

### **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. GP/F44/004

Electromagnetic Methods of Log Survey in the Study of Oil and Gas Wells under the Complex Geological Conditions

Project Manager: Myrontsov, M.L.

The methods of electric and inductive logging are developed by large commercial corporations (*Schlumberge*, *Halliborton*, and *Backer Huges*) which do not disclose information on their techniques. In Ukraine, the need for such job is constantly debated in academic and industrial circles. However, not any practical steps in this direction have been done yet.

The idea is based on using new types of equipment that is innovative with respect to both the method of measurement (pulse method with measuring in the three spatial directions, etc.) and the characteristics (high resolution, wide range of setting the geo-electric parameters of oil- and gas-bearing formation, etc.). These ideas were worked out at the level of modeling. A highly effective way of solving the direct and inverse problems of electric and inductive logging by method of integral currents developed by the project manager has been used to create algorithms and software.

Not any consequential studies have been conducted before that in Ukraine. The work is relevant and attractive from both the research and the practical standpoint. A highly effective method of electromagnetic logging during the geophysical survey has been developed. Two applications for patent of Ukraine have been submitted. A fundamentally new model of electromagnetic logging apparatus has been manufactured.

The project can be used by national and international geophysical companies engaged in logging.

### PROJECT NO. GP/F44/008

### Fuel Disperse Systems Based on Highly Concentrated Coal Slurries Project Manager: Savitskyi, D.P.

The fuel disperse systems based on highly concentrated coal slurries are used to solve the problems of efficient consumption of natural coal and utilization of coal waste.

To implement the results of research in the industry it is necessary to work out a regime of burning of highly concentrated coal slurry in pilot facilities available at the institutes of the NAS of Ukraine. In Ukraine, the development of infrastructure for production of fuel dispersed systems based on natu-

ral coal is possible in the following areas: burning in boilers with power capacity up to 20 MW and burning in thermal power plants and CHP boilers with power capacity over 20 MW. In the first case, the financial cost will be spent only for minor refurbishment of ready-made design of boilers in which solid fuel is burnt. The second one requires significant modernization of equipment depending on selected method of burning. The implementation of fuel dispersion systems based on highly concentrated suspensions is appropriate primarily for the boilers that use ineffective layer-wise method of coal burning, as well as for power generating facilities of thermal power plants and CHP plants operating on gas or oil in order to replace expensive energy sources. In addition, it is possible to perform combined combustion of coal slurry with gas.

#### PROJECT NO. GP/F44/010

### Development and Clinical Studies of Nanocomposite Materials for Medicine Project Manager: Pogorelov, N.V.

The transplantation of organs and tissues has been still an unsettled issue in most countries.

The use of artificial materials to replace damaged or lost organs is an optimal solution to this problem. Orthopedic plastic reconstruction is the leading field using artificial implants among the surgical procedures. Thus, only in the European Union, about 600 thousand operations are performed annually. Therefore, the development of new materials for orthopedic plastic reconstruction is an actual medical and biological problem of today. Chitosan is one of the most promising materials for the synthesis of artificial implants. However, not a single sample has passed the full-cycle research which includes physical and chemical analysis of materials, model animal tests, and clinical application. Therefore, there have remained unresolved issues related to optimal drug synthesis formula, dependence of drug properties on the structure, and material interaction with living bone tissue. This project is aimed at solving this problem.

For the Ukrainian market of osteoplastic materials the use of chitosan is innovative. The advantage of this polymer is the ability to form pores of different diameters and to produce implants with varying texture and shape. However, adding the apatite component makes it possible to produce implants with high biomechanical properties. The advantages of new osteoplastic material are the presence of nano-apatite, as well as the explicit implant's osteo-conductive and osteo-integration properties which have been testified by a variety of biophysical and histological methods. One of major material characteristics is its low cost and satisfactory biological properties which allow the specialists to widely use implants in orthopedics and traumatology.

### PROJECT NO. GP/F44/014

# The Development of New Organic-Inorganic Luminescent Nanosystems Based on Hetero-Nuclear Complexonates of Lanthanide with p-Metals Project Manager: Smola, S.S.

The main idea of the project is to develop methods for obtaining hetero-nuclear lanthanide-containing complexes in silica nanoparticles with effective emission characteristics.

The presence of p-metal-complex chromophore capable to absorb and to transfer excitation energy to radiating states of lanthanide and silica matrix ions can significantly reduce non-radiating energy loss on high frequency vibrations of solvent molecules. As compared with previously known materials an advantage of proposed organic-inorganic systems based on lanthanide-containing complexes is a

possibility to significantly increase the quantum yield of luminescence at a much lower concentration of emitting (i.e. lanthanide) centers.

The specific fundamental problem solved by the project is the development of strategies for directed synthesis of hetero-nuclear complexes of lanthanides with p-metals (Ge (IV) and Sn (IV)) based on amino-poly-carbon acids of different structure, as well as of silica-polymeric nanosystems containing given complexes.

The results obtained in the course of the project make it possible to do target search of lanthanide-containing fluorescent compounds with practically useful properties. The developed methods for the synthesis of organic-inorganic systems containing lanthanide fluorescent complexes are useful for designing the functional materials of high-tech optics, molecular devices for light convertion, and so on.

### PROJECT NO. GP/F44/015

# Diagnostics of Coalescence Fractured Dissipative Structures Based on Meso-Mechanics Approaches

Project Manager: Maruschak, P.A.

Based on the combination of phenomenological approaches and methods of mathematical statistics the cracking of materials is described as a synergistic process. This has allowed the researchers to evaluate the kinetics of material damage accumulation at different (micro, meso, and macro) levels and to offer technological approaches to the formation of stable state of cracked surface.

The synergistic approaches used in this work make it possible to consider the fractured structure as multilevel hierarchical systems whose elements determine the functional meso-structural levels of deformation. The use of this approach has made it possible to develop a method for diagnosing the support ability of structure with multiple crack-like defects during continuous production cycle and to forecast strength, ductility, and residual durability of structures of heavy-loading facilities.

The research relevance is caused by the need to improve the accuracy of diagnostics of current structure physical conditions and to extend the residual life of metallurgical equipment.

#### PROJECT NO. GP/F44/016

Development of Scientific Framework for Environmental Safety of Natural and Anthropogenic Geo-Systems in Ukraine's Carpathian Region and Adjacent Areas

Project Manager: Prikhodko, M.M.

Under the conditions of almost total reclamation of Ukraine's territory (especially, environmentally vulnerable mountain and foothill areas in Ukraine's Carpathian region and adjacent zones) the study of issues related to human impacts on the environment (natural geo-systems), the development of environmental risks, and the ecological safety of geo-systems is of paramount importance. To develop a model of environmentally friendly use of nature and to harmonize the anthropogenic impact on natural and anthropogenically modified geo-systems with the environmental regulations we need to elaborate the scientific framework for environmental safety of natural and anthropogenic geo-systems because they predominate in the structure of geo-systems which shape the environment.

The scientific approaches and recommendations on environmental safety of natural and anthropogenic geo-systems can be used by regional offices of the State Land Agency and the State Water Agency of Ukraine, regional environmental protection administrations of the Ministry of Environment

of Ukraine, as well as by executive bodies and local self-governing authorities to substantiate the economic activities and scope of utilization of natural resources and to elaborate the strategy for sustainable socio-economic development of Ukraine's Carpathian region and adjacent areas.

### PROJECT NO. GP/F44/025

### Engineering of Mechanical Stresses in Semiconductor Hetero-Structures as the Basis of Modern Nano-Device Architecture

Project Manager: Kuryliuk, V.V.

The key project outputs are as follows:

Spatial dependence of strain tensor components in SiGe hetero-structures with quantum dots of different morphology and component composition has been established. The quantum dots which are heterogenic by germanium content have been showed to be less strained than the nano-islands of constant composition. In addition, the heterogeneity of germanium content leads to the redistribution of strains within the quantum dots with corresponding restructuring of edges of SiGe hetero-structure energy zones.

The changes in density of germanium quantum dots grown on pre-oxidized silicon surface have been established to significantly affect the depth of localization of electrons in silicon substrate due to redistribution of elastic fields. This fact opens the horizons for controlled influence on the processes of recombination in hetero-structures by changing their stress state.

The elastic strain in the silicon-germanium hetero-structures has been experimentally showed to cause reorganization of photo-EMF kinetic dependences as a result of deformational changes in the structure of hetero-junction energy bands.

The project results can be used as scientific framework for the manufacture of photo- and thermoelectric converters based on hetero-structures with quantum dots, the operation of which is determined by recombination processes in the structures. Engineering of mechanical stresses will make it possible to monitor the above mentioned processes to improve the effectiveness of photo- and thermoelectric conversion.

#### PROJECT NO. GP/F44/027

# Intelligent System for Early Warning of Bankruptcy of Ukrainian Enterprises

Project Manager: Matviichuk, A.V.

Among the potential users of developed intelligent system for early warning of bankruptcy of enterprises there are banks, investment companies, credit unions, government bodies, industrial enterprises and organizations, and holdings.

The intelligent information system for early warning of bankruptcy of enterprises can be used by risk management units of banks in order to select reliable borrowers. It allows them to objectively assess the financial status of enterprises, probability of borrower bankruptcy and default on loans.

Also, the information system can be used by managers or analysts of companies and holdings for making managerial decisions. It allows them to identify the existing internal problems of financial nature and to take the preventive measures. Geographically, the market size corresponds to the territory of Ukraine. In the case of further improvement of proposed information-analytical system towards the incorporation of specific features of each country the market can be extended to any country provided there exists the respective statistical framework and the model is adjusted to it.

### PROJECT NO. GP/F44/038

# New Bacterial Bio-Sorbent for Extraction of Uranium (VI) and Strontium from Aqueous Media Project Manager: Shevchuk, I.A.

As of today, there has been known a lot of different sorbents that can be used to remove heavy metals and radionuclides from aqueous media. However, their use has both positive and negative effects. Thus, the main drawbacks of using the clay minerals as sorbents are their low sorption capacity with respect to activated carbon and radionuclides, high cost and complicated disposal of waste materials, and so on. In this regard, the possibility of using biological methods of water purification draws attention of domestic and foreign scientists. The most promising is the use of biotechnologies based on sorption processes with natural microbial associations or pure culture as sorbents. The advantages of using the microbial sorbents are high effectiveness of metal ion removal, small amount of waste, sustainability, accessibility, and low cost.

The results can be used to develop a new and effective environmental technology to clean up radioactively contaminated natural and artificial waters and to reduce anthropogenic impact on the environment. In the course of project, there was justified the principle technological scheme for purification of water systems from soluble compounds of uranium (VI) and strontium by bio-sorbent based on cells of *B. polymyxa*, which involves the use of periodic configuration of the process followed by separation of biomass by centrifugation. The ceramic technique has been proposed for disposal of waste radioactive bio-sorbents.

#### PROJECT NO. GP/F44/054

### Calixarenes as Effectors of ATP-Hydrolytic Smooth Muscle Systems Project Manager: Shkrabak, O.A.

Failure of contractile function of uterus smooth muscle (myometrium) often causes various pathologies: slow labor, spontaneous abortion, premature birth, miscarriages, atony, uterus hypo- and hyper-tonus. These pathologies are conditioned by dysfunction of membrane-bound cation transport systems, as well as of contractile apparatus of uterus smooth muscle. Hence, the creation of pharmacological products that can modify the myometrium contractile function in the case of these pathologies is promising direction of research.

The dependence of calixarene inhibitory properties with respect to  $Ca^{2+}$  and  $Mg^{2+}$  ATF activity of the plasma membrane of myometrium cells on the structural organization of calixarene molecule has been studied. The results obtained allow the researchers to directly enhance the effector properties of calixarenes and to create new biologically active compounds.

The pharmacologic agents for treatment of pathologies associated with impaired myometrium contractile function can be created on the basis of the respective calixarenes.

### PROJECT NO. GP/F44/064

### New Oligomeric Systems with 1,3,5-Triazine-Containing Derivatives of Thiopyran [2,3-D] Thiazol-2-on as Potential Anticancer Agents

Project Manager: Skorokhoda, T.V.

The methods for synthesis of thiopyran [2,3-d] thiazol-2-on have been developed; the influence of temperature and solvent on the course of cyclic condensation reaction has been studied. This allows the researchers to achieve a maximal yield of target product with minimal material and energy costs.

New linear and branched block co-oligomers with controlled functionality and molecular weight distribution have been obtained by radical grafting polymerization; their structure and colloid-chemical properties have been studied; and the possibility of their use as carriers in the transportation system of medicines has been considered.

The synthesized oligomeric carriers can be used in various systems of drug delivery because their structure allows them to bind the drug by one of three mechanisms: solubilization, complexation or covalent binding.

#### PROJECT NO. GP/F44/086

### The Molecular Nature of Point Mutations Induced by Modified DNA Bases: Quantum Chemical Simulation Study

Project Manager: Brovarets, O.O.

The results open up new possibilities for designing highly efficient mutagenes — analogues of target-action nucleotide bases that can selectively induce errors of replication or errors of inclusion. This is important for both the development of new cancer control strategies using the phenomenon of "mutational catastrophe" and the applied molecular genetics, particularly, for selective breeding. The results obtained will allow the biophysicists and molecular biologists to plan experiments on differentiating the errors of inclusion and the errors of replication, on the mutations occurring during genome replication and when storing the genetic information, as well as experiments on site-directed mutagenesis for studying the physical mechanisms of DNA biosynthesis accuracy. In addition, the mechanisms will make it possible to predict the frequency of induced mutations caused by chemicals, including by the environmental pollutants which are potential mutagens.

### PROJECT NO. GP/F44/095

# Technique for Removal of Dying Cells as a Promising Way of Autoimmune Disorder Treatment Project Manager: Bilyi, R.O.

In the course of research, there has been developed a technique for formation of abzymes with sialidosic activity through immunizing by hapten-protein conjugate of sialidosic reaction transition analogue. Half-preparative amount of abzymes with sialidosic activity has been obtained; their purification and characterization have been made. The treatment of cells with abzymes has been showed to cause their induced desialylation. The treatment of apoptotic cells has been established to enhance eferocytosis (phagocytosis of dying cells) by macrophages differentiated from venous blood monocytes. An application for Ukraine's patent on invention by no. a201210528, priority of 06.09.2012 «Catalytically active antibodies with sialidosic activity and methods for their production» has been submitted.

The technology has showed that it is possible to create the abzymes with sialidosic activity for therapeutic use, in order to prevent autoimmune diseases.

#### PROJECT NO. GP/F44/107

### Physical and Technological Features of Integrated Optoelectronic Systems Based on Organic Electroluminescent Devices

Project Manager: Cherpak, V.V.

The fundamental problem of research is the need to create new economical organic information displays and to make in-depth analysis of the processes of input and distribution of light radiation

generated by organic light emitters in fiber waveguide, including the processes that occur in organic electronic devices.

The specific fundamental objective of research is to develop a technological framework for the organic elements of integrated optics and displays based on the study of physical aspects of distribution of light radiation generated by organic electroluminescent structures directly in optic environments; to manufacture and to study integral optical devices containing organic light-emitting structures acting as generators of optical radiation integrated in optic systems.

For the first time, there has been developed a technique for formation of white glow OLED of ITO /THCA (24 nm) / periodic film Alq3 (10 nm) / Ca (140 nm) / Al (200 nm) structure the brightness of which with CIE coordinates (0.36, 0.38) close to the natural white light (0.33, 0.33) is equal to 300  $cd/m^2$  at 7 V and a current efficiency of 2.2 cd/A.

The proposed light-emitting structure can be used by international and national companies specializing in the manufacture of displays (*LG*, *Samsung*, *Panasonic*, etc.) or lighting devices.

### PROJECT NO. GP/F44/127

Studying the Impact of Transplantation of Testis Steroidogenic and Germinal Cells Using Conventional Pharmaceutical Products of Replacement Therapy for Correction of Different Conditions of Experimental Hypogonadism

Project Manager: Pakhomov, A.V.

Polyetiology of male infertility, complexity of the course of disease, and functional interdependence of male gonads on all the systems and organs create significant difficulties in developing adequate therapies [Rajfer J. Cambell's, 1992]. Variety of techniques used, lack of common approach, and wide range of tissue and cellular techniques have drawn attention to the subject of cell transplantation.

Among the tasks of this project, there is the study of effectiveness of hormone replacement and stimulating therapy in combination with a promising modern method, the cell transplantation, for the correction of hypogonadism of different origin.

The results allow us to analyze different states of sexual disorders associated with a decrease in androgen levels and fertility and to predict how to adjust the treatment (for example, to reduce the dose of testosterone in case of hypergonadotropic hypogonadism caused by absence of gonads as a result of trauma or surgical removal because of malignant neoplasms), as well as to reduce doses of chorion gonadotrophic hormone to remove symptoms of hypogonadism caused by the action of toxic factors (e.g., by administration of chemotherapy drugs or poisoning by salts of heavy metals). Due to the method of transplantation it is possible to remove the symptoms of testosterone deficiency, to mitigate possible negative effects of replacement therapy (emotional mood swings as a result of androgen level fluctuations, adverse effect on prostate, premature closure of bone epiphyses, early puberty, edema, hypercalcemia, dizziness, nausea, thrombophlebitis, cholestatic jaundice, increased level of aminotransferase), and to prevent inhibition of steroid-producing cells.

### PROJECT NO. F47/021

Mechanisms of Medicine Trans-Membrane Permeability under the Action of Thermo-Trophic Liquid Crystals

Project Manager: Kravchenko, I.A.

The biological membrane is the major barrier separating the internal environment from the external influence. It has a complex structure. Creation of favorable conditions for drug penetration through bio-membranes is the main function of trans-membrane permeability amplifiers.

Understanding of the mechanisms of influence of thermo-trophic liquid crystals on molecular structure of lipid matrix will solve the problem of creating an optimal amplifier of permeability of drugs penetrating mainly through the lipid matrix. Therefore, the fundamental scientific problem to be solved in this project is to elucidate the mechanisms of enhancement of drug penetration through intact bio-membranes, in particular through intact skin.

Optimization of drug penetration into the organism and its impact on target organs depends largely on the way in which it is administered. The use of intravenous and oral medications does not always mean optimal impact on the organism. In this regard, such alternative methods as intranasal, transbuccal, rectal, and transdermal administration of drugs are of special interest of researchers. Using these methods is one of ways to optimize drug therapy of various diseases.

The results can be used to create new drugs. The most active compounds will be offered for an extended pharmacological research in order to obtain permission for pre-clinical tests.

### PROJECT NO. F47/045

### New Technique for Ethanol-Oil Based Biodiesel Fuel

Project Manager: Patryliak, L.K.

The main goal of research is to develop new technologies for producing biodiesel by ethanol interetherification of various oils with the stage of glycerol self-separation from reaction mixture, production of consolidated pilot batches of fuel, fuel tests on real engines, and evaluation of its energy effectiveness and environmental impact.

A new technology of biodiesel production by ethanol inter-etherification of vegetable oils on solid zeolite catalyst has been developed. The product is obtained as a mixture with petroleum diesel fuel. In the whole concentration range it surpasses the latter by anti-detonation and environmental characteristics.

The optimal conditions of inter-etherification of crude rapeseed oil by commercial ethanol have been established under the laboratory conditions, on the cheap and easy prepared solid catalyst.

The laboratory technique has been implemented on pilot plant for producing large batches of biodiesel by heterogeneous catalytic inter-etherification of rapeseed oil by ethanol. The results have proved the feasibility of implementing heterogeneous catalytic inter-etherification of vegetable oils by ethyl alcohol. The product has a proper quality and can be used as biodiesel in the pure state or be mixed with mineral fuel.

### PROJECT NO. F47/053

### The Development of Modified Protective Polymer-Composite Corrosionand Wear-Resistant Coatings for Shipbuilding

**Project Manager**: Buketov, A.V.

The properties and the control of structure formation as a result of modification of binders, fillers, and composites by external magnetic field and ultraviolet irradiation have been studied and substantiated from scientific standpoint. The regularities, mechanisms, and features of enhancing the performance of epoxy-composites as a result of improved interfacial interaction during the formation of materials have been established.

The results can be implemented at the leading enterprises, such as Kherson Shipyard, *Pallas* Shipyard (Kherson), the Black Sea Shipyard (Mykolaiv), *61 Communards* Shipyard (Mykolaiv), and *Zaliv* Shipyard (Kerch) dealing with testing of structural elements and enhancing corrosion- and

wear-resistance characteristics of process equipment, as well as at the enterprises of chemical, food processing, oil refining, and radar engineering industries for increasing the service life of equipment.

#### PROJECT NO. F47/066

### Changes in Functioning of T-type Calcium Channels in Nociceptive Neurons of Rats with Different Forms of Diabetic Neuropathy

Project Manager: Voitenko, N.V.

The dysfunction of peripheral nervous system, particularly, in case of neuropathy, is one of the important problems of present-day health care system. Peripheral diabetic neuropathy (PDN) is widespread among the diabetics and is often accompanied with impaired perception of pain. To identify the causes and to develop the methods for prevention of pain syndromes in case of various diseases, including diabetic neuropathy is fundamentally important tasks of modern physiology. Despite the huge amount of experimental and clinical materials accumulated on these issues over the recent ten years (Limanskyi 1986, Milan 1999), the question about how the pain appears still has not been answered ultimately. The study of mechanisms, processes, and phenomena in those brain systems which perceive and process information about the influence of pain factors on the organism can provide a significant progress in solving this problem.

The theoretical value of the project results is connected with the fact that they explain in detail the molecular mechanisms of impairment of pain sensitivity in case of various forms of diabetic neuropathy at the level of calcium channels functioning. The practical value of results is their usefullness for the development of drugs aimed at alleviating the condition of patients suffering from various forms of diabetic sensory neuropathy. The obtained data and their interpretation can be the basis for developing highly selective pharmacological approaches to the treatment of aforementioned pathologies. The substances influencing the operation of plasma membrane calcium channels are suggested to be used for the treatment of sensory neuropathy of patients suffering from diabetes.

### PROJECT NO. F47/069

### Improved Methods for Reducing the Anthropogenic Environment Pollution by Oil and Gas Sector

Project Manager: Shkitsa, L.E.

The dependencies for determination of basic parameters of drilling fluid and equipment, which affect the intensity of emission of hazardous substances into environment have been obtained. Methods for mathematical simulation of drilling fluid vapor emission to the atmosphere and a methodology for experimental research of evaporation intensity have been proposed. A model-based method for evaluating the formation of gas contamination area and air pollution by leaks from pipelines has been developed. The operation safety and risk of destruction of long-term usage main oil pipelines have been estimated. An environmental impact assessment for the oil and gas sector in the region has been made in order to optimize the ecological conditions.

A method for determining pollution has been elaborated taking into consideration the design and operating parameters of the pump and circulation system when performing different processes by rig. This methods provide for:

♦ New design of vibrating sieve to reduce emissions of harmful substances to the air in the working area of drilling rig;

→ Forecasting of the environment conditions based on the mathematical models proposed for the main pipelines.

### PROJECT NO. F47/072

Studying the Role of Cell Signaling Mechanisms in the Response of Plants to the Action of Ultraviolet B as a Critical Factor for Improving Their Productivity

Project Manager: Yemets, A.I.

The methods to address the issues raised in the project will lay foundation for the further development of strategies for preserving the existing flora and producing high yields of important agricultural and industrial crops to overcome the lack of food, against the background of constant world population growth and to use alternative sources of biofuel production under the conditions of growing deficit of energy in the majority of countries. To understand the molecular mechanisms of perception and response of cells to the action of UV-B is necessary for developing new approaches to genetic and biotechnological improvement of plants, which will be used to create new lines with high flexibility and/or resistance to the action of UV light. This will enable their introduction in the dwelled areas with high UV-B level. The proposed research is original and unparalleled anywhere in the domestic and foreign markets. Thus, the project scientific and social impact is obvious and extremely high. The possible scope of application includes agriculture and energy industries.

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