crystalline phase of pollucite.

SYNTHESIS, CHARACTERIZATION, ELECTROCHEMICAL AND PHOTOPHYSICAL PROPERTIES OF 4,4-DİFLUORO-8-(4′-BROMOPHENYL)-3,5-DIETHYL-4-BORO-3A,4A-DIAZA-S-INDACENE (BODIPY)*

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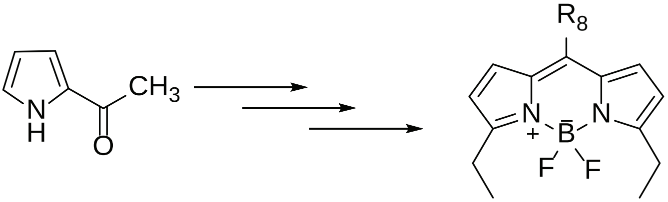

In this study, 2-ethyl-1H-pyrrole was prepared from the reaction of methyl 2-pyrrolyl ketone, hydrazine hydrate and KOH in ethylene glycol at 150 °C.

Different substituated 3,5-dimethyl BODIPY at mezo position was obtained from the reaction of 2-methyl-1H-pyrrole with different acyl clorides. Structures of these compounds were done by ^{1}H NMR, ^{13}C NMR, IR spectroscopies.

**This study was supported by TUBITAK (Scientific and Technological Research Council of Turkey) with project no 114Z176*

References:

[1] Goud, T.V., Tutar, A., Biellmann, J.F., *Tetrahedron*, 62, 5084-5091, 2006.
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[3] Arbeloa, T., Banuelos J., *J. Org. Chem.*, 80, 5771−5782, 2015.

NMS-P-58

THEORETICAL STUDY OF EXCITATION PROFILES OF COHERENT ANTI-STOKES RAMAN SCATTERING AND APPLICATIONS TO SOME CAROTENOIDS

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Many experimental and theoretical studies have been devoted to analyses of resonance Raman excitation profiles (REPs) and coherent anti-Stokes Raman (CARS) profiles, which allow to determine changes in the equilibrium geometry of molecule in its excited states to be determined (the inverse problem of vibronic spectroscopy).

The effect of inhomogeneous broadening due to the surrounding on the excitation profiles of resonance Raman and CARS was theoretically studied. Analytical expressions for the REPs and CARS excitation profiles with an arbitrary relation between the relaxation constant of the vibronic levels and the parameter, characterizing the inhomogeneity of the environment, obtained by us [1], are presented.

CARS spectroscopy is a nonlinear optical technique that has provided to be a valuable tool for the investigation of many different systems, important for chemistry and biology. It is well known that the excitation profiles of resonance CARS are mostly used to estimate the origin shift parameters with electronic excitation for vibrations having resonantly enhanced Raman components, which provides information about the molecular structure and its changes in an excited electronic state. Therefore, it is important to have an adequate theoretical model taking into account the joint (simultaneous) influence of different broadening mechanisms [1]. In this work we review our results, suggest some new relations and apply the theory to some carotenoids.

References:

[1] M.G.Zakaraya and G.M.Chonishvili (2014), Bulletin of the Georgian National Academy of Sciences, vol. 8, no 1, 2014.

THE COMPLEX STUDY OF ANTIOXIDANTS AND MINERAL COMPONENTS IN GEORGIAN RED WINES

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The mechanism of action of the most common antioxidants (aromatic amines, phenols, naphthols, etc.) consists from the breakage of reaction chains: molecules of antioxidant interact with active radicals to form inactive radicals.

At present, the scientifically substantiated and the developed different technological modes, allowed to extract the antioxidants from the grape. Therein grape wines are being enriched with biologically active substances. At the same time, the mineral components of the wine - it is a significant part of it, affect to the aging process and taste and in a much more depends on the composition of the soil, water and atmosphere pollution degree, i.e., from the environment ecology. From this point of view it is urgent both the determination of the total content of antioxidants (AO), and close thereto integral index - antioxidant activity (AOA) of the test object, and the complex analysis of the chemical composition of wines, taking into account not only the content but also the specific activity of each component in it. Minerality of wine - a complex issue, is still not sufficiently studied and is very interesting.

So, the aim of this work is to determine mineral components and preliminary identification of main phenolic antioxidants in Georgian red wines Saperavi and Kindzmarauli, using HPLC, photocolorimetry, spectrophotometry, conventional chemical analysis methods.

To determine the influence of soil composition on the mineral component of red wine from the eastern region of Georgia - Kakheti (place Mukuzani and Sabue) on the first stage, the complete chemical analysis of the soil samples, taken at a depth of 5 and 25 cm was carried out. It was found that content of SiO_2 is practically the same for all studied samples, the content of aluminum varies in limits 10-17%. The content of calcium in soil of Mukuzani vineyard is twice less in the depth 25 cm, than in near-surface layer, but in soil of Sabue vineyard the content of calcium doesn't depend from depth of sampling. The quantity of potassium and sodium doesn't depend from depth also and varies from 1 to 2%. The quantity of potassium in grape leaves and in seeds is twice less, than in soil, the content of sodium an order of magnitude lower.

The initial experiments to determine the mineral composition in soil, grape leaves and bunch (stem, skin, and seeds) indicate on nonhomogeneous distribution of Na^+, K^+, Ca^{2+}, Mg^{2+}, SO_4^{2-}, Cl^- ions along whole chain from the soil to the wine. Total content of mineral components in wines varies in limits 1.2 – 2.8 g/l, that less at 50% than in grape. Content reduction of mineral components is continuing at treatment and aging of wine.

Identification of phenolic compounds was carried out using HPLC (Agilent 1260) at 280 and 360 nm with Zorbax Eclipse XDB C18-01 column and acetonitrile/bidistilled water/acetic acid as mobile phase.

22 phenolic compounds were identified in bunch, seeds and in Saperavi wine of Sabue vineyard, 28 in stem. The main components are following: gallic acid, protocatechuic acid, cafferic acid, syringic acid, ferullic acid, dehydroquercetin, rutin, O-Coumaric acid, sinapic acid, myricetin, (+)-catechin, ellagic acid. Were detected the trace quantities of vannilic acid, p-hydroxybenzoic acid, resveratrol and others. The detailed analysis of more interesting components of red wines – polyphenols (phenolic acids, flavonoids, anthocyanins, flavanols, including procyanidole and catechins, chinoin, coumarins, resferatrol) – is the subject of following study.

The work is carried out in the frame of Project No DI/38/7-220/14, financed by SRNSF

NMS-T-02

SPATIAL MEMORY IMPAIRMENT AND HIPPOCAMPAL CELL LOSS INDUCED BY OKADAIC ACID

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In the present study, we evaluated and compared effect of intracerebroventricular (ICV) and intrahippocampal bilateral microinjection of okadaic acid (OA) on spatial memory function assessed in one day water maze paradigm and hippocampal structure in rats. Rats were divided in following groups: Control(icv) - rats injected ICV with aCSF; Control(hipp) - rats injected intrahippocampally with aCSF; OAicv - rats injected ICV with OA; OAhipp - rats injected intrahippocampally with OA. At the end of the behavioral experiments OA treated and control rats were deeply anesthetized with pentobarbital and perfused through the ascending aorta with 300 ml saline followed by 600 ml 4% paraformaldehyde in 0.1 M phosphate buffer (pH 7.4)). The surviving pyramidal cells in the hippocampus of rats were visualized by Nissl staining. The number of the hippocampal pyramidal cells in Nissl staining sections was counted at X 400 magnification. Nissl staining of hippocampal sections showed that the pyramidal cell loss in OAhipp group is significantly higher than that in the OAicv. The results of our behavioral experiments showed that all rats exhibited a decreased latency to find the hidden platform across the eight training trials and OA treatment did not affects probe-test performance 30s after training. In marked contrast, the present experiments indicate that OA treatment affects probe-test performance 24 h after training. These findings suggest that OA treatment did not affect learning process and short-term spatial memory but induced impairment in spatial long-term memory. OA-induced spatial memory impairment may be attributed to the hippocampal cell death. Based on these results OA induced memory deficit and hippocampal cell loss in rat may be considered as a potential animal model for preclinical evaluation of antidementic drug activity.

NMS-T-03

DETERMINATION OF COMPOSITION OF MINERAL WATER OF VILLAGE BABILI, LENTEKHI DISTRICT

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Production of natural mineral waters is one of the most important sectors of Georgia's industry, which can significantly contribute to the development of the whole economy.

In order to study therapeutic activity of natural mineral waters and their influence on the human organisms first of all it is necessary to determine water characteristics. The main parameters are ionic and gas composition, temperature, and radioactivity. As soon as these parameters are known, it is necessary to determine the unique microcomponents of mineral water in order to establish functional relationship between these microcomponents and other substances of mineral water. Mineral waters are formed deep underground and reach the surface due to hydrostatic or gas pressure.

One of the most important subjects is the stages of formation of mineral water. The same mineral water formed under influence of different environmental and natural processes may significantly vary in its chemical composition. The mineral waters one of which is formed deep underground and another one closer to the surface may differ in content of specific microcomponents. The high temperature of the mineral water may not definitely serve as a proof of its being formed in deeper earth layers. Physical and chemical processes undergoing in the Earth's crust do noticeably change chemical composition of mineral waters. Namely these processes determine the difference in composition of various mineral waters.

The main goal of the study was to examine and determine chemical composition of mineral water of village Babili, Lentekhi District according to international standards.

Various timed-tested methods were applied for analysis. Hydrogen ion concentration (pH) was determined by means of potentiometric titration (diphenylcarbazone applied as indicator).

Concentration of hydrocarbonates was determined by use of acidometric titration (methyl orange applied as indicator).

Concentration of calcium and magnesium ions as well as the total hardness of water was determined by application of complexonometric titration. The influence of heavy metals was avoided by addition of sodium sulfate.

Concentrations of biogenic substances were determined by means of photometric analysis: Nessler's reagent was used for , Griess reagent for-, diphenylamine for, and ammonium phosphomolybdate for .

Concentration of iodide ion was determined by application of Reznikov's method.

Total concentration of organic substances was determined by the method of permanganometry (oxidation-reduction titrations).

Concentration of dissolved oxygen was determined by use of iodometry. The results of analysis are provided in the below.

Table 1. Chemical composition of mineral water of village Babili, Lentekhi District

	mg/l										μg/l
pH	Permanganometry	Dissolved oxygen	Mg^{2+}	Ca^{2+}	HCO_3^-	Cl^-	NO_2^-	NO_3^-	NH_4^+	PO_4^{3-}	I^-
5.6	1.92	0.98	17.25	3.45	19.96	0.73	-	-	-	-	0.85

As the results of analysis show the concentration of abovementioned ions is within a normal range and the mineral water can safely be used for human consumption.

NMS-T-04

CLEARING-TREATMENT OF QUARRY WATERS OF COPPER-PYRITE DEPOSITS

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It is known that the sulfide ore deposits are one of the most significant source of toxic pollution. Besides, residuals of heavy and non-ferrous metals compounds tens of thousands of tons, which represents the serious economic problem while ore operations, considering also an environmental damage in an area.

The copper sulfide deposit Madneuli (Georgia) is a typical example of deposits existing worldwide with technocratic impacts on the environment. According to the researches, the indexes of the contamination of the soils and water objects by toxic elements (Cu, Zn, Cd, Fe), is much greater than maximum permissible concentrations, that is revealed in very high level of sickness rate of population in the area.

The analysis of existing methods for purification of quarry waters of sulfide deposits shows that at present, there is no efficient and economic method for purifying from the ions of heavy metals. At the same time, quarry waters of Madneuli deposit belong to low-concentrated ones and are considered as non-profitable for extraction of heavy metals.

Based on the above, for clearing-treatment of quarry waters of copper-pyrite deposits we have selected reagent (sulfide) method.

Upon fulfilled researches, there has been set optimal parameters for purification of waters. Also, there has been obtained pyrite-polymetallic sulfide sediment and quarry waters with concentration of metal sulfates below the concentration limit allowed for water reservoirs.

Based on retained results, there has been worked out a principal technological scheme for quarry water cleaning-treatment.

NMS-T-05

INFLUENCE OF CHEMICAL COMPOUNDS APPLIED AGAINST THE POTATO RING ROT ON THE CAUSATIVE BACTERIUM – *CLAVIBACTER MICHIGANENSIS* Subsp. SEPEDONICUS

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Potato ring rot caused by a phytopathogenic bacteria *Clavibacter michiganensis* subsp. *sepedonicus* is serious problem [1]. Despite the fact that, chemicals applied for the disease treatment and storage disinfection in Georgia and other countries are from ecological point of view, chemical pesticides are often used as there is no resistant cultivars and cultural practice is no effective [2-4]. The aim of the study is to evaluate the effect of chemical agents, particularly solution of blue copperas and fungicide Kauritil on bacteria was studied. It was found that the solution of blue copperas at a ratio 1:1 had no suppressive effect on bacteria after 5 min of exposure with bacterial culture (10^9cells/ml). During 2-hour exposure, the loss of growth ability was observed and 5-hour exposition had a lethal effect on pathogen. At higher concentrations of blue copperas (at a ratio 2:1), growth ability of bacteria was reduced. At a ratio 3:1, the loss of growth ability was observed for 5 min of exposition, and in 2 hours, blue copperas had a lethal effect on bacteria. As for Kauritil, this compound, compared with blue copperas, revealed even stronger bactericidal activity. During 5 min of exposition, its effect to the bacterial culture at a ratio 2:1 was lethal (Table 1).

Table 1. The influence of blue copperas and Kauritil on a bacterium *Clavibacter michiganensis* subsp. *sepedonicus*

Strain #	Exposure time	Mixture of Blue copperas and bacterial culture of 10^9 cells/ml			Kauritil and bacterial culture of 10^9 cells/ml		
		1:1	2:1	3:1	1:1	2:1	3:1
6520, 50	5	+++	++	++	++	-	_
	120	++	++	-	+	-	-
	300	-	-	-	-	-	-

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NMS-T-06

OBTAINING AND CHARACTERIZATION OF NOVEL ANTIBACTERIAL HYBRID COATINGS

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The aggressive microorganisms and viruses have adverse effects on the environment and human together with three global dangers for humanity: energy crisis, food crisis and ecological disasters.

The novel inorganic-organic hybrids were created in order to elaborate non-traditional functional materials with specific properties for protection of cultural heritage and museum exhibits [1, 2]. Biocorrosion stability was achieved by combining different molecular building blocks in various ratios and by controlling their mutual arrangement.

As bioactive components, were used heterometal coordination compounds of some biogenic elements and ligands simultaneously containing metallocene [bis(η^5-cyclopentadienyl)iron] and polycyclic asymmetric fragment. The industrial silicon-organic oligomers with side functional groups were selected as modifiers. They characterized with a good compatibility to various hetero- and carbochain polymer matrices (polyurethane, polyepoxy, fluorine-containing copolymers, etc.). That allows us to develop principally new generation of multifunctional antibacterial coatings with good thermal stability, hydrophobicity and mechanical properties.

The work temperature interval of the obtained composites was established by investigation their thermo-physical properties. The thermal stability of the obtained composites was investigated by Thermal gravimetric analysis (TGA). Based on TGA results polyurethane matrices and their hybrids are quite stable up to 200^{o}C and the weight loss does not exceed 5-6 wt.%. Intensive destruction process of samples takes place above 300-350^{o}C with total weight loss more than 45 wt.%. Composites based on fluorine-containing copolymer are more thermostable than composites based on epoxy or polyurethane matrices: their weight loss starts above 230-240^{o}C and intensive destruction process takes place above 370-400^{o}C with total weight loss of 30-35%. The complete thermal degradation of the tested composites occurs above 600^{o}C.

Differential scanning calorimetry (DSC) method was used to locate the phase and glass transition temperatures. The analyses of DSC curves show that endothermic picks correspond to the glass transition temperatures of the tested samples (T_g). All obtained coatings have glass transition regions above 50^{o}C. The modification of chosen matrices with silicon-organic oligomers causes shift the peak position of the glass transition to lower temperatures compared to non-modified polymer matrices. Developed composites are amorphous substances at room temperature (the working temperature for using of the antibacterial coatings as protectors of museum exhibits). This is very important as crystallization can worsen their optical properties.

According to the obtained results, elaborated inorganic-organic hybrid coatings are characterized with good adhesion to the surfaces of various synthetic and natural materials, high strength, elasticity and stable mechanical properties, hydrophobicity and resistance to photo- and thermal aging. These materials do not produce harmful gases during exploitation, are relatively cheap and available.

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OBSERVATION THE YOUNG MEN PHYSICAL DEVELOPMENT IN HIGH-FREQUENCY ELECTROMAGNETIC WAVES OF CELLULAR BASE STATIONS TRANSMITTING ANTENNAS IN THE SECURITY ZONE

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Rapidly progressive technologies, such as cellular telephone connection, is a subject of dispute. Their impact on human health is still controversial. They belong to the nonionized electromagnetic field. In the surrounding area of the cellular radio stations there are constantly held the electromagnetic field measurement. The measurements field have shown that the intensity of the control, is the maximum permissible level 3-20 times lower, than the permitted level of work safety [1, 2, 3, 4].

In 1999-2003 years were analyzed 108 youths physical development. During a considerable period of time (3 years) 14 of them for a long time were in the high-frequency electromagnetic waves in a safe under the influence. .Based on these calculations the cellular radio communication systems may be belonged to the environmentally safe and life safe communication systems. So, we were dealing with the factors of the physical development that caused the age adjustment. All of them were the city residents. Their body length was marked by the high rate of these youths thigh bone x-ray. It was clear , the early ossification among the same age seniors, which amounted to 2,5-4 years [1,2,3,4,5,6,7].

Similar observation was conducted in the years 2006-2015. Among the 32 young residents of the city, within the same length and the same influence. These contingent in comparison with other seniors (meaning 1999-2003years), revealed high intensity of early ossification process (3-4 years). Thus, we can conclude: for a long period of time under the high-frequency electromagnetic waves in a safe influence, as revealed in the accelerated development of physical-acceleration signs, The bones of the skeleton, particularly the thigh bone ossification the high length of the body.

According to our data acceleration interpreter Electromagnetic Theory confirmation. This Theory of modern technology, taking into account the impact on the human body, needs fundamental study of the material needs extensive, long-term research and observational studies [1, 4, 5].

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NMS-T-08

PRESCHOOL CHILDREN’S PHYSICAL DEVELOPMENT INDICES REVIEW

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Many scientists agree that the last hundred years, people have dramatically changed the environment of the earth through their actions. For one’s part our organism is constantly under the influence of the external universe and experiencing some amendments, including one physical development indicators. In the last 20 years we performed the observation to the youth and infants physical development. The study was complex, and the result of each section was reflected step by step. The results showed the existence of acceleration in infants as well as youths. [1, 2, 5, 6]

Therefore there was a question of pre-school children observation. Research is also complex, in addition to physical development indicators (body length, weight, head circumference and chest circumference), attention was paid to a number of factors. Provided the parents’ physical health and development indicators, the prenatal period, the sequence of pregnancy, the period between pregnancies, abortions and pregnancies among others. Extensive survey was collected from the parents’ detailed information.

The study included Kutaisi two pre-school facilities, 3 to 5 years of age. The number of examined children with relatively complete analysis is 115. Among them were 60 girls and 55 boys. The reviewed data on this stage, we only focus on physical development indices figures, besides the contact with the other factors. (Relationship analysis will be reflected in the near future in the works) physical development indices have been grouped in the form of a table, for each age category and sex.

Age	Body length		Body weight		Chest circumference		Head circumference	
	girls	boys	girls	boys	girls	boys	girls	boys
3year	97,2	97,5	16,8	15,4	52,5	51,2	54,5	52,2
4year	98,2	103,2	16,4	17,9	52.8	54,4	51,8	52,4
5year	107,2	111,5	18,1	18,6	55.7	56,2	52,1	52,1

The data have been compared with the last 2-3 years, the beginning of the century, the last century 70’s and 90’s data. The result was that the pre-school children physical indicators belong to the medium and high data. This indicates that in this age category physical development is rapidly going on [1, 2, 3, 4, 5, 7].

Of course, a more complete and reliable data needed to conduct much greater quantity of children, including other methods of engaging in research. This will be the subject of our work in the coming 5 years, after this we can release more exhaustive information.

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RADIO RESISTANCE TO ULTRASONIC RADIATION

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Increasing resistance of the human body to ionizing radiation becomes highly relevant to the development of nuclear energy, not immune to accidents, the long stay of the astronauts in space orbiting the Earth, with the upcoming mission to Mars. Today the radio protectors (mainly synthetic) are already known, many of which are toxic, have side effects and require careful application.

There are, however, non-toxic natural compounds, which are very promising for use as radiation protectors in the form of biologically active food supplements.

NMS-T-10

DEVELOPMENT OF HPLC METHOD FOR DETERMINATION OF CAFFEINE IN ENERGY DRINKS

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Products, containing caffeine, a natural origin alkaloid of purine group, are widely represented on the retail market. In recent years it has become popular to add caffeine into energy drinks. Thus, optimization of methods is very important for qualitative and quantitative determination of caffeine. In the current work, it is represented the developed rapid and sensitive HPLC method for caffeine determination.

Chromatographically optimal condition was achieved by using mobile phase of acetonitrile-water (40%: 60%) under following conditions: UV detection was conducted at 254 nm; flow rate of mobile phase -0.7mL/min; column size with solid phase is following: Phenomenex® Luna® 5 µm C18(2) 100 A/ LC Column 250 x 4.6 mm; column temperature - 25ºC; sample injection volume - 20µl.

In given conditions, the possibilities of quantitative determination of Caffeine was studied; the procedure revealed linear and correlation coefficient R^2, which is 0.998.

Based on the received data we can conclude that the developed method can be used for qualitative and quantitative determination of caffeine in different type Energy Drinks.

THE QUALITATIVE AND QUANTITATIVE ASSAY OF ORGANIC ACIDS IN ACTIVE PHARMACEUTICAL INGREDIENT OF „CAMELYN M"

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On the basis of conducted studies using the method of gas chromatography-mass spectrometry (GC-MS), organic acids were identified in Camelyn 100% solution. For quantitative determination of total organic acids potentiometric titration method was applied.

On the basis experimental studies have been selected the optimal conditions of GC-MS method for analysis: mobile phase- helium, flow rate-1ml/m, injector temperature- 250°C, transfer line temperature-295°C, oven temperature-40°C, retention was during 3 min. Temperature gradient-15°C/min → 150°C,retention-1min, 20°C/min → 250°C, retention 1min, 35°C/m →310°C retention-2mn. Sample injection volume 1µl, ion registration regime- TIC. Ion detection ranged between 45.00 – 470.00 amu.

Conducted studies give us opportunity to add in the normative document of Camelin's active pharmaceutical ingredient the specification of qualitative and quantitative determination of organic acids.

NMS-T-12

SEPARATION OF ENANTIOMERS OF SELECTED CHIRAL TRIAZOLE DERIVATIVES WITH POLYSACCHARIDE-BASED CHIRAL STATIONARY PHASES AND AQUEOUS MOBILE PHASES

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Every year ½ of world's food supply undermines and grazes by plant pests, diseases and weeds. Agricultural and vegetable crops productivity is heavily dependent on the protection against them. For this purpose combat chemical methods are used. Pesticides are substances meant for attracting, seducing, and then destroying any pest. They are a class of biocide. The most common use of pesticides is as plant protection products (also known as crop protection products), which in general protect plants from damaging influences such as weeds, fungi, or insects. Although pesticides have benefits, some also have drawbacks, such as potential toxicity to humans and other species. Triazole group of chemicals-Fungicides are actual nowadays.

Here are explored chiral triazoles: Bitetranole, Diclorbutazole, Difenoconazole, Diniconazole, Fenbuconazole, Metconazole, Penconazole, Prothroconazole, Triadimenole, Triadimefone, Vinclozoline, Itraconazole, Etconazole.

Used mobile phases: Methanol 100%+ Diethylamine 0.1%, Methanol-Water 97-3%+Diethylamine 0.1%, Methanol-Water 95-5%+Diethylamine 0.1%, Methanol-Water 90-10%+Diethylamine 0.1%, Methanol-Water 85-5%+Diethylamine 0.1%, Methanol-Water 80-20%+Diethylamine 0.1%, Methanol-Water 75-25%+Diethylamine 0.1%, Methanol-Water 70-30%+Diethylamine 0.1%.

The separation of enantiomers of 13 triazole derivatives was studied using polysaccharide-based chiral stationary phases and aqueous-organic mobile phases in high-performance liquid chromatography (HPLC). The major emphasis was made on the role of chemistry of a chiral selector and the mobile phase on elution order and separation mechanism of enantiomers. For the most of chiral triazole derivatives studied the retention and separation factor of enantiomers increased with increasing content of water in the methanol as the mobile phase. An interesting effect was observed for the stereoisomers of difenconazole on the Lux Cellulose-3 column. In particular, in methanol containing 0.1% (v/v) diethylamine all four stereoisomers were baseline separated while separation worsened with increasing content of water and when water content in the mobile phase reached 20% only two separated peaks were observed. For the enantiomers of triadimephone separation of enantiomers increased with increasing content of water in methanol, reached the maximum at 15% water content, then decreased again and disappeared at the water content of 20%. For several analytes with two chiral centers all for stereoisomers were resolved baseline with various combinations of mobile and stationary phases.

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SUMMARY SELECTIVE LESION OF GABAERGIC NEURONS IN THE MEDIAL SEPTUM BY GAT1 SAPORIN IMPAIRS SPATIAL LEARNING IN A WATERMAZE

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Given the central role the hippocampus plays in declarative memory formation and the strong input to the hippocampus from the medial septum (MS), it is tempting to hypothesize that this input is critical for memory processes. The septum and the hippocampus are heavily interconnected through the fimbria-fornix and are functionally coupled, often referred to collectively as the septohippocampal (SH) system. The aim of this study was to investigate the role of the medial septal (MS) GABAergic cells in hippocampal dependent spatial learning using the immunotoxin GAT1-SAP to produce selective lesions of GABAergic MS neurons. In current study rats were trained in a visible platform version of the Morris water maze in which either a place or cue strategy could be used to escape successfully. Immunohistochemical studies showed that intraseptal injection of GAT1-SAP extensively damaged GABAergic MS neurons and spared most cholinergic neurons. The rats' responses on the competition test were classified as either cue or place, based on the swim path for those trials. An overview of the data from both competition trials for each group show that the control rats in 14 trials out of 16 competition test trial used place strategy, while MS-lesioned ones used this strategy in 2 trials only. Decreased place-bias in MS-lesioned rats compared to the control rats was significant ($P<0.01$). The data obtained in the control and GAT1-SAP lesioned animals in the present study, demonstrate that lesioned rats were impaired in hidden platform trials during training, and displayed a pronounced cue-bias in competition tests. Therefore, above data suggest involvement of the MS GABAergic neurons in organization of the spatial map-driven behavior and this structure, along with the hippocampus, should be viewed as a constituent of the functional system responsible for the cognitive types of spatial memory.

CONTAMINATED SOIL REMEDIATION BY SELF-CLEANING PROCESSES ACTIVATION

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Pollution of various dangerous substances increasingly influences soil fertility and hence the sustainability and productivity of agricultural plants. Increased share of contaminated soils makes it necessary to use more and more environmentally safe chemicals, which provide fastremediation.

In recent years, humic compounds are used for soil remediation and reinstatement. Interest in them has grown since it was revealed that the humic compounds are capable of binding heavy metals' (zinc, lead, arsenic, chromium, nickel, etc.) radionuclides and toxic forms. Formatted compounds and complexes stay stable and remain sustainable for more than 100 years towards chemical and microbiological impact. Another effective solutions are humic compounds to organic eco toxicants. As a result of their exposure to petroleum hydrocarbons and oil, contamination of the substrate decreases 6 times in 1,5-2 months, while the content of pesticides in soil and chloricbiphenyls - nearly 100 times in 50-60 days [1].

While treating the contaminated soil with humic compounds, the ion-exchange, adsorption and coagulation processesare going at the same time, which provide effective soil readjustment (detoxification). Layers are formed, in which a variety of toxicants and humic compounds produce (in pH wide range), practically non-migratory, stable and steadycompounds - hardly accessible for microorganisms [2].

The research aims to develop a method of ecosystem restoration for polluted soil fertility saving methods.

Multicomponent pollution cleanup requires natural ecological systems self-activation process, when all three soil biological agents (bacteria, fungi, plants root system) are supplied with food substrates with easily digestible form. We will use local coal and peat oxidized forms, enriched with micro-elements. Disintegrative compounds usually degrade easily and quickly, buthigh-molecular part requires more time.

Accelerated phytoremediation process is necessary because of the long period of degradation. In this case we will provide high silicon containing natural concentrates that accelerate the growth of the plant's root system, resistance to stress, improve mechanical strength. In addition, adding natural boronminerals will also reduce the number of toxins [3].

It is possible to increase efficiency in humic compounds with active silicon. High silicon-containing supplements can be produced using natural diatomaceous earth in Akhaltsikhe. Changing silicon containing mineral (diatom) to liquid silicon dioxide decreases acids content in humic compounds. This compounds could be used together as an innovative research project.

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A MATHEMATICAL REPRESENTATION OF ELECTROANALYTICAL FUNCTION OF THE SAFRANIN-MODIFIED RADICALLY-PRETREATED MATERIAL TO HYDROQUINONIC COMPOUNDS

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Conducting polymers (CP) are one of the most studied classes of materials during the last 5 decades [1]. As they have "tunable" properties, they have vast and rich spectrum of use.

One of the most important aspects of their use is the development of chemically modified electrodes for sensor and biosensor. For the case of CP, the modification may be realized by:

- covalent modification;
- entrapment;
- doping;
- adsorption.

In the mentioned cases, the modifier and modification technique were correspondent to the analyte nature. For example, for quinone-hydroquinonic system many modifiers were developed [2 – 3] - each one with its own advantages and disadvantages. The elaboration of these techniques includes some difficulties, like the indecision in the action mechanism and the sensor and the presence of different electrochemical instabilities. The both problems may be resolved with the help of the mathematical model, adequately describing the electroanalytical system.

In the work [3], the safranine-modified polymer electrode has been used, and its supposed mechanism may be represented below:

In this work, it was shown, that the best electrochemical response for safranin modified polymedic electrode may be given in neutral pH range. The oscillatory and monotonic instabilities in this system are provoked by DEL-structure changing factor.

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NMS-T-16

THE MATHEMATICAL REPRESENTATION OF THE ELECTROANALYTICAL FUNCTION OF IONIC LIQUIDS IN THE HYDROQUINONIC COMPOUNDS´ DETECTION

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The use of chemically modified electrodes is one of the tools, frequently used in the electrochemical analysis. Its principal advantages are flexibility in use, versatility in formation and affinity to the analyte [1 – 3]. On the other hand, the polyelectrolytes and ionic liquids are one of the mostly used electroanalytical modificators, due to their reactivity and conductivity. Nevertheless, its function strongly depends on pH and also may be affected strongly by possible electrochemical instabilities. Thus, a theoretical evaluation of the modificator mechanism of action is necessary for the development of an electroanalytical technique.

In the works [1, 2] the ionic liquid was used without quitosane and in the work [3] it was used. Comparing the current – pH curves, obtained for both of cases, the pH of the peak for the work [3] was shifted towards the lower values, than in the works [1 – 2] (Fig. 1).

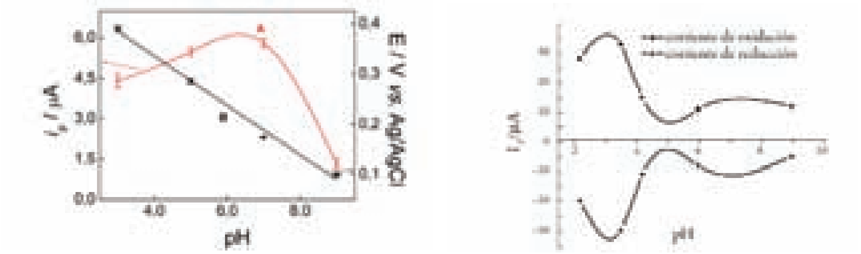

Fig.1. The I – pH curves of the electroanalytical system of carbon paste electrode, modified with ionic liquid without [1] (leftwards) and with [3] (rightwards) quitosane

It may mean that quitosane, a strongly basic polyelectrolyte, affects strongly the electroanalytic system, participating in the acid-basic equilibrium.

In this work, this influence is studied by mechanistic theoretic means, by development of a mathematical model, including the presence of quitosane, and its comparison with the model, referring to the system [1], described in [2].

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A THEORETICAL EVALUATION OF CoO(OH) WORK AS AN ELECTRODE MODIFIER FOR ELECTROANALYTICAL PURPOSES

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Chemically modified electrodes are an excellent tool for electroanalytical purposes for different compounds. Their advantages are efficiency, rapidity, exact and precise response and affinity to the analyte (due to the key – lock principle). The last factor is principal in the matter of choosing the electrode modifier [1].

On the other hand, cobalt(III)oxyhydroxyde (CoO(OH)) is seen by researchers as an alternative for titanium (IV) oxide, cause it is a p-type semiconductor and may be used as a photo, photoelectro and electrocatalyst. The investigation of its electroanalytical function has begun recently [2 ,3].

Nevertheless, there are some difficulties in possible use of CoO(OH) as an electrode modifier. Firstly, its electroanalytical properties´ investigation has been commenced recently, so there is still indecision, concerning the most probable mechanism of its action. Secondly, its electrosynthesis may be accompanied by electrochemical instabilities, also characteristic for the oxidation of small organic molecules and heterocyclic compounds´ electropolymerization [4]. Both problems may obtain their solution, if the electrochemical system gains a rigid theoretical base, which may only be given by a development and an analysis of a mathematical model, capable to describe adequately the system´s behavior.

So, the aim of our work is the theoretical investigation for the procarbazine electrooxidation on CoO(OH).

It´s possible to prove, that the optimal analytes for CoO(OH) are those capable to be oxidized in neutral or lightly alkaline media ($7<=pH<12$). Acidic and strongly alkaline media may lead to material dissolution. The electrochemical oscillations in this system are possible, caused by surface and electrochemical factors.

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NMS-T-18

CONSUMER FERTILIZER – ZEOLITE NANO-MATERIAL SATURATED WITH MACRO- AND MICROELEMENTS

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The effective way to achieve the nutrition regime of plants is to use mineral and organic fertilizers. Their effectiveness is quiet low: after introduction in the soil part of nitrogen fertilizers goes washed, and part of phosphoric fertilizers is easily eliminated by the soil which turns it into insoluble iron or aluminum phosphorus salts. That’s why the coefficient of utilization of such fertilizers is as low as 15-25%.

Natural zeolites are widely used in agriculture. Bringing mineral fertilizers along with zeolite provides the duration and reduces leaching of fertilizer and nutrition elements from the soil.

New nano technological method for preparation of anionic exchangers is proposed, which is based on involving ammonium dihydrogen phosphate into zeolite structure without disrupting the structure of zeolite and formation of new phase with anion exchanging properties. Due to molecular-sieve features of zeolite, ammonium cations and phosphoric anions involved in its structure transfer in the soil gradually, interaction of anions with ions in the soil happens to a minimum level that maximizes the effectiveness of fertilizer.

New material preserving zeolite structure, enriched by phosphorus and nitrogen, and containing boron, zinc, manganese, molybdenum and copper on nano level is proposed. Such microelement-containing fertilizer due to its multifunctional universal characteristics can be used for almost all types of agricultural crops both in open field and greenhouses, as well as in sapling farming and at home on decorative plants.

NMS-T-19

INHIBITORY EFFECT OF RESVERATROL FOR ALUMINUM CORROSION IN ALCOHOLIC SOLUTIONS

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This paper presents experimental results obtained using resveratrol as corrosion inhibitor for aluminum in ethanol solutions. Resveratrol (3,5,4′-trihydroxy-trans-stilbene) is a stilbenoid, a type of natural phenol, and at the same time a phytoalexin produced naturally by several plants as a response to the injury or attacks by pathogens such as bacteria or fungi [1-2]. As a chemical entity, it is known since 1940, when it was first isolated from the roots of white hellebore (Veratrum grandiflorum) and later from Polygonum cupsidatum, a medical plant [3]. Food sources of resveratrol include the skin of grapes, blueberries, raspberries and mulberries, as well it can be found in wines [4].

Resveratrol exists in two isomeric forms, as trans- and cis-resveratrol, whereas the trans-form is the most abundant one [5-6]. Both isomeric forms have been detected in wines. However, trans-resveratrol can be easily converted into its cis-isomer under the influence of heat and UV-light [6].

The electrochemical behavior of resveratrol in ethanol solutions was examined by cyclic voltammetry on platinum and aluminum electrodes. The oxidation process of resveratrol on platinum or a both electrodes is complex, pH dependent, and all its steps are irreversible.

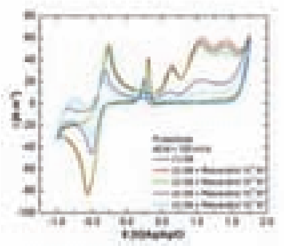

Figure 1. Cyclic voltammograms (5 cycles) in 0.25M Na_2SO_4 (SB) in absence and presence of resveratrol different concentrations, scan rate 100 mV s^{-1}.

Further, the inhibitory effect was studied by linear polarization and Tafel method in order to determine the kinetic parameters, providing information about the inhibitory mechanism. The diminution of corrosion rate of aluminum in the presence of resveratrol can be attributed to the adsorbtion of resveratrol on the metal surface, blocking the active sites, or depositing corrosion products on the aluminum surface.

The inhibitory properties of resveratrol on aluminum corrosion process offers considerable prospects for the wine or other alcohol industry, also, defining it as a natural or eco-friendly corrosion inhibitor in alcoholic media.

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ESC

ENERGY SOURCES, CONVERSION AND STORAGE

THE FORMATION OF INTERMOLECULAR C-C BONDS AS A FUNCTION OF TEMPERATURE WITH PARTICIPATION OF C_3-C_4 ALKANE

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It is known that, conversion of gaseous hydrocarbons to aromatic and alkylaromatic hydrocarbons occurs on modified HZSM-5 zeolite catalyst. Also it is known that, sulphated and tungstened ZrO_2 can activate C_3-C_7 alkanes at low enough temperatures. Combination of features of these catalytic systems can enable to make contacts which are capable to involve gaseous alkanes for making valuable liquid hydrocarbons at relatively low temperatures.

Current report is dedicated to study the influence of temperature on activation of conversion propane to liquid hydrocarbons on composite catalysts ZSM-5/WO_4^{2-}(SO_4^{2-}) ZrO_2 (HZSM/(W/S)Z) and their components.

Conversion of C_3H_8 and C_3H_8:CH mixture (where CH=C_6H_6, C_7H_{16}), also the mixture of natural gasoline with associated petroleum gas were studied at prototype laboratory catalytic installation provided with quartz reactor. The experiments were done with varying temperature from 140º to 600º and reactant delivery rate from 250 $h^{-1}$to 1000h^{-1}. The analysis of conversion products are carried out chromatography.

Conversion of propane (I) and its mixture with benzene (II) and n-heptane (III) and their components by forming intermolecular C-C bonds were studied at temperature range of 140º - 600º by using composite catalysts (CC) ZSM-5/WO_4^{2-}(SO_4^{2-})ZrO_2 (HZSM/(W/S)Z) and their components. Unlike aromatization of (I) (400-600º) and alkylation of (II) (300-450º), involving (I) to process with (III) happens at 140-220º. Possibility of involving (I) and butane (4-10%) to low temperature processes (140-220º) with C_{7+} alkanes were shown on the example of conversion joint natural gasoline and associated petroleum gas by forming C_5-C_6 alkanes-isomerization and disproportionation products. It was assumed that reaction of aromatization of (I) and alkylation of benzene with (I) including initial activation of (I) on the zeolite component of CC, but involving to the process forming intermolecular C-C bonds of C_3-C_4 alkanes is connected to bimolecular activations of the C_3-C_4 with participation of oxygen W/(S)Z of CC component.

Stages realization reactions by forming intermolecular C-C bonds between I-C_4 and C_{7+} on the CC can be foundation to produce high-quality gasolines from associated petroleum gas.

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PHOTOVOLTAIC MODULE

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Barack Obama nominated U.S. Energy Initiative. In accordance with this emphasis should be placed on solar energy. Vast deserts of Arizona and Nevada to be covered with solar panels. According to the plan put forward by 69% of all electricity and 35% of the heat energy in 2050 will be provided to solar energy. It was under this will be, first and foremost, “sharpened” American nanotechnology program. By 2015, on current forecasts the market nanotechnology products to exceed $1 trillion dollars. A significant portion of those will be made in the USA. According to U.S. estimates it would require training of about 800,000 professionals to work in this area. Therefore especially important to develop photovoltaic module. The photovoltaic module is used in energy, namely solar power plants with radiation concentrators designed for power, autonomous or centralized power system. Established PV module design [1], cost-effective, technologically simple, reliable virtually created so that the Fresnel lens made of silica glass are rounded and separated from each other, heat sink plate with connecting parts in contact with the cooling element in the form of a copper rectangular tube. Fresnel lenses collect the sun’s rays at the focal point. Each lens has its own solar cell, mounted on a metal cooling plate and each lens is firmly connected to the terminals. Light-receiving surface of the solar cells are located at the focal point of the lens. A solar cells, in turn, are located in the centers of the heat-removing metal plates. Heatsinks with photocells, located on the iron plates, which are connected rods. Iron plates connected with the water-cooling system with connector parts. Centralized water cooling system keeps most of the solar cell heating. Photovoltaic module includes round lenses of silicate glass, photovoltaics. Heat metal plates, centralized water, connecting rods, and a metal reflector plate outside, and the lenses are separated from each other and have a round shape. This increases their safety. The module has a thin outside reflector plates welded Kemp, tight. Heatspreader with connecting parts in contact with the cooling element. It’s a copper tube with a thin hole for the flow of water during the centralized system of modules for cooling through a central pumping station. This system allows full use of quantum energy. Sun, which fell into the module. Most of the quantum of energy absorbed by photocell is converted into heat. This heat energy is transferred to the cooling plate with high thermal conductivity and photo converters using plate heat water, which flows through the copper pipe. As a result, the quantum energy is converted into electrical energy used to heat water. This process is designed to work modules in large quantities and in a centralized system. The result is to increase the energy performance of PV modules, ensuring quality and reliability in emergencies, relief, need technology with high accuracy, using simple and inexpensive materials, facilitate technology structure and assembly. Fresnel lens perpendicular to the sun’s rays fall. The rays are concentrated and collected in one spot. Collected flows beam fall on the photocell and obtained photovoltaic effect, electrons are released and there is current in the circuit.

Reference:

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SPINELS $LiM_xNi_{0.5-x}Mn_{1.5}O_4$ – Type (M=Co+Cr, Al AND Cu; $0<x\leq 0.4$) AS PROMISING CATHODE MATERIALS FOR Li- ION BATTERIES

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Modern development of high technologies in the field of chemical power sources is associated with elaboration of new materials. Application of these allows to: decrease weight and dimensions of power sources, increase their energy capacity, capability and resourcefulness. Nowadays batteries represent very important technological object. Electrodes (anode and cathode) and electrolyte are the three major components of most batteries, including lead-acid batteries used for startup of car engines, as well as wildly used compact lithium cells widely used in different applications (e-books, watch, etc.). All developed countries intensively search for the above components that would be efficient in terms of price and operational performances, to apply them in the new types of batteries. Lithium-ion batteries (LIB) are now ubiquitous.

The goal of the work was elaboration of phase pure nanosized modified $LiM_xNi_{0.5-x}Mn_{1.5}O_4$ type compounds (M=Co+Cr, Al и Cu) based on lithium, manganese, nickel acetates and dopants. These compounds will be able to provide high cyclic and electrochemical characteristics as cathode materials of LIB. In order to elaborate samples, we used two step method based on thermal decomposition of eutectic mixture of initial reagents (Li, Mn, Ni acetates and dopants –Co, Cr, Cu and Al).

The carried out investigations confirm that simplified synthesis methods enable preparation of nanosized (d=10÷20 nm), phase pure substituted lithium manganese spinels. The multiple doping causes a decrease of lattice parameter. The above mentioned can promote increasing of spinel's stability during cycling at elevated current densities, as well as while storing with the contact with electrolyte. It can be assumed that doping helps to remove impurities and stabilizes the spinel structure at the stage of the synthesis of samples of a given composition. Stabilization of structure and increase of theoretical capacity due to smaller molecular wage of dopen elements (Cu,Al), compared to nickel, can improve the discharge capacity. The developed compounds can be used as cathode materials in the 5V region of potentials. Since role and importance of LIB increases not only for portable electronic devices, but also for application in high power electric vehicles, the developed compounds could be of interest for next generation of Li-ion batteries.

ESC-O-04

PRODUCTION OF BIODIESEL USING SUPERCRITICAL FLUIDS TECHNOLOGY

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Biodiesel is mono-alkyl esters of long chain fatty acids derived from vegetable oils or animal fats, i.e. bio resources though the process of esterification. Biodiesel is a high quality fuel which can be used in any segment of industry where petro-diesel is used, including the internal combustion engines.

Development of biodiesel industry can contribute towards growing national GDP; create new businesses and new jobs, strengthening the country's energy and economic independence.

The greatest advantage of biodiesel is the consequence that biodiesel is an eco-friendly fuel. Biodiesel is renewable and sustainable and can significantly reduce danger of environmental disasters.

Recently Georgia has signed the Paris Climate Agreement 2016 and has taken obligations to reduce GHG emissions and develop renewable, eco-friendly energies, therefore by launching and developing biodiesel in the country Georgia will meet these obligations and responsibilities.

In 2012-2015 years a pilot project "Biodiesel in Georgia"started at Ilia State University. A new lab for producing biodiesel was launched and today it is fully operational. The lab can produce up to 0.5 tons of biodiesel daily. The preliminary analysis of biodiesel received from both plant oil and the secondary cooking oil, have shown that the characteristics of biodiesel both B100 (pure biodiesel) and B20 (a blend 20% biodiesel mixed with 80% petroleum diesel) are quite similar to those of petroleum based diesel fuel. The test showed that biodiesel **B100** produced in the lab of Ilia State University met standards defined as ASTM D 6751. Thus the project of Ilia State University has theoretically proven and practically demonstrated that Georgia can start production of its alternative, renewable eco-friendly fuel – biodiesel and bring economic and ecological benefits.

Since biodiesel is intended to be used in internal combustion engines, the physical and chemical parameters and characteristics of pure biodiesel - **B100** and the **B20** blend were further carefully analyzed and compared to those of a conventional petroleum diesel fuel. Each character was studied according to the existing standards. The physical and chemical parameters of biodiesel were analyzed using ***SPECTRUM Version 10.4.2.PerkinElmer.*** As the results have shown, the spectrum of **B100**, **B20** and petroleum diesel are quite similar.

The composition of fatty acids in B100 and B20 were defined by using a liquid chromatographer and the functional groups by **Spectrum Two spectrometer**. The conducted analyses and results have clearly demonstrated that the physical and chemical parameters of both **B100** and **B20** were within the standards of EN 14214, ASTM D6751 and EN 590.

For the industrial scale production of biodiesel the modern method of Saka-Dadan has been analyzed. This method, named Supercritical Fluids Technology, uses supercritical methanol as the area for esterification reaction. This innovative method ensures quick esterification of the fatty acids of the oil in the area of supercritical methanol, where the reactions of transesterification and esterification run successfully and quickly, without catalyzers.

The traditional method with catalyzers implies two necessary steps – cleaning and washing, whilst for the supercritical fluids these two steps are no more needed and the total time of reaction is reduced to 4-10 minutes all that can significantly reduce production expenses and the final price of biodiesel too.

Thus the research has shown that the modern method of supercritical fluids i.e. esterification of the fatty acids in supercritical fluids, has good potential to be used in the industry for biodiesel production.

ESC-O-05

SYNTHESIS OF TiO_2 NANOTUBES BY Ti FOIL ELECTROCHEMICAL DISSOLUTION FOR DYE-SENSITIZED PHOTOELECTROCHEMICAL SOLAR CELL

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The growing demand for clean energy in combination with the depletion of fossil fuel resources and climate change issues such as global warming have prompted an urgent need for environmentally sustainable energy sources. Renewable energy can be obtained from sustainable resources. Solar energy from the sun holds the most promise as an alternative energy source because the supply is essentially unlimited and free.

Goal of the project is the preparation of TiO_2 nanoparticles for dye-sensitized photoelectrochemical solar cell. In the work is describing a new method of TiO_2 electrogeneration from Ti foil anodic dissolution. TiO_2 naoparticles have been obtained by Ti foil anodic dissolution in 0.1-1M HCl solution, where 30% hydrogen peroxide solution drop by drop has been added, cathode was stainless steel foil, and current density in different tests has been changed from 0.2 A/cm^2 to $1A/cm^2$, voltage has been changed from 8v to12 v correspondingly. Electrochemical processes have been carried out at 90^oC degree with steering rate 800 rpm. TiO_2 directly has been obtained in electrolyte solution. This method gives us opportunity to control size of generated TiO_2 particles by changing of process current density and hydrogen peroxide addition rate. TiO_2 nanoparticles have been investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM) and dye-sensitized photoelectrochemical solar cell has been made. The TiO_2 particles with sizes 50-500 nm have been obtained.

Dye-sensitized photoelectrochemical solar sell was made by using TiO_2 with particles sizes ~50 nm and 250 nm. The photo anode (4x4 cm) was made by two layers TiO_2. The first layer was TiO_2 with particles size 50nm and the second layer consist particles with ~250 nm. The photo anode substrate was ITO glass. The cathode was made by ITO glass and Pt catalyst. As a dye was used Ruthenizer 535-bisTBA (from Solaronix SA). $I^-/I3^-$ acetonitrile solution was used as a electrolyte. As a light source was used Xe lamp with power 50 mvt/cm^2.

Electrochemical properties (i-V and I-P c curves) of solar cell are shown in the figure 1. Open circuit voltage is 0.63v, short circuit current is 12 mA/cm^2, maximum power is 4 mvt/cm^2 and current at the maximum power is 7.5 mA/cm^2. Fill factor ff - 0.538, light energy convert efficiency - 8.01%.

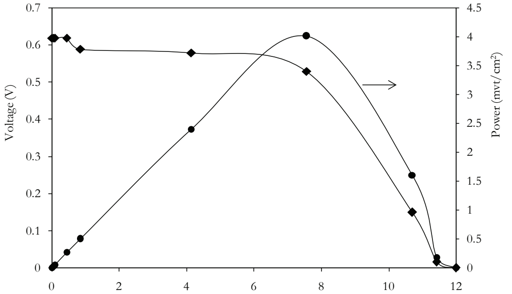

Figure 1.Electrochemical properties (i-V and I-P c curves) of solar cell

ESC-O-06

AN ELECTROCHEMICAL METHOD OF OBTAINING OF THE ACTIVE MANGANESE DIOXIDE POWDER FOR CURRENT SOURCES

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The electrochemical way of synthesis of the manganese dioxide (MD) can be briefly presented as two successive reactions:

$$Mn^{2+} - e^{-} = Mn^{3+} \qquad (1)$$
$$2Mn^{3+} + 2H_2O = MnO_2 + Mn^{2+} + 4H^{+} \qquad (2)$$

Industrial way includes its obtaining as a compact sediment at the anode from the solutions containing relatively low concentration of sulfuric acid (20-40 M) at the temperature of about 90 °C and the low anodic current density (80-100 A / m^2). Under conditions of high concentrations of sulfuric acid (~ 200 M), at the room temperature and the high current density (600-1000 A / m^2), the equilibrium of reaction (2) is strongly shifted to the left, the intermediate Mn^{3+} ion is more stable and has time to go into the solution where reactions of disproportionation and hydrolysis take place (2). This method provides getting the fine powder of manganese dioxide. It can be used as an adsorbent, catalyst, oxidizing agent, etc. However, it is not suitable for the current sources.

The aim of this work was preparation of active manganese dioxide powder in the electrolyte solution, acceptable for power sources. This method has a number of significant advantages over the anodic electrodeposition of compact manganese dioxide: the energy is not wasted on heating the solution, there is no evaporation of the electrolyte (which creates environmental problems) and, most importantly, there is no need of mechanical removal of manganese dioxide precipitate from the anode surface (which often leads to damage of the electrode) and further grinding of large pieces.

We studied the effects of organic additives in the working solution on the electrochemical properties of obtained manganese dioxide powder. A number of organic substances, mainly hydroxyl group-containing (starch, sucrose, glucose, ethylene glycol) greatly improved its electrochemical characteristics. The activity of manganese dioxide was explored in the alkaline battery model. Electrode, prepared on the basis of MD powder was served as a cathode and zinc powder was used as an anode. The discharging of the battery was occurred in the galvanostatic conditions at 50 mA current up to 0.9 V. The electrochemical activity of MD was evaluated by the time spent on the discharging. It was demonstrated that MD powder, produced without any additives, was discharged for 90 minutes, while our best examples discharged within 150-160 minutes. The discharging time of the Industrial samples is 140 minutes, on average.

SOLID POLYMER ELECTROLYTES ON THE BASIS OF BRUSH TYPE ORGANOSILOXANE POLYMERS

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There is extensive information in the literature about brush type methylsiloxane polymers with various organic nature branching fragments which are used as solid polymer electrolyte membranes as an electro storage devices in Lithium elements. Because of that, the synthesis of new organosilicon copolymers with various lengths of side electro donor branching fragments is relevant. Polysiloxanes having side acrylate and methacrylate groups can reveal electro donor properties, as well as it is possible chemical reactions on the esteric groups.

Presented work is dedicated to synthesis of comb-type methylsiloxane oligomers with various ester side fragments and investigation of their properties. It must note that the acrylate and methacrylate are conjugated systems and the hydrosilylation reaction may proceed differently.

The hydrosilylation reactions of α,ω–bis(trimethylsiloxy)methylhydrosiloxane (PMHS) ($n \approx 35$) with acrylate and methacrylate in the presence of platinum hydrochloric acid and platinum on the carbon Pt/C have been investigated at various temperatures. It was established that complete hydrosilylation of all active ≡Si-H groups do not take place and various-linked oligomers are obtained. For hydrosilylation reaction the reaction order, rate constants and activation energies were found. The structure of synthesized oligomers was determined by FTIR and NMR spectral data. For oligomers with long side groups by NMR spectra data the existence of conformers was confirmed. For synthesized oligomers gel permeation chromatography, differential scanning calorimetric and wide-angle X-ray roentgengraphic investigation has been carried out.

On the basis of synthesised oligomers solid polymer electrolyte membranes have been obtained via sol-gel processes of oligomer systems doped with lithium trifluoromethylsulfonate (triflate) or lithium bis(trifluoromethylsulfonyl)imide. For solid polymer electrolyte membranes the dependence of ionic conductivity as a function of temperature and salt concentration has been investigated. It has been found that the electric conductivity of the polymer electrolyte membranes at room temperature changes in the range $4x10^{-5}$ – $6x10^{-7}$ S/cm.

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ESC-P-02

ELECTROCATALYTIC PROPERTIES OF NANOSIZED TITANIUM DIOXIDE FILMS MODIFIED BY La AND Nd

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Titanium dioxide is a promising material for application in environmental photocatalysis, for the generation of electricity in the solar and fuel cells, gas sensors, optical and protective coatings, electrochemical devices, as oxygen reduction catalyst etc. [1, 2]. The catalytic activity of titanium dioxide increases greatly when nanoparticles are used. This paper presents results of studying the electrocatalytic characteristics of electrodes based on nanosized titanium dioxide films modified by La and Nd in the case of oxygen electroreduction.

Electrocatalytic films based on nanosized titanium dioxide modified by La and Nd were produced by sol-gel method on a Ti substrate from solutions containing titanium chloride, lanthanum and neodymium nitrate; after which the electrodes were annealed in air at 430-500^{0}C. The prepared samples were characterized by using transmission electron microscopy, x-ray diffraction, x-ray photoelectron spectra, and ultraviolet-visible photocurrent spectra. The average size of nanoparticles was no more than 10 nm, the average thickness of the deposited layers was 300 – 1000 nm. The XRD results indicated that TiO_2, TiO_2/La and TiO_2/Nd electrodes calcined at 430°C consisted of anatase as the unique phase. The photocurrent spectra of the TiO_2/La and TiO_2/Nd electrodes showed a stronger current in the UV range and a shift in the flat-band potential (E_{fb}) towards more negative values than that of TiO_2 electrodes (Table 1).

Catalytic properties of TiO_2, TiO_2/La and TiO_2/Nd electrodes were investigated in the processes of oxygen electroreduction in physiological (0,9 %) solution of NaCl. It has been found by I-E curves measurements that the potential of oxygen reduction varies from the film composition (Table 1).

Table 1: Influence of Nd and La on electrocatalytic characteristics of TiO_2 films in 0,9 % solution of NaCl. $T_{anl.}$=430^0**C**

№ п/п	Sample	Potential of oxygen electroreduction E_{O2}, V	Width of "electrochemical window" ΔE, V	Flat-band potential, E_{fb}, V	Band-gap E_g, eV
1	**TiO_2**	**-0.60**	**0.17**	**-0,3**	**3,2**
2	**TiO_2/Nd**	**-0.49**	**0.24**	**-0,54**	**3,1**
3	**TiO_2/La**	**-0.43**	**0.25**	**-0,60**	**3,2**

By XPS measurements it has been found that the surface of TiO_2 electrodes is formed from non-stoichiometric titanium oxide $TiO_{1.91}\cdot(OH)_{0.09}$ and its hydroxide phase. Therefore the high electrocatalytic activity of TiO_2 nanoparticles in the oxygen reduction process may be due to the formation of catalytically active Ti^{3+} centers and to the presence of OH groups in the oxide matrix.

It is shown that modifying of TiO_2 films by neodymium and lanthanum improves catalytic activity of TiO_2/Nd and TiO_2/La electrodes in the reaction of oxygen electroreduction, which is manifested in decreasing of oxygen reduction potential E_{O2} and increasing of dynamic range of O_2 electroreduction potentials («electrochemical window» ΔE). The correlation between electrocatalytic activity of electrodes and energy position of conduction band E_{fb}, is determined.

The modifying TiO_2 electrodes characterized by a high sensitivity to dissolved oxygen ((4-5)$\cdot 10^{-6}$ g/l) and high reproducibility of characteristics in long-time cycling. These electrodes are promising for use in electrochemical sensors for the determination of oxygen in liquids, for example, in blood plasma.

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CATALYTIC CONVERSION OF BIOETHANOL INTO VALUABLE PRODUCTS

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Currently, due to the increasing global consumption of fossil fuels and the reduction of oil reserves being an active search for a replacement of traditional hydrocarbons. One of the available alternative sources of raw material is biomass, a major transformation in the traditional way which is its fermentation into bioethanol. Using catalytic methods it is available to produce from ethanol aromatic and aliphatic hydrocarbons of different structure [1]. This process is analogous to methanol conversion process MTG (methanol - to-gasoline) known as ETG (ethanol-to-gasoline) [2].

In this paper, we tried to evaluate the possibility of the production of olefins and aromatics from bioethanol - one of the most promising alternative raw material sources. In this regard, the following are of producing aromatic hydrocarbons from ethanol over different catalysts.

The studies of the catalytic conversion of ethanol was carried out on an automated flow installation. We used catalysts of the following composition: CuO / γ -Al_2O_3; CuO / SiO_2; ZnO / γ -Al_2O_3; ZnO / SiO_2; ZrO_2 / γ-Al_2O_3; ZrO_2 / SiO_2. Testing the activity of the catalysts in the conversion of ethanol, which is characterized by the conversion of ethanol, was carried out on an automated flow catalytic unit (PKU - 2). The feedstock used 95% ethanol.

The best yields of liquid and gaseous products are observed on bioethanol conversion process at temperatures of 250-300° C and a space velocity of 60 hr^{-1}. The results showed that the yield of aromatic and gaseous hydrocarbons depends on the catalyst composition and process conditions of the process. The optimal catalyst at reaction condition of the T_r = 250° C, W = 60^{-1} in bioethanol reforming for producing aromatic hydrocarbons was ZrO_2 / γ -Al_2O_3, where the concentration of xylene in the reaction products was 26.5 vol.%. The best catalyst for producing ethylene among the studied catalysts is ZnO / SiO_2, where the yield of C_2H_4 is 57.8 % at 300^0C. The highest yield of hydrogen (25.1 vol.%) is observed over the 1% CuO / γ -Al_2O_3 catalyst.

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ESC-P-04

NEW APPROACHES AND TOOLS FOR REHABILITATION OF CHEMICALLY CONTAMINATED SOILS

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Elaboration and development of the cleansing technology from chemical contaminants, also prevention of environment is the key and challenging ecological problem of the mankind. Successful and ecologically friendly method of cleansing of environment is a phytoremediation – selection and purposeful planting of those plants, roots of which provide uptake and enzymes to transform the molecules of toxicants from environment.

Phytoremediation in comparison with other nonbiological and biological technologies has great advantages. Nowadays it is very actual to use complex approaches, which provide effective and successful remediation technologies.

Presented work is directed to expel the shortcomings of phytoremediation and by this way provide effective resolution of the problem of soil/water contamination at different cases of contamination.

Nowadays contamination of environment by oil hydrocarbons, pesticides and heavy metals is important problem for Georgia.

Elaboration of a new type phytoremediation technology, giving in presented work, based on joint application of natural sorbents, microorganisms and plants. They will allow avoiding the problem of chemical contamination of soils. It will provide restoration of polluted environment and cease for long period of time avoid dissemination of toxic compounds from pollution hotbeds. Presented complex biotechnology has preventive importance. This technology can be applied to polluted soils by heavy metals, oil hydrocarbons, explosives, pesticides and other pollutants.

The main idea and novelty of the carried out work is development a novel approach for the ecological safety. The approach based on using natural minerals composites which are comprised of natural mineral rocks, microorganism strains having high detoxification ability and plants-phytoremediators. In this composite material, the function of the sorbent is to uptake the pollutant and ceases its distribution into the environment. The role of the microorganisms is to accomplish first stage of organic contaminant biodegradation and then application of phytoremediation as a unique cleanup strategy. Natural sorbent can be applied during the initial stage cleaning of polluted soil, followed by application of a phytoremediation technology through planting of purposeful vegetation. This results in the total assimilation and mineralization of pollutants and/or their intermediates of their partial transformation by microbes.

According to presented work, it was used wide spectrum of contaminants: heavy metals – Cu and Pb, organochlorine pesticide – DDT, explosive – 2,4,6 trinitrotoluene (TNT) and oil hydrocarbon (hexadecane). Attention have been paid to enhancement of soil fertility, which improves microorganism and plant growth conditions and is important for bioremediation processes providing soil total rehabilitation.

ELECTROCHEMICAL CO-DEPOSITION OF ANTIMONY WITH SELENIUM FROM TARTRATE ELECTROLYTES

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Creation of different semiconductor materials, high-quality films is one of the main tasks of modern semiconductor electronics and solar photovoltaics.

The advantage of electrochemical method for preparing these semiconductor films is that it allows solving the problem of producing photoconverters of solar energy in large areas.

One of the most promising representatives of semiconductors is antimony selenide (Sb_2Se_3). For obtaining thin films on the basis of $Sb_2Se_3$from tartaric acid electrolytes, particularly, we separately studied the kinetics and mechanism of antimony electrodeposition and selenium. Cyclic voltammetry method was used to study the electrochemical reduction of these ions from tartaric acid ($C_4H_4O_6$) solutions.

Polarization curves show, that cathodic reduction of antimony in these solutions begins at potential of -0.44 V and proceeds up to maximum -0.54 V. It means that reduction of Sb on Pt electrode occurs at single stage (fig. 1).

However, during cathodic reduction of selenium on investigated electrode, 2 peaks were recorded on polarization curves. These peaks show, that deposition of selenium on Pt electrode is 2 step process (fig. 2).

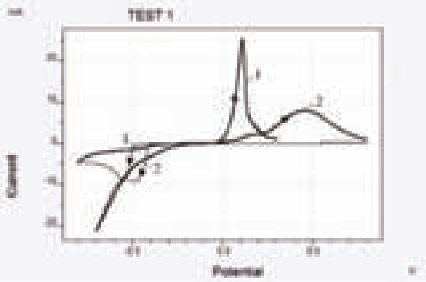

Fig. 1. Polarization curve of antimony (1) and alloys antimony-selenium (2).Composition of solution (mol/l): 1- 0.05 SbOCl+0.007 $C_4H_4O_6$; 2- 0.075 SbOCl+0.025 H_2SeO_3 + 0.007 $C_4H_4O_6$, scan rate - 0.02 V/s, pH=1.7, T=296 K.

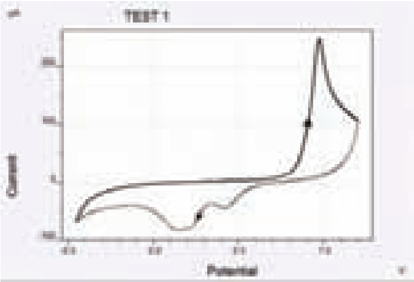

Fig.2. Polarization curve of selenium. Composition of solution (mol/l): 0.08 H_2SeO_3+0.007 $C_4H_4O_6$, scan rate - 0.02 V/s, pH=1.7, T=296 K.

Fig. 1 (curve 2) demonstrates the cyclic polarization curve of the electrochemical co-deposition of antimony with selenium. As can be seen, electrochemically co-deposition of these elements from tartaric electrolytes takes place single stage that begins at -0.47V potential.

Furthermore, the influence of different factors on the cathodic reduction process of the antimony and selenium ions separately and on their electrochemical co-deposition.

ESC-P-06

PUBLIC UNDERSTANDING OF NUCLEAR ENERGY

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The role of social sciences in energy studies is more and more appreciated and it is noted that such studies must become more socially oriented, interdisciplinary and heterogeneous. Problem-focused research activities that centre on both physical and social processes, include diverse actors and mix qualitative and quantitative methods, have a better chance of achieving analytic excellence and social impact [1,2].

The practice of social life shows that the growing impact of energy technology has brought science ever more into our daily lives. However, the public is left with nothing to counterbalance the pervasive influence of science and technology. The role of science communication is to remedy this lack and bring achievements of science into the public eye and to the attention of important stakeholders such as politicians and industry.

Therefore, in the present study we have conducted a review of scientific papers in terms of public understanding of science and technology including public understanding of nuclear energy, we have identified several major areas of problems including public understanding of science and technology [3], risk perception and communication [4], stigmatisation and decision-making processes [5].

European countries which have nuclear power plants use various tools for information distribution, communication and involvement of stakeholders in nuclear projects. This diversity is connected with many factors, among which are: the democratisation level of the state, social expectations about the commitment level, energy culture, political culture, the experience of the countries in nuclear projects implementation or stakeholder involvement and the decision-making phase [6]. Distinguishing marks of good communication and participation in energy projects include the recognition of different interests and perceptions of the local community; understanding of local communities; communication addressed to specific groups vital from the point of view of acceptance; transmission of information by means of tools and channels compatible with the needs of the population; continuous dialogue with local groups, especially those who are in opposition. The indicated factors should be taken into account both at the national and local level, as the differences in national and local contexts create different conditions for the emergence of social acceptance. The issues of inclusion of stakeholders are recognised, among others, by international organisations such as the Organisation for Economic Cooperation and Development [8] or supranational ones like the European Union (EU) which attempt to develop public debate and show the value of inclusion of stakeholders in decision making processes related to energy issues.

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HYDROGEN GENERATION FROM THE HYDROLYSIS OF SODIUM HYPOPHOSPHITE USING CoB_2O_4 CATALYST

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The goal of the work involves a radically new approach – establishment of possibility of the use of sodium hypophosphite (NaH_2PO_2) as hydrogen source and study of the process of its reforming: synthesis of corresponding catalysts and their testing for generation of hydrogen. It is well known that in the process of chemical nickel plating at 80-95 ^{0}C, in the course of an interaction between sodium hypophosphite and water the formed atomic hydrogen reduces nickel on the surface of the plated metal. Nickel plating with the participation of sodium hypophosphite is self-catalytic [1]. Overall catalytic reaction of the interaction between hypophosphite and water may be presented as follows:

$H_2PO_2^- + H_2O \rightarrow H_2PO_3^- + H_2$ (1)

It is well known that in the absence of nickel-ions in the hypophosphite solution, and with the use of so-called Raney nickel catalyst, an intensive separation of hydrogen is possible at high temperatures (80-95 0C), but at room temperature the process practically stops. It was synthesis CoB_2O_4 catalyst, which can produces hydrogen from hypophosphite solution at room temperature and its use in fuel cell is possible.

The hydrogen separation at catalytic interaction between water and hypophosphite proceeds by electrochemical mechanism (the process occurs by electron transfer), according to which the hypophosphite-ion presents the distorted tetrahedron in the centre of which a phosphorus atom is located and at the ends of tetrahedron two hydrogen and two oxygen atoms are placed. Hypophosphite-ion is adsorbed at metal (catalyst) surface, hydrogen atom of which is connected with catalyst surface by covalent bond, attenuates P-H bond and finally cleaves it; hydrogen is replaced by hydroxide-ion from water (2, 3) which causes hypophosphite transformation in phosphite. Electron, atomic hydrogen and proton, formed by the reaction (3), produce molecular hydrogen (reaction 4):

$H_2O = H^+ + OH^-$ (2)
$H_2PO_2^-ads + OH^-ads = H_2PO_3^-ads + Hads + \bar{e}$ (3)
$Hads + H^+ads + e- = H_2$ (4)

Boron containing cobalt catalyst was synthesized [2,3], in an ultrasonic setup where a chemical beaker with 1 M $CoSO_4$ solution was placed. 20 mL of 0.6 M $NaBH_4$ solution was added dropwise into the beaker at the room temperature under the conditions of intensive mixing. The formed pulp was washed by distilled water. After drying, the deposit was annealed at the temperature of 450°C and finely dispersed black powder was obtained. In X-ray phase analysis of the sample, small peaks were observed in the X-ray diffraction pattern. They corresponded, according to the ASTM standard, to CoB_2O_4 (2.88,2.44, 2.03, 1.86 Å). In the work, the hydrogen evolution from aqueous solution of sodium hypophosphite was studied at 10-30 ^{0}C by CoB_2O_4 catalyst. In case of 2M NaH_2PO_2 solution hydrogen evolution rate was 3.4-3.6 ml sec^{-1} g^{-1}, which was enough for 0.6 W $H_2–O_2$ fuel cell operation.

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ESC-P-08

FUEL CELLS FOR ENVIRONMENTAL PURPOSES. PART I. SULFIDE AND NITRATE DRIVEN FUEL CELL

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Hydrogen sulfide and nitrates are persistent pollutants from various origins – domestic, industrial and natural. There are different methods for their elimination, but most of them are expensive and energy inefficient. The present study is an attempt for their removal with energy generation at the same time. By recombination of the waste fluxes of sulfides and nitrates the treatment of both of them can be achieved. The sulfides are oxidized to sulfates and the nitrates are reduced to nitrogen. The milestones in the processes for creating such a fuel cell are the choices of optimal design of the fuel cell and effective electrodes for minimizing the internal losses.

In this investigation a configuration that consists of two concentrically arranged compartments separated by a membrane situated at the bottom of the inner unit was studied. The experiments were carried with different electrodes and improved electroconductivity of the solutions by adding NaCl. A commercially available Celgard 3510 membrane was used. The electrical resistance of the fuel cell was decreased from 850 to 76 Ω after using pyrolized activated paddling and activated carbon instead of graphite rods for electrodes. The results for the depletion of the waste substances as well as the electrical indicators are given.

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THE FUNDAMENTAL AND TECHNOLOGICAL ASPECTS OF THE PROCESSING OF FLY ASH OF THERMAL POWER PLANTS TO PRODUCE NEW VALUABLE PRODUCTS FROM IT

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The most original and perhaps the most valuable components of fly ash from coal combustion at thermal power plant – hollow aluminosilicate microspheres (HAM), which are a hollow, nearly perfect form silicate beads with a smooth surface, with diameters from 10 to several hundred micrometers, an average of about 100 microns. The wall thickness from 2 to 10 microns, the melting temperature of 1400-1500 °C, the density 580-690 kg/m^3. The value of HAM is determined by the fact that they are perfect fillers for a wide variety of materials.

Fractional separation of aluminosilicate cenospheres of fly ash thermal power plant is performed on the developed laboratory installation in the upward vortex flow of the separation medium with superposition of multiple pulsation and the magnetic field of certain intensity. Using modern methods we studied the composition and structure of narrow fractions of definite composition, sorption properties of cenospheres optimal for obtaining a multifunctional porous materials in which the obtained powder and block materials with a regular porous structure.

On the basis of microspheres selected from fly ashes from the combustion of coal or lignite to thermal power we develop technology of preparation of modified catalysts: cracking of residual oil or heavy oil, allowing obtaining a fuel oil of up to 64 mass % of light fractions, including 14.5 % of gasoline and up to 85 % of light fractions from heavy oil, including 37 % of gasoline fraction; hydrocracking, hydroconversion and hydrotreating of hydrocarbons, which allows to increase the yield of gasoline with an octane rating of 83.1 to 54.2 mass %; the paraffins dehydrogenation in a fluidized bed, allowing to obtain at 580 ºC to 54-55 mass % of isobutylene from isobutane and 37% of propylene from propane; polymerization of ethylene with the yield up to 1,000 kg of polyethylene per gram of catalyst; the Fischer-Tropsch synthesis in the reactor with suspended layer with a CO conversion above 80 % and the target hydrocarbon selectivity C_2-C_4 + C_5 94.4 mass %; the oxidative chlorination of ethylene, allowing to obtain up to 98.4 mass % dichloroethane in the efficiency of use of C_2H_4 to 93.8 mass %; oxidation of methanol to formaldehyde, allowing optimal conditions to increase the yield of formaldehyde is up to 99.9 % with 100 % selectivity in the oxidation of methanol to formaldehyde; oxidative conversion of methane, which allows to increase the selectivity of the formation of C2-products to 67.4 % at a methane conversion of 23.8 %, which corresponds to the best known catalysts for the oxidative condensation of methane; microspherical catalyst for cracking of oil residues allowing to increase the overall yield of distillate fractions to 58.0 mass % at boiling temperature up to 350 ºC, the yield of gasoline – 18 mass %, the octane number up to 82,5; the oxidation of sulphur dioxide by atmospheric oxygen, allowing the temperature interval 40-60 °C clean flue gases from the CHP SO_2 when the degree of conversion of SO_2 89-95 % with simultaneous production of sulphuric acid.

As part of our research we developed microspherical carriers with a perforated shell of variable thickness and porosity, selective sorbents on their basis, as well as promising carriers of sorption-active components of the processes: cleaning the flue gas from SO_2, NO_x, in the process of sorption the degree of absorption of NO_x is up to 93 %, SO_2 up to 95 %; adsorbent for the extraction of oil from oil-water emulsions, allow a single extraction of oil to the residual oil content in the water layer of no more than 3-4 % of the initial mass of oil, i.e. the water is purified to a state suitable for use for technical purposes – the method is characterized by the ease of regeneration of aluminosilicate microspheres; we have developed the modified aluminosilicate microsphere highly selective sorbent of mercury, allowing to extract up to 100-120 mg per 1 g of ash microspheres.

ESC-P-10

NEW SOURCE OF ALTERNATIVE ENERGY – PLANT “EICHORNIA”

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Nowadays, utilization of alternative sources of energy and namely, biomass becomes the main direction for development of the World Energy for containment of accelerated rates of global climate changes. During the estimation of technological processes of biofuel production for conditions of Georgia, it was revealed that from the environmental and economical point of view, the most effective method of biofuel production if cultivation of water plant “Eichornia” (Eichornia Crassipes) and use of its biomass for production of biogas. “Eichornia” is a representative of a supreme water plant, floating plant – typical hydrophyte. By its bioproductivity, no other existed plant is able to compete with “Eichornia”. “Eichornia” is characterized by the highest intensity of photosynthesis. One plant of “Eichornia” is able to make more that 400 vegetative shoots for 30 days. It’s possible to obtain from 300 to 1500 tones of green mass from 1 ha per season and during processing, it’s possible to gain 70 000 cubic meters of biogas. Because of such high productivity, industrial cultivation and biotechnological conversion is considered as one of the most perspective directions in the field of biofuel production [1]

At the same time, cultivation of “Eichornia” bears a certain environmental danger which means its fast reproduction and overgrowth, resulted with covering of surfaces of basins by solid layer of the plants. It makes worse the oxygen condition of basins and destruction of the other habitats. “Eichornia” is represented in the list of 36 most dangerous invasive species of the plant kingdom. The list is prepared by the group of experts of the International Union for Conservation of Nature (IUCN) [2]. Following the recommendations of the Biodiversity Convention which underlines that biofuel production and utilization must not exert the negative effect on biodiversity and socioeconomic conditions of people and also, it is mentioned that introduction of invasive allogenic species requires following of safety measures and estimation of the risk. On these issues it was put into practice an experiment. [3]

The main target of the experiment was the revelation of resistance of vital capacity of “Eichornia” in natural and climate conditions of Georgia (*in situ*) and also abilities of its cultivation in laboratory conditions (*in vitro*). Experiment was held in a self-contained basin formed in the foundation pit of an abandoned sand-pit open-cast mine in March, April and May on the territory of Adjara. All of the 40 plants of “Eichornia” set down on the basin were perished during 12-16 days (the average temperature of air was 7^0 c in March, 10^0 in April and 17^0 c in May).

Conclusion – “Eichornia”can’t naturalize even in subtropics of Georgia with temperature below 20^0 c and can’t survive in open basins. In conditions of certain safety measures and monitoring, it can be cultivated in basins of Georgia and also, biomass can be harvested. The experiment in the laboratory conditions showed that keeping temperature within 26-30^0 c and providing illumination during 12-14 hours, the plants in plastic containers with water (mixed with peaty soil) are begeted well. Creation of such conditions in greenhouses can make possible to gain the seedlings of “Eichornia” in necessary quantities.

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ELABORATION OF BRIQUETTE FUEL COMPOSITIONS AND TECHNOLOGIES FOR THEIR PRODUCTION

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Saving of traditional energy resources and decreasing of ecological tension of the environment are very important tasks of the present-day energetic. A successful way for solving both of these problems is manufacturing from many accumulated in the environment carbonaceous solid, non-merchantable wastes (industrial, oil-refining and mining enterprises, agricultural, biological, household and other) by well-known from the ancient times, well-proven method of production of alternative composite fuel – briquettes. This is highly effective and profitable technology and it is widely used in the world.

The purpose of the presented study was preparation of briquette fuel on the basis of wastes of various carbon-bearing raw materials available on the territory of Georgia. Elaboration of the optimal technological scheme, assessment of physical and chemical, as well as technical characteristics of the obtained fuel, determination of ecological effect and indices of saved energy.

Location and stocks of major combustible materials, resources of their suitable for usage wastes, in particular of the fine-grained wastes of charcoal, wood residues (sawdust, wood chipboard millings), grounded corn plant roots are studied in Georgia for the first time. The binding materials and cheap and available local raw materials needed for modification of combustible briquettes were also studied.

Several compositions had been produced and investigated and seven of them had been selected as being the best ones: three bio- and four coal containing compositions: wood chipboard millings, grounded roots of corn plant, sawdust mixed type briquettes (compositions containing fine-grained coal fractions together with several binders and modifiers in a specified proportion).

Fuel briquettes were assessed in terms of ecology and economics as well. In particular, on the basis of the elemental analysis the thermal capacity of fuel briquettes in MJ/kg; maximum quantity of harmful gases COx, NOx, SOx exhausted during combustion of briquettes and an energy saved by usage of the briquettes were calculated. It has been found that the obtained briquettes were more effective by all data compared with the raw material, and this is the uniqueness of the fuel briquettes in general. The best from the obtained briquettes by their thermal capacity, stability, and amount of exhausted gases were ones prepared on the basis of ground roots of corn plant and sawdust. They burn almost 4 times longer in comparison with the raw material, are characterized by low smoke, are humidity-resistant. The obtained combustion ash is the best potassium containing fertilizer and the savings of electricity makes up to 1805,3 kWh/T. Mixed composition briquettes containing coal wastes are characterized by high thermal capacity, so they can be used in a relatively powerful industries, energetic, drying equipment, etc. Stability of this briquettes depends mainly on pressure and temperature conditions of pressing.

It should be noted that roots of corn plants and wood chipboard millings, as well as polyethylene as binding material in mixed composition briquettes have been used for the first time. The obtained fuel can be used in housing and communal sector (stoves, fireplaces), in small enterprises and energetic, for heating of different function buildings, in drying installations, in heat and power plants, in agriculture (greenhouses, farms), in passenger trains, etc.

As a result of the performed investigational analysis it can be concluded that on the basis of utilization of secondary carbonaceous wastes present in Georgia it is possible to develop and obtain high-calorific alternative briquette fuel. The obtained samples are in line with the standard requirements in terms of economy and ecology. They can be used to obtain additional thermal energy, which provides development of energy efficient technology and reduction environmental tension.

We hope that this work will contribute to development of briquette technology in our country.

ESC-P-12

THE LIQUID SORBENT CONDITIONAL SYSTEMS ON GEOTHERMAL WATER BASE

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The World energetic crisis forces the countries to look for new alternative energy sources. Such sources can be clear, non-traditional energy resources, like: solar, wind, bio and geothermal. Our object of research in this article concerns the geothermal energy resources. Geothermal energy provides a huge, reliable, renewable resource, unaffected by changing weather conditions. It reduces reliance on fossil fuels and their inherent price unpredictability and when managed with sensitivity to the site capacity, it is sustainable. Geothermal energy is relatively environmentally friendly. The use of conventional polluting fuels such as oil and coal can be reduced if geothermal and other alternative energy forms be used (reducing pollution).

Georgia is rich by geothermal resources, but today they are not used effectively. One of the ways of effective use of geothermal water resources suggested by us is their use in refrigerating equipment of fruit and vegetable store-houses. Besides, the scheme is already developed for using geothermal water for drying and cooling cereals in grain-elevators. For cooling atmospheric air the special air-cooling units are developed.

NEW CATALYTIC AND ADSORPTIVE TECHNOLOGIES OF HYDROCARBON RAW PROCESSING

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Last years requirements to ecological safety and production properties of commercial oil product, process gases and gas distillate, submit to gas lines, against magnification of a fraction of high-sulphur raw stock have sharply increased. In connection with this, we have elaborated following catalytic and adsorptive systems for the development of quality of gas distillate, fuels and oils.

1) Hydrofining of natural and associated gas with high content CO_2 in Fe-Ni-Mo and Fe-Co-Mo catalysts, adapted for raw material of Mubarak GPP, will provide the drop of the maintenance of mercaptans in tank gas to new rigid conditions (0,015 g/m^3). There have been correlated the texture, phase composition, dispersity of active phase and surface characteristics of catalysts in the oxide and sulfided form, ready serial imbibition of carriers by combining of metals of groups VI and VIII of the Periodic system, single imbibition by solutions of heteropolycombinations of row 6 [1-3] and «surface assemblage» through the stage of forming of interim chelate complexes [4]. The variation of temperature (300 - 350 ° C), pressure (0.01-2 MPA), and the volume rate of gas distillate (2000-5000 $hour^{-1}$) there have been determined conditions for drop of the maintenance of sour sulfur from 0.005 % to 0.00001 %.

2) Water extraction from process hydrocarbon gases. The method of synthesis of the adsorbent, based on recrystallization of Angren kaolin in zeolite NaA in strongly alkaline condition in pellets, has been developed without binding application [5]. The zeolite adsorbents which sorption capacity on water vapor reaching 25-30 g/ 100 g of a sorbent that are comparable with indexes of import zeolites have been obtained.

3) Enhancement of the quality of commercial products and economic efficiency at fluid hydrocarbon raw processing. Results of monitoring of experimental-industrial test of trimetal So-Ni-Mo catalyst of hydrofining, and Ni-Mo catalyst of hydrodearomatization allow to obtain basic oils of high-quality have been exposed . The role of the dimensional factor in the formation of active phases of catalysts Ni-Mo and Ni-Mo-W with the point of view of activity and stability at the enrichment by hydrogen tri - and bicyclic aromatic hydrocarbons has been discussed. It has been determined that the developed catalysts provide the production of Jet A-1 airkerosene and oils II of group on the classification of API.

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ESC-P-14

INFLUENCE OF MODIFICATION OF Co-Mo AND Ni-Mo OF CATALYSTS ON THE HYDRODESULFURIZATION OF FLUID AND GASEOUS HYDROCARBON RAW

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The aggravation of an ecological situation in the modern world demands advancing of purifying processes of hydrocarbon raw from toxic admixtures. The overwhelming majority of oilfields and gas distillate in Uzbekistan are classified as sulphur and high-sulphur. Naturally, it creates fixed difficulties at obtaining of high-quality liquid and gaseous fuel, demands advancing of processing technology, including development of modern domestic catalysts of hydrodesulfurization. Thus, it are necessary to consider an adverse combination of corrosion-active mercaptans in the composition of crude gases and gas condensates with the water saturated with acidic components: O_2, H_2S and CO_2. With the point of view of secure exploitation of plants, this factor seems to influence on the fracture velocity of an internal surface of machinery and transport mainlines. Negative affecting of aggressive substances on catalytic processes consists in an irreversible poisoning of Co-Mo and Ni-Mo of catalysts of hydrofining of fluid hydrocarbon raw products of corrosion. Presence of CO_2 - substances with the cokegene properties, promote the formation of the carbon-bearing depositions and to convertible blocking of active sites of catalysts. Efficiency of purification of gas distillate from mercaptans by means of absorbents of alkali nature decreases, and in certain cases it could be and not profitable. In accordance with, the maintenance of CO_2 in gas distillate of fields in Uzbekistan could reach 4,5 %, and in currents of ethane-bearing gas, refined in the Shurtan Gas-chemical complex to 9,7 % a mol [1].

We have developed a serial of the molybdenum-bearing catalysts, the promoto ions of nickel, cobalt and iron for processes of demercaptanization of gas distillate and the gas condensate, efficiently decomposition C-S bonds in molecules of mercaptans in the presence of carbon dioxide without an essential carburizing of active sites of hydrocracking. The influence of hydroxides of aluminium of various origins on the porous structure and mechanical strength of the alumokaolinborate carriers and phase composition of Ni-Mo and Co-Mo of catalysts, the promotor Fe_2O_3 have been investigated. Catalysts have been synthesized by single dip by combined solutions of inorganic salts of the transitional metals, stabilized by phosphoric acid [2], and also serial drawing on carriers of oxalic acid, oxalate of molybdenum and nitrates of members of group VIII of the Periodic system - «surface assemblage».

It has been shown that the peak dispersity as aluminum oxide, and molybdates of nickel and a cobalt, reaches at the use of deposition pseudoboehmite and drawing of active components by the method of «surface assemblage» by means of oxalic acid. Catalysts on the basis of aluminum hydroxides of alcoholate origin do not correspond to endurance capability criterion. Hydrodesulphat activity of Fe-Ni-Mo, Ni-Mo, Co-Mo, Fe-Co-Mo and Fe-Mo of catalysts in the course of hydro refinement of diesel distillate, gas condensate and gas distillate have been compared.

It has been proved the positive role of modification of Ni-Mo and Co–Mo catalysts of hydrodesulfurization ions of iron from the point of view of regulation of surface acidity and stable activity at mercaptans removal from the gas distillate contain 5 % of CO_2. It has been observed only additive increase of activity at the modification of Fe_2O_3 in the course of sulphur removal from gas condensate (kerosene) and diesel distillate.

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THE SEQUENCE OF THE PREPARING PROCESS OF OPTIMAL COMPOSITION OF ANTISUBLIMATION COATINGS FOR SEMICONDUCTING BRANCHES OF THERMOELEMENTS

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The sequence of the technological process for preparing optimal chemical composition of electroinsulating antisublimation coatings based on inorganic vitreous enamels have been developed for protecting all types semiconducting branches of thermoelements against sublimation. Proposed method gives possibilities to create antisublimation coatings in a short time with using the minimum amount of materials, which perfectly satisfy requirements. They are characterized by high level of protection in prolonged working conditions [1,2].
Table 1 shows experimental results of vitreous enamels of five systems.

Table 1. Characteristics of vitreous enamels and their properties

System	Composition of vitreous enamels	Tempera-ture, °C		$R_{inter.}$ x 10^3 Ohm				Tensile strength kg/cm²	Specific resistance Ohm·cm
			Branches of p - type		Branches of n - type				
		Melting interval	Defor-mation of coating Melting	After for-mation of coating	Defor-mation of coating	After forma-tion of coating			
1	Na_2O- B_2O_3-PbO	290-400	340	5,3	5,4	8,4	8,6	65	10^{-5}-10^{-11}
2	Na_2O-SiO_2-Bi_2O_3-PbO	320-395	330	5,4	5,3	8,1	8,1	70	
3	Na_2O-TeO_2-PbO - SiO_2	305-370	330	5,4	5,5	8,3	8,2	60	
4	Na_2O-B_2O_3–TeO_2- PbO-SiO_2	275-354	325	5,4	5,5	8,3	8,2	60	
5	Na_2O-B_2O_3 – Bi_2O_3-TeO_2 PbO - SiO_2	245-355	325	5,5	5,5	8,5	8,4	70	10^{-5}-10^{-11}
--	BiSbTe	-	597	-	-	-	-	-	$1{,}2 \times 10^{-4}$
--	BiTeSe	-	585	-	-	-	-	-	$O{,}3 \times 10^{-4}$

Table shows, that vitreous enamels from the pointed system and also technological conditions of their formation practically does not effect on their electrical characteristics of n - and p – types branches of thermoelements.

It was established, that vitreous enamel especially based on Na_2O-B_2O_3–Bi_2O3-TeO_2-PbO-SiO_2 is the best material for application as electroinsulating antisublimation coating of lowtemperature branches of thermoelements of n- and p-types. Vitreous enamel based on pointed system, prepared on liquid glass provides assembly of thermobatteries at room temperatures.

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ESC-T-02

VOLTAMMETRIC STUDIES OF Ca DOPED Y-114 LAYERED COBALT PEROVSKITE ELECTRODES WITH CATALYTIC EFFECT FOR ETHANOL ELECTROOXIDATION IN ALKALINE SOLUTIONS

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In this paper, ethanol anodic electrooxidation reaction on $Y_{0.5}Ca_{0.5}BaCo_4O_7$ electrode in aqueous alkaline solution was investigated using voltammetric studies. The catalytic activity of ethanol anodic oxidation becomes a serious issue, mainly for the operation of layered cobalt perovskite electrodes in fuel cells. The research is necessary to understand the oxidation mechanism on the surface of these type of compound electrodes. Electrochemical behavior has been studied by cyclic voltammetry, linear polarization.

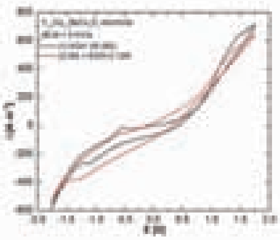

Figure 1. Cyclic voltammograms in 1M KOH (BS) and in BS + 0.12M EtOH, scan rate 5 mV s^{-1}.

M. Valldor synthesized for the first time the $Y_{0.5}Ca_{0.5}BaCo_4O_7$ compound, defining it as a semiconductor. It was prepared by replacing half of the quantity (in moles) of Y^{3+} ions with Ca^{2+} ions, in $YBaCo_4O_7$ cobalt perovskite, achieving the change of average valence state of the cobalt ions [1]. Experimental determinations and calculations made by Valldor confirmed that the stoichiometry of this compound is $Y_{0.5}Ca_{0.5}Ba(Co^{2+})_{2,5}(Co^{3+})_{1.5}O_7$ [1-4]. This stoichiometry recommend $Y_{0.5}Ca_{0.5}BaCo_4O_7$ perovskite for electrochemical studies, aiming to oxidize the Co^{2+} ions to Co^{3+} inside its structure. Due to their structural, magnetic and electrochemical properties, the mixed cobalt oxides can be used as membranes with high oxygen permeability, oxygen sensors and also as fuel cells electrodes.

Direct alcohol fuel cells (DAFCs) are considered to be advanced sources of energy for a variety of applications. Methanol was examined as a primary fuel for DAFCs because of its low cost and easy storage, but the aspect of toxicity remains crucial. Ethanol is also considered an attractive alternative fuel because of its low toxicity and possibility to be produced from a broad variety of biomass products [5].

The results provided basic information in understanding ethanol oxidation reaction (EOR) on 114 cobalt layered perovskites catalysts.

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ESC-T-03

VOLTAMMETRIC STUDIES OF METHANOL ELECTROOXIDATION IN ALKALINE SOLUTIONS ON SKELETAL NICKEL BASED 6 LAYERS PLATINUM NANOPARTICLES ELECTRODE

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In this paper, new aspects of the electrocatalytic oxidation of methanol on skeletal nickel based 6 layers platinum nanoparticles electrode in aqueous alkaline solution was investigated using voltammetric studies. Pt and its alloys are the most commonly used catalytic materials in the anode of DAFCs taking into account their excellent adsorption properties and easy methanol dissociation. The cost of this type of electrodes is a major impediment in the fuel cell technology commercialization, because it cost alone approximately 54% of the total fuel cell stack price [1-4]. Methanol oxidation research is in progress and it is impossible to cover every aspect of the new electrode developments [4]. Activity, selectivity, and stability are critical issues for any catalysts proposed to be used in DAFCs [4]. The research is necessary to understand the oxidation mechanism on the surface of these electrodes. Electrochemical behavior has been studied by cyclic voltammetry and linear polarization.

Electrochemical tests were performed at room temperature using a SP-150 potentiostat/galvanostat (Bio-Logic, SAS, France). A 100 mL typical glass cell was equipped with three electrodes: working electrodes consisting of skeletal nickel based 6 layers platinum nanoparticles samples, Ag/AgCl reference electrode and two graphite rods used as counter electrodes. For performed experiments, the exposed surface of working electrode was 0.5 cm^2. Nickel-platinum based electrodes have been prepared by spray pyrolysis technique Different concentrations of methanol were added: 0.125, 0.25, 0.5, 1 and 2 M, all prepared from Sigma-Aldrich reagent p.a. min 99.8%.

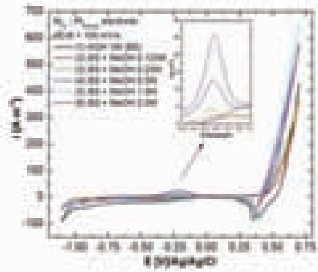

Figure 1. Cyclic voltammograms in 1M KOH (BS) without and with MeOH different concentration, scan rate 100 mV s^{-1}. Inserted anodic peak for formaldehyde to formate oxidation.

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LIST OF ABSTRACTS

PLENARY (PL) AND ROUND TABLE (RTL) LECTURES

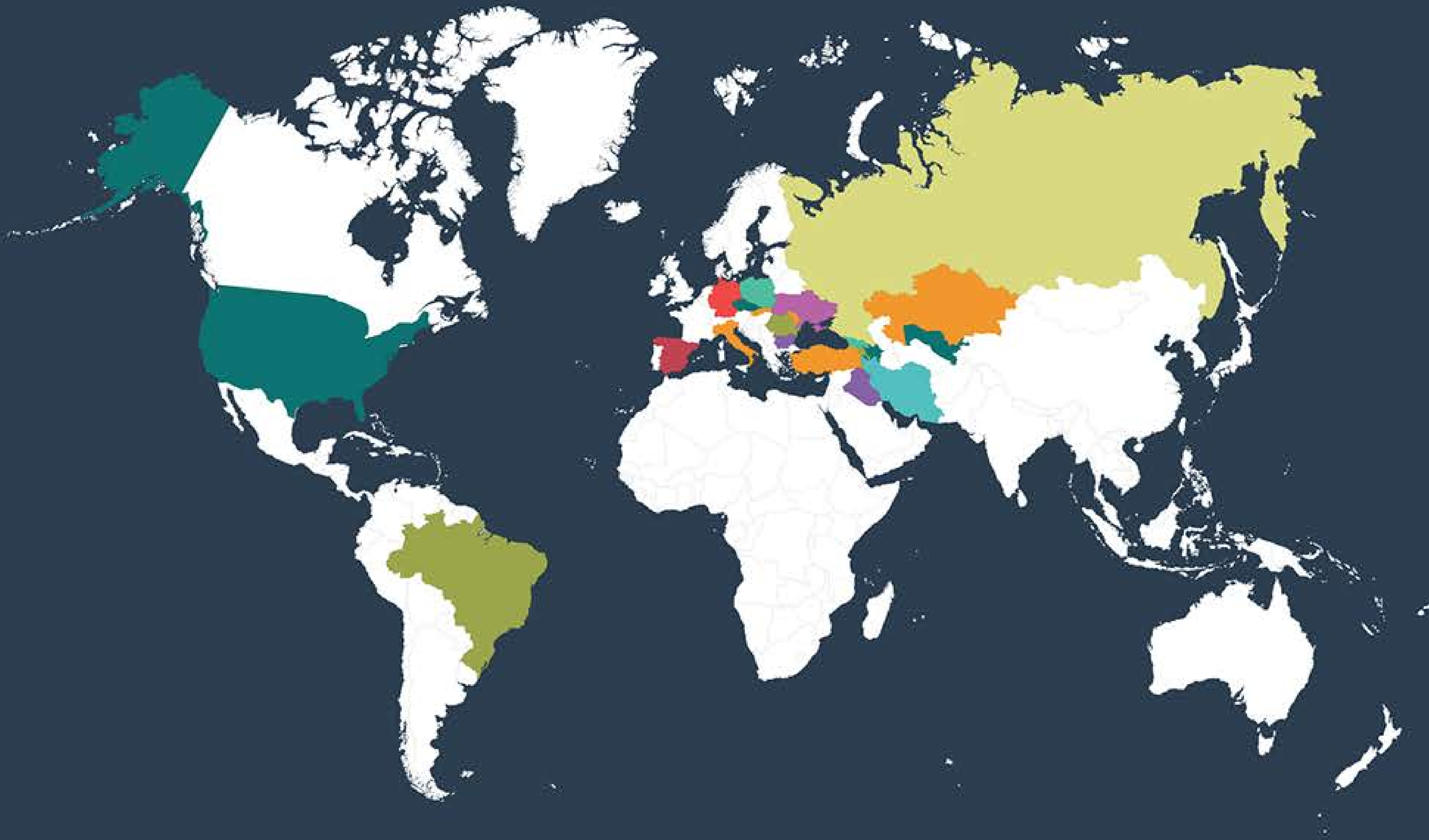
NPN
NANO PROCESSES AND NANOTECHNOLOGIES

FTA
FUNDAMENTAL AND TECHNOLOGICAL ASPECTS OF PROCESSING OF MINERAL PRODUCT AND SECONDARY RAW MATERIALS

NMS
NEW METHODS FOR ECOLOGICAL AND RADIATION SAFETY, MEDICAL AND AGRARIAN RESEARCHES

ESC
ENERGY SOURCES, CONVERSION AND STORAGE

AUTHORS INDEX

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