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INNOVATION-ORIENTED PROJECTS

The proposed database contains the annotated reports on completed research projects of the State Foundation for Basic Research (SFBR), which, in the expert opinion of Foundation Board members, have been brought to a certain level of practical implementation and regarded as innovative ones.

PROJECT NO. F40.1/004

AN INTEGRATED APPROACH TO ANALYSIS AND VERIFICATION OF TELECOMMUNICATION SOFTWARE SPECIFICATIONS FOR THE SINGLE-PROCESSOR AND THE MULTIPROCESSOR SYSTEMS

Project Manager: *Letychevskyi, O.A.*

The purpose of project is to develop an integrated approach to the analysis and verification of telecommunication system software based on formal methods with the use of self-deduction, insertion simulation, and model validation. The methods of analysis and verification of specifications for telecommunication systems have been elaborated in terms of imperative sequential and parallel applications, as well as in terms of the basic protocols and MSC-charts. The main stages of research include the development of multi-insertion protocol models and applications of telecommunication systems, the development of deductive methods for verification of protocols and applications by data structures, the preparation and performance of experiments in the insertion simulation system developed at the Glushkov Institute of Cybernetics of NASU. The software prototypes for the analysis and verification of specifications have been created.

The project results have been presented at conferences, in publications, and in research reports.

PROJECT NO. F40.1/043

DEVELOPMENT OF INDICES AND INDICATORS OF SUSTAINABLE DEVELOPMENT OF REGIONS OF RUSSIA AND UKRAINE ON THE BASIS OF COMBINED USE OF CAUSAL AND PROBABILISTIC SEMANTICS

Project Manager: *Zgurovsky, M.Z.*

There have been obtained the results of studying the hazardous factors and risks of complex man-made systems in global and regional contexts to be used for building up an information resource on the basis of World Data Center-Ukraine. The approach used in this study involves the consideration of development of the Russian Federation and Ukraine from the standpoint of providing stability and balance in three dimensions: *the economic, the environmental,* and *the socio-institutional*. To coordinate

and to balance the three specified dimensions is a strategic task and the most important current challenge for the national governments, the competent international organizations, and all the progressive people of the world. The project is aimed at addressing the fundamental scientific problems of creating the indices and indicators characterizing the sustainable development of territories, which would allow the decision makers to justify a particular strategy and further plans for socio-economic development. Within this framework, the risks threatening the sustainable development in the regions of Ukraine have been estimated with the use of developed methodology for assessing the consistency of expert evaluation. The research has been carried out within the framework of the World Data System of International Council for Science.

PROJECT NO. F40.2/023

FOCUSING OF INTENSIVE BEAMS OF NEGATIVELY CHARGED PARTICLES BY ELECTROSTATIC PLASMA LENS

Project Manager: *Goncharov, A.A.*

A new improved model of lens with spatial charge on positive ions have been developed and manufactured. A model of source issuing the negatively charged particle beams has been developed and the beams of electrons and negative ions have been obtained. The current density has been experimentally showed to increase 1.8 times on the axis of wide-aperture electronic beam. It has been experimentally proved that there are no potential dips on the axis of new lens model. Thus, the aberrations in lens have been significantly decreased. The plasma of spatial charge cloud has been established to stabilize the electron source and together with the lens focusing force it allows one to compress a 100-ampere, wide- aperture (initial diameter 6 cm) beam to a size of 1 cm and to get a beam current density greater than 100 A/cm^2. A numerical model of focusing beams of negatively charged particles in electrostatic plasma lens with dynamic spatial charge cloud has been developed. It allows the researcher to calculate the accumulation of spatial charge in plasma lens and the interaction of cloud and the charged particle beam passing through the lens aperture considering the new positive ions continuously arriving at the cloud. The model-based test calculations have been showed to be in line with the well-known data from literature and with the experimental results. The numerical experiment has proved that it is necessary to take into account the magnetic field within the lens. Its value is critical for the separation of electrostatic and magnetic focusing. The experiment has showed the importance of keeping the right balance between the bulk charge of lens and the focused beam. If the beam bulk charge exceeds the lens one the focusing mode of plasma lens is broken. The effect of plasma lens based on electrostatic trap for positive ions on the electron beam with a small current up to 100 mA and average energy of 10-15 keV has been demonstrated.

PROJECT NO. F40.2/045

RESEARCH AND DEVELOPMENT FOR MODERNIZATION OF BELLE-2 DETECTOR CALORIMETER FOR STUDYING THE B–MESON PHYSICS

Project Manager: *Hektin, O.V.*

The aim of research is to analyze the factors that are very important for obtaining CsI crystals with high radiation resistance to maintain stability of the detector under increasing burden on calorimeter. The objects of research are the unalloyed CsI crystals obtained industrially, as well as the experimental samples with added impurities grown by the Czochralski and Bridgman techniques. The analysis of data indicates a significant dependence of absorption, luminescent, and scintillation parameters of crystals on cationic and anionic composition of admixture material. The offered ways to

reduce the content of undesirable oxygen impurities allow one to propose the use of divalent europium ions as scavenger leading to the purification of molten CsI before crystal growth. This, in its turn, enables to improve significantly IR transparency and to get rid of the slow scintillation pulses in crystals, thereby improving the Fast/Total ratio that is the criterion of suitability for the use of CsI as scintillator. The effect of irradiation on changing light output of CsI own luminescence has been studied. The CsI crystals with low extraneous cation and oxygen containing impurities have been showed not to change significantly their optical characteristics under the influence of ionizing radiation. Measuring the Fast/Total parameter in initial crystals makes possible, to some extent, to predict the radiation resistance level of CsI crystals.

PROJECT NO. F40.3/017

CREATING THE NANOSTRUCTURED CALIXARENIC RECEPTORS FOR HIGHLY SELECTIVE DETECTION AND BINDING OF ORGANIC MOLECULES IN THE GASEOUS PHASE AND IN THE SOLUTIONS

Project Manager: *Kalchenko, A.I.*

The stability of anionic calixarene adducts in the gaseous phase and in the solutions has been theoretically predicted. New types of calixarenes with polyfluorophenyl substituents on the upper crown of macro-cycle have been synthesized. Their structure has been studied by nuclear magnetic resonance and X-ray diffraction methods. The conformations of fluorophenyl calixarene derivatives in gaseous phase, the energy of their "*guest-host*" interaction with nucleophilic molecules, and the mechanisms for stabilization of created adducts have been calculated with the use of quantum-chemical methods. Highly effective synthons based on thiacalixarenes have been synthesized. The molecular and crystal structure of synthesized compounds has been studied by X-ray analysis technique. The results can be used to create highly sensitive sensors for anion detection. In addition, they can be useful for creating the highly sensitive sensors suitable for detecting amino acids and derivatives of uracil and adenine in aqueous solutions, as well as for studying the complexing properties of (thia)calixarenes with biologically important compounds under their binding and detection in biological environment, as well as in objects of pharmacology and medical industry. The studies allow the researches to use the above types of water-soluble (thia)calixarenes as modulators for proteolytic separation.

PROJECT NO. F40.3/034

DEVELOPMENT OF NEW ENANTIOSELECTIVE BIO- AND ORGANIC CATALYZERS BASED ON SUBSTANCES OF THE SYNTHETIC AND THE NATURAL ORIGIN

Project Manager: *Kolodiazhnyi, O.I.*

The methods for enzymatic separation and bio-catalysis of alpha- and beta-hydroxyl-containing phosphorus compounds have been studied. The methods for bio-catalytic separation of phosphonates by *Burkholderia cepacia* lipase have been developed.

1. A method for the enzymatic separation of racemic compounds into enantiomers using of acidification of secondary alcohols by internal cyclic anhydrides of dicarboxylic acids has been developed. It allows one to avoid the chromatographic purification of compounds. The method can be used to separate large quantities of compounds within multigram range.

2. There has been developed a method for the synthesis of all possible stereoisomers of cis- and trans-vicinal cyclic alkenes (n = 4—6) with the absolute configuration 1R, 2R; 1S, 2S, 1R, 2S; 1S, 2R, which are the essential chiral synthons for synthesis of leukotrienes and prostaglandins and are used in total synthesis of (+) — Estrone and (+) — Desogestrel.

3. The new organic catalyzers based on L-tyrosine and its derivatives which catalyze aldol reactions in hydroxyl-containing environments, including the aqueous solutions, have been designed.

4. The research results have practical significance and lay foundation for upcoming introduction into the industry.

PROJECT NO. F40.3/041

NEW BIOMIMETIC CATALYSTS FOR SPLITTING MACROERGIC PO AND CN BOUNDS BASED ON MODEL COORDINATION COMPOUNDS OF TRANSITION METALS

Project Manager: *Frytskyi, I.A.*

The development of new, highly efficient method for splitting the macroergic PO and triple CN bonds is an important task of modern chemistry. Currently, the advanced effective high selective methods of splitting these bounds are in great demand in genetic engineering (hydrolysis of DNA and RNA), chemical ecology (neutralization of organophosphoric pesticides and toxic substances, derivatives of hydrocyanic acid) and in organic synthesis. Within the framework of project a new synthetic system for efficient splitting of phosphester, nitriles, and isonitriles has been developed. It combines the cooperative involvement in catalysis of metal-containing active centers and additional uncoordinated functional groups that can act as intramolecular nucleophiles. The proposed catalysts are based on mono- and binuclear chelate with original and binuclear ligand systems containing additional donor groups (carboxyl, oxime, hydroxamate, and hydrazide), in addition to metal-carrying complexes. The target coordination compounds can be considered as a model of metal-containing active centers of enzymes catalyzing the split of a wide range of phosphoesters and triple CN bonds. There have been studied the rational synthetic ways for obtaining the target compounds and their characteristics with the help of combining different analytical, physical, and chemical techniques to study the structural and magnetic properties, as well as to study the kinetics of catalytic split of organophosphoric pesticides and other phosphoester substrates, nitriles, isonitriles, and cyanides. The correlations between structural, spectral, and magnetic properties of synthesized complexes and their catalytic activity have been established. The factors influencing the catalytic effectiveness of metal complexes have been found to facilitate the rational design of functional models of metal enzymes and the creation of new biomimetic catalysts.

PROJECT NO. F40.6/010

METHODOLOGY OF PROCESSING THE SEISMIC AND GRAVIMETRIC DATA WHEN STUDYING THE CRUST AND THE UPPER MANTLE OF THE DNIEPER-DONETS BASIN AND THE SIBERIAN PLATE

Project Manager: *Egorova, T.P.*

The main goal of project is to develop new methods and techniques for integrated processing and interpretation of geophysical data on the structure and dynamics of the crust and the upper mantle. The methods shall be based on the seismic and gravimetric techniques that have been used for processing the materials of deep seismic sounding of different tectonic structures within the territory of Ukraine and Russia: the Dnieper-Donets basin and the crystalline shields of Moesia plate and the Siberian plate. The new techniques (migration of refracted and supercritical reflected waves, building of high-speed profiles and profiles of the upper mantle density with the Earth spherical shape taken into consideration and with the use of unique records of peaceful nuclear explosions, mathematical modeling of fields, etc.) allow the researchers to investigate in detail the structure of the main seismic boundaries in the Earth's crust, in the upper mantle, and in transition zone from the upper to the

lower mantle, as well as to build the comprehensive three-dimensional models of the upper mantle in Russia and to get a 2D-model of density distribution in the upper mantle and in the transition zone in three profiles (Quartz, Kraton and Kimberlite). These new data will help to study in detail the Earth's upper layer dynamics and to understand the history of formation of different types of geological structures.

PROJECT NO. F40.7/041

CRYSTAL CHEMISTRY, CRYSTAL GENESIS, AND BIOMIMETIC SYNTHESIS OF ORGANOPHOSPHOROUS NANOCOMPOSITES CREATED IN LIVING ORGANISMS

Project Manager: *Dubok, V.A.*

A collection of samples of phosphate bio-fertilizers of biogenic origin and their synthetic analogues has been gathered. The samples were annealed within the temperature range of 500—1100 °C. The general properties and crystal chemistry of bio-fertilizers as mineral-organic nano-associated systems have been studied. With the help of XRF and IFS methods the structures of the synthetic and the biogenic apatite have been demonstrated to be similar. It has been showed that within the range of temperature from 600 to 800 °C the biogenic apatite mostly consists of hydroxyl-carbon-apatite, while at higher temperatures it consists of hydroxyapatite, whereas the synthetic material consists of hydroxyapatite with admixture of tricalcium phosphate. Under heat treatment with a lack of oxygen the nitrogen-containing radicals are formed in biogenic hydroxyapatite. They are included in the structure of biogenic hydroxyapatite through isomorphic substitution, with nitrogen being a substitute for phosphorus in the structure of hydroxyapatite. The heat treatment with excessive oxygen does not lead to the formation of radicals. New data on the conditions of formation of nitrogen center in biogenic hydroxyapatite have been obtained. The computer simulation of cationic and anionic isomorphic substitutions in the structure of hydroxyapatite has been made. The results of computer simulations are in good agreement with the experimental data. The work on the synthesis and study of the characteristics of the biogenic and the synthetic HAP has showed that the resulting synthetic material possesses the properties quite similar to those of the bio-apatite and can be used as biocompatible implant. The results of research can be used in materials science, nanotechnology, medicine, nano-mineralogy, and in nanophysics.

PROJECT NO. 41.1/001

OSCILLATION OF METALLIC AND COMPOSITE SHELLS DURING INTERACTION WITH ELASTIC AND LIQUID FILLER

Project Manager: *Kubenko, V.D.*

The complex processes of degrading stability of composite material shell elements almost have not been studied with consideration of design and structural features revealed during their application. The project involves the development and implementation of appropriate mathematical tools, which allow the researches, on the one hand, to build a new adequate computational model of object, the elastic fluid; and, on the other hand, to study the impact of design features and external factors on critical velocity of fluid and on the characteristics of divergent and dynamic loss of object's stability.

The new results obtained within the framework of project are important for predicting dynamic behavior of shell structures with metallic and composite materials during the interaction with elastic and liquid (steady and unsteady flow) environments.

The research results can be used for saving energy when transporting liquids by selecting the optimal pumping regimes in the areas of dynamic instability of pipelines and in the resonance zones.

They are important for the prediction of operational reliability of different liquid transporting pipeline systems to prevent accidents that can cause significant environmental pollution.

PROJECT NO. 41.1/006

SYNTHESIS AND PROPERTIES OF BIONANOMATERIALS BASED ON APATITE-LIKE SYSTEMS MODIFIED BY METALLIC NANOPARTICLES, FULLERENES, AND CARBON NANOTUBES

Project Manager: *Karbivskyi, V.L.*

A series of Ca-HAP-carbon nanomaterial composites has been synthesized for the first ever time, with their physical and chemical properties, as well as atomic structure being studied. Preliminary functionalization of nanotubes has been established to be necessary for a more optimal interaction of apatite with carbon nanotubes during the formation of composite. The introduction of carbon nanomaterials in calcium hydroxyapatite leads to the formation of molecular complexes and the structural ordering. The effects in the evolution of valence band structure and charge status of atoms have been established depending on the type and degree of isomorphic substitution in isovalent cation sublattice of stoichiometric apatite matrix. The correlation of locations and form of lines of the calculated and the experimental data indicates preferential location of 3d-metals in Ca(2) position of the apatite structure.

Thus, the project results provide scientifically substantiated preconditions for creating a new generation of bionanomaterials, namely bio-implants, biosensors, and medical drugs of adaptive and sustained action.

PROJECT NO. 41.1/009

TECHNIQUE, SPECTRAL AND THERMOELECTRIC PROPERTIES OF MULTILAYER LOW-DIMENSIONAL HETEROSTRUCTURES BASED ON LEAD CHALCOGENIDES

Project Manager: *Freik, D.M.*

The fundamental regularities of the formation of lead chalcogenide semiconductor low-dimensional structures by vapor-phase methods have been studied. The process conditions that ensure the optimum values of thermoelectric parameters: electrical conductivity, Seebeck coefficient, thermoelectric power, thermal conductivity, thermoelectric Q factor have been established. The structure formation of hetero-systems based on lead chalcogenides with desired topological characteristics has been investigated. The developed techniques for nanostructure formation have been protected by patents of Ukraine.

The results can be used in higher schools for special courses, be discussed at joint seminars, published in joint research papers in collaboration with researchers from other organizations. Also, they may be interesting for manufacturers of micro-and nano-electronics from the standpoint of the practical application of results.

PROJECT NO. 41.1/015

PHYSICAL PROPERTIES OF $BiFeO_3$-BASED SOLID SOLUTIONS NEAR MORPHOTROPIC PHASE BOUNDARY

Project Manager: *Eremenko, V.V.*

The purpose of project is to obtain new lead-free magnetoelectric and piezoelectric materials. The expected results will be used in the development of segnetomagnetic and piezoelectric materials for microelectronic devices and sensors which are sensitive to magnetic and electric fields and strain.

The optimum modes for obtaining segnetoceramics based on bismuth ferrite with low dielectric losses suitable for the use in high electric fields have been developed. The magnetic and crystalline

structures of solid solutions obtained by methods of diffraction of neutrons, electrons, and synchrotron X-rays have been determined. A technique for introducing micro-admixtures to reduce dielectric loss due to the presence of iron ions of different valence in samples has been developed. The magnetic, optical, and dielectric properties, as well as magneto-electric effect in a wide range of concentrations of alkaline earth metal ions have been studied. The magnetic properties and magneto-transport properties have been investigated within the range of temperature from 1.5 to 700 K in magnetic fields up to 14 Tesla.

PROJECT NO. 41.1/019

DEVELOPMENT OF PHYSICAL AND ENGINEERING FRAMEWORK FOR FORMING MULTICOMPONENT NANO-MICRO-STRUCTURAL PROTECTIVE COATINGS BASED ON TI-HF-SI-N AND ZR-TI-SI-N WITH HIGH HARDNESS ≥ 40 GPA, THERMAL STABILITY OF ≥ 1000 °C, AND HIGH PHYSICAL AND MECHANICAL PROPERTIES

Project Manager: *Pohrebniak, A.D.*

Creation of multifunctional, nanocrystalline or nanocomposite materials with multicomponent composition and ordered structure is a very important task for modern material science. These new coatings shall have high performance properties modifiable by changing the parameters of their composition and structure.

Using the advanced techniques the structured nano-coatings have been obtained. Depending on technique (ram or separated ion-plasma flow) the crystallite size in the Ti-Hf-Si-N coating varies from 10 to 4.5 nm, while in the coatings based on Zr-Ti-Si-N it ranges from 15 to 20 nm. This makes it possible to obtain new coatings with high physical and mechanical properties, such as hardness. The coatings based on Ti-Hf-Si-N have been obtained using the ram flux H = (48.4 ± 1.4) GPa; modulus of elasticity E = (520 ± 12) GPa.

The obtained nanostructured coatings can be used to protect the tools and turbine blades at *Turbomechanical Works,* in Poltava, and for helicopters and *Mi*-6 at *Aviakon,* in Konotop.

PROJECT NO. 41.1/025

ULTRAFAST ELECTRONIC PROCESSES AND NONLINEAR OPTICAL PHENOMENA IN PHOTOPOLYMER COMPOSITES WITH METAL NANOPARTICLES AND PERIODIC STRUCTURES BASED ON THEM

Project Manager: *Smirnova, T.N.*

The polymer nanocomposites with nanoparticles of noble metals allow one to create new materials for photonics and optoelectronics. The holographic arrangement of similar nanocomposites gives an opportunity to create photonic-crystalline structures of different dimensions (1D, 2D, 3D) combining the diffraction and the special properties of nanoparticles. The research results lay foundation for further development of controlled light diffractive elements and new generation of lasers.

Currently, all over the world, there are being developed the lasers with photonic crystalline resonator using the plasmonic structures to improve the energy characteristics of lasers, including to reduce the generation threshold and to increase the efficiency of lasers. In addition, the plasmonic resonance excitation leads to an increase in non-linear medium response and in intensity of luminescence, as well as to the stimulated Raman scattering. Therefore, to obtain new results on nonlinear optical properties of nanocomposites and 1D-, 2D- structures of metal nanoparticles and to study the properties of lasers with controlling structures based on them are the further tasks related to the development of light-controlled diffractive elements and new generation of lasers.

PROJECT NO. 41.1/031

STABILITY AND DEVELOPMENT OF METHODS FOR SOLVING MULTIOBJECTIVE DISCRETE OPTIMIZATION PROBLEMS

Project Manager: *Serhienko, I.V.*

The research conducted within the framework of this project can be used as basis for decision-making under conditions of uncertainty. Particularly, they can apply to the theoretical and economic study within the framework of mathematical modeling of transition in Ukraine's economy and to the identification of new patterns of the economy as a whole and its individual components. Also they can be used in the course of decision-making at various levels of economic activities. The development of new mathematical methods for the identification and regulation and resolution of incorrect vector models of discrete optimization is an important tool to support decision-making in various fields of human activities and all the participants of the process, from the government bodies to the business entities and consumers, in the context of Ukraine's transition economy characterized by imbalance between the old production processes and the new conditions of management, as well as by a lack of proven mechanisms of market self-regulation, which have been evolved over decades in the advanced market economies. This support includes the complete and accurate information provided as a result of its analysis, structuring, and correction, as well as the specific recommendations for rational management decisions.

PROJECT NO. 41.1/044

TOPOLOGICAL SELF-ORGANIZATION OF COVALENT LATTICE STRUCTURE AS BASIS FOR THE DEVELOPMENT OF HIGHLY RELIABLE INFRARED PHOTONIC MEDIA

Project Manager: *Vakiv, M.M.*

This project is aimed at developing the methodology of selection of highly glass-forming alloys based on germanium chalcogenides for the use in modern IR telecommunication equipment, optoelectronics, and photonics.

The specific fundamental problem solved in the project is to study the experimental and quantum-mechanical methods of topological self-organization processes in the structure of chalcogenide glasses while changing their chemical composition.

These results have important implications for modern infrared photonics, telecommunications, and optoelectronic materials science. The importance of this research is associated with approval of new approach to determine the most optimal and highly reliable compositions of chalcogenide glasses for practical application. It allows the researchers to predict the boundaries of self-organized phase in chalcogenide glasses with more complex composition. The specifications of prepared samples of chalcogenide glasses are prevalent over the known world analogues due to increased resistance to physical aging and service reliability under the action of external factors.

PROJECT NO. 41.2/014

STUDY OF STRUCTURE FORMATION AND PROPERTIES OF LASER EXPOSURE ZONE FOR HYBRID PROCESSES OF LASER WELDING

Project Manager: *Sheliagin, V.D.*

The project is aimed at studying the structure and properties of laser exposure zone in hybrid processes of laser welding and deposit welding. It is expected that the planned research will establish

the patterns of forming the structure and properties of materials in exposure zone for hybrid processes of deposition and welding with the use of laser radiation.

The development of equipment and tools for control, management, and mutual adjustment of components of hybrid welding and deposition will allow one to control the parameters of two sources of energy, which will result in formation of required weld or deposition zone with the help of new process design with predictable molten pool and quality of deposited layer, which prevents the formation of cracks and guarantees strong mechanical properties.

The techniques developed on the basis of research results will be commercialized through executing the individual orders or organizing turnkey stations while providing necessary equipment according to customer requirements. The commercial implementation of project results provides for equal rights of parties to the results of operations.

PROJECT NO. 41.2/017

STRENGTHENING AND RESTORATION OF METAL SURFACES BY ELECTRO-SPARK DOPING METHOD WITH ADDITIONAL ULTRASOUND EXPOSURE USING MULTIFUNCTIONAL ELECTRODE SYSTEMS DOPED WITH IRON, COBALT, AND NICKEL

Project Manager: *Paustovskyi, O.V.*

The project is aimed at developing the basic principles of using the cutting-edge technique of multi-component electrodes based on intermetallics and spark coatings made of them with high performance characteristics.

The project studies have made it possible to establish the basic patterns of creating electrode composite materials containing intermetallic compounds, especially, forming their phase composition and structural conditions.

The implementation of techniques for electrode material production, which have been developed within the framework if this project and the application of these materials in order to strengthen and to restore the worn parts will make it possible to reduce the cost of repairing the equipment 5—6 times, as well as to increase the wear-resisting properties 2-4 times and the heat resistance 5—6 times. This allows one to do significant savings of material and energy resources in engineering industry. The results can be used in machine-building, metallurgy, and mining complex for ensuring the maximum durability of processed products and electro-erosive machining of worn parts of manufacturing equipment.

PROJECT NO. 41.2/018

DEVELOPMENT OF RESEARCH BASIS FOR INTEGRAL TECHNIQUES FOR TEMPLATE NANOSTRUCTURES OF INTEGRAL OPTOELECTRONIC ELEMENTS BASED ON III-NITRIDES

Project Manager: *Osinskyi, V.I.*

The new nano-element and nano-electronic techniques for producing light emitters in the visible and near ultraviolet ranges which can be integrated into advanced microelectronic element basis have been developed.

The technique for obtaining the ordered arrays of III nitride semiconductor nanostructures on large-diameter silicon wafers. The nanolayers of AlN, AlN_xO_{1-x} and Al_2O_3 have been experimentally obtained. A possibility of substitution of nitrogen atoms for oxygen ones at a relatively low temperature of ion energy has been showed for the first ever time. The nanostructures have been obtained in nitrogen plasma with energies of 1—150 eV during 5—10 minutes at a temperature of 150—200 °C. The structures of AlN/ AlN_xO_{1-x} are formed within nano-peroxide of aluminum.

It has been experimentally showed that under the action of N+2 low energy ion radiation the molecules of aluminum oxide are dissociating, which speeds up the chemical reactions by 2-3 orders as compared with the thermal activation. At the same time, the mutual solubility of Al_2O_3 with AlN increases, which promotes the formation of quantum-dimensional structures, particularly, the quantum dots. This technique can be used to create quantum computer elements.

PROJECT NO. 41.3/005

DESIGN OF VISIBLE LIGHT SENSITIVE PHOTOVOLTAIC CELLS BASED ON QUANTUM DOTS OF CHALCOGENIDES OF METALS, WIDE-ZONE OXIDE SEMICONDUCTORS, AND GRAPHENE DERIVATIVES

Project Manager: *Kuchma, S.Ya.*

Within the framework of project the following tasks have been made:

a) New methods for the synthesis of quantum-dimensional chalcogenide semiconductors and partially reduced graphene-oxide have been elaborated with the use of chemical, photochemical, photocatalytic, and photo-electro-catalytic approaches, as well as the processes of sequential ion adsorption;

b) New methods of formation and techniques for electrochemical monitoring and characterization of complex composite film structures based on mesoporous titanium and zinc oxides, quantum-dimensional particles of cadmium, zinc, and lead chalcogenides, and on partially reduced graphene-oxide have been developed;

c) The visible light sensitive film photo-electrodes which are promising for the use in the third generation of solar cells have been obtained.

The dynamics of charge transfer in electrolyte / nanoparticle / metal system have been studied; electrocatalytic activity of these systems in redox processes has been investigated. The main factors determining the effectiveness of spatial separation and transport of photo-generated charges in nanostructures with graphene derivatives have been established.

The optimal modes of operation model for photovoltaic cells based on films consisting of mesoporous titanium oxide and zinc chalcogenide nanoparticles and partially reduced graphene-oxide.

PROJECT NO. 41.3/008

ARYLATION PRODUCTS OF FUNCTIONALIZED FURAN, THIOPHENE, AND PYRROLE DERIVATIVES IN MOLECULAR DESIGN OF NITROGEN CONTAINING HETEROCYCLES

Project Manager: *Obushak, M.D.*

The main idea of project is to design the complex heterocycles, including new heterocyclic systems, with the use of functional derivatives of aryl-furan, aryl-pyrrole, and aryl-thiophene. The high reactivity of these compounds makes it possible to synthesize a complex of multinuclear heterocyclic derivatives with high potential for biological activity. Depending on the nature of functionalization the listed reagents act as the amine and carbonyl (aldehyde) components in cyclization. The variation of other cyclization components has generated the approaches to synthesis of various heterocyclic systems, including multi-nuclear ones with different heteroatoms.

It should be noted that the arylation of pyrrole derivatives by arene-diazonium salts were described in literature and there were only a few examples of involvement of thiophene derivatives in this reaction, where the target products were obtained with a low yield. The complications encountered were associated with high acidofuge factor of pyrrole ring. Based on their experience in this field, the authors have suggested the possibility of successful project implementation of reactions; developed this hypothesis; and successfully implemented it.

Compounds with new heterocyclic ensembles, which are promising with respect to screening of biological activity have been synthesized. The direction and selectivity of cyclization have been studied. Effective methods of synthesis of new reagents for heterocyclizations based on the use of different options of arylation of pyrrole, furan, and thiophene derivatives have been developed. The functionalized 5-aryl-pyrroles (thiophenes, furans) tested as structural units in the molecular design of nitrogen-containing heterocyclic compounds (thiazole, thiadiazine, oxazine, triazole, triazole [3,4-b] -1,3,4-thiadiazole) have been obtained.

PROJECT NO. 41.3/013

PALLADIUM PHOSPHONATES (II) IN NEW TECHNIQUES OF DIAGNOSIS AND TREATMENT OF CANCER DISEASES

Project Manager: *Pekhnio, V.I.*

Within the framework of project the following tasks have been solved:

The coordinating features of phosphonic acid derivatives have been defined on the basis of data on structure, composition, stability, and spectral characteristics of complexes;

The concentration conditions for creating the solutions of palladium (II) complexes with 1- hydroxyethylidene-1, 1-diphosphonic acid, which are sustainable and have a stable composition, have been developed. The concentration conditions for synthesizing the complexes of palladium (II) with derivatives of phosphonic acids have been established on the basis of the distribution diagram of equilibrium concentrations of complexes;

The most promising complexes for creating new anticancer drugs have been selected on the basis of biological activity screening. Hence, as a result of project, new promising medicine palladium complexes with derivatives of phosphonic acids have been obtained and studied. Their effect on the healthy and the tumorous tissues has been established.

PROJECT NO. 41.4/023

STUDY OF CORRELATION BETWEEN FORMATION OF THIAMINE OXIDIZED DERIVATIVES AND METABOLIC DISORDER UNDER ADVERSE CONDITIONS TO DEVELOP THE CORRECTION WAYS

Project Manager: *Donchenko, G.V.*

The mechanism of influence of reactive nitrogen and hydrogen on the oxidation of thiamine and its derivatives has been studied. The release of fluorescent metabolites, thiamine, and thiamine-disulfide after exposure of thiamine aqueous solutions and bank blood to ionizing radiation and ultrasound (880 kHz, intensity 0.2—2 W/cm^2) has been determined. The possible role of xenobiotics (for example, paracetamol) in the oxidation of thiamine derivatives in tissues has been studied. The ability to protect blood proteins from nitration of tyrosyl residues under unfavorable conditions by administering therapeutic doses of thiamine has been investigated.

These data justify the use of thiamine, its hydrophobic metabolites (thiochrome and oxodihydrothiochrome), and their complexes with other biologically active compounds, such as the antioxidants, to inhibit nitration of protein tyrosine residues under exposure to X-rays or γ- radiation in inflammatory processes. A test on metabolic disorders caused by exposing the human organism to nitrogen dioxide and peroxynitrites formed under the action of ionizing radiation and other adverse environmental factors accompanied by oxidative and nitrosyl stress has been developed.

On the basis of results a new colorimetric method for determination of thiamine and TDF in pharmaceutical preparations will be proposed. In addition, the researchers intend to develop a diagnostic test to determine the radiation dose received by the human being and the fact of being exposed to such action.

PROJECT NO. 41.4/028

DEVELOPMENT OF PRINCIPLES AND METHODS FOR ASSESSING IMPACT OF OPERATING NUCLEAR POWER PLANTS ON HYDRO-ECOLOGICAL SYSTEMS

Project Manager: *Protasov, O.O.*

The main fundamental idea underlying the project is that the anthropogenic tech-ecosystems play as important role in the biosphere as the natural ecosystems do. However, their structure and function have not been understood and studied sufficiently. To a large extent, it concerns the tech-ecosystems of NPP. The system for NPP EIA can be developed only on the basis of a thorough study of the structure and functioning of integrated tech ecosystem.

A comprehensive assessment of NPP impact on environment based on the tech ecosystem conception has been proposed for the first time. The criteria framework for expert evaluation and methodology for evaluation based on the Water Framework Directive EEC have been elaborated; the national methodology used for assessing the quality of aquatic environment has been used. The concept of NPP tech ecosystem has been elaborated and is used in Hydrobiological Monitoring Regulations.

In the course of project the basic principles of hydro-biological monitoring of NPP heat tanks, cooling, and industrial water supply systems have been developed. They have been included in the document titled «Regulations for hydro-biological monitoring of heat tanks, cooling system, and service water supply system of Khmelnitsky NPP» no. O.LO.6211.RH-12. Similar regulations can be prepared for all the nuclear power plants and thermal power plants of Ukraine proceeding from the above basic principles. The main provisions of the regulations can be implemented at the Belarusian energy facilities as well.

PROJECT NO. 41.4/042

ROLE OF GENES AND PHOSPHOLIPID AND CARBOHYDRATE METABOLISM ENZYMES IN PLANT GROWTH AND TROPISM

Project Manager: *Kolesnikov, Ya.S.*

The gene expression and beta-glucosidase enzymatic activity in different plant organs (and in different organ areas) of growing young plants have been characterized. The effect of different light conditions on gene expression and on activity of beta-glucosidase enzyme has been studied. The peculiarities of beta-glucosidase functioning (at the level of enzymatic activity and gene expression) at the initial stage of plant (leaf) growth during ontogeny under different conditions of plants lighting have been established. The involvement of beta-glucosidase in controlling the metabolism of phyto-hormones and its role in tropism reactions has been estimated.

The analysis of results has showed that the processes of plant tropism in response to changing the direction of vector of gravity involve D phospholipase. The local increase in auxin hormone in plant tissues intensifies gravitational tropism impeded by adding a phospholipase D 1-butanol inhibitor.

The research results can be used to develop the methods for growing plants under conditions of microgravity and during long-term space flight.

PROJECT NO. 41.4/043

ROLE OF PTTG GENE IN LIVER PRECANCEROUS PATHOLOGIES

Project Manager: *Sybirna, N.O.*

Chronic liver disease (CLD) is a serious problem in modern medicine, insofar as for a long period it proceeds asymptomatically and being untreated leads to liver cirrhosis (LC). Recently, there has

been recorded an increase in experimental works related to the efficiency of gene therapy for treating fibrosis and cirrhosis. The role of many signaling cascades in pathogenesis of liver fibrosis remains unclear. Among the signaling factors a special attention should be paid to pituitary tumor transforming gene (PTTG) which has been discovered recently and is involved in a wide range of physiological and oncogenic functions, including regulation of the cell cycle, DNA repair, angiogenesis, and oncogenesis. The PTTG expression correlates with invasiveness and tumor stage, which allows the researchers to use the PTTG protein analysis as a prognostic marker indicator.

In this regard, the effect of PTTG gene on liver fibrogenesis and organogenesis has studied by the example of an experimental model of liver fibrosis of mice, for subsequent use as a method of gene therapy. The research results constitute a scientific framework for the development of methods for correcting hepatocyte functional state in the course of treatment of patients with precancerous lesions and liver cancer pathology by means of correcting PTTG gene expression.

The results can be used for further research to find a method for inhibiting the PTTG gene expression in experimental models.

For more information, please, contact the State Fund for Fundamental Research: office 404, 16 Shevchenko Blvd., Kyiv; phone: +38 (044) 246-39-27, 246-39-29, 246-39-30; web page: www.dffd.gov.ua