

# PROJECT

# Research and development of new functional materials based on nanodimensional modifications of carbon FR - Oxigraphenes

# Development of a highly economical, environmentally friendly method for the preparation of a nano carbon material FR - Oxigraphen

# **Urgency of the project**

The project is a priority and relevant area in the field of applied and fundamental scientific research, development and production of nano carbon materials and quantum structures based on graphene and its derivatives.

It is expected that the receipt of new materials and instrumental structures based on graphene can provide promising breakthroughs in such scientific areas as nano electronics, nano photonics, information, space and military technologies.

The graphene market belongs to the High Tech sector. Many experts predict graphene and graphene oxides the phenomenal growth of commercial consumption. For example, in the report "Global Graphene Market (Product Type, Application, Geography) - Size, Share, Global Trends, Company Profiles, Demand, Insights, Analysis, Research, Report, Opportunities, Segmentation and Forecast, 2013-2020" Market from \$ 20 to \$ 149 billion, or 44% per year.

In the world market, the leading companies are CVD Equipment Corporation, Graphene Nanochem PLC, Vorbrck Materials, XG Sciences, Haydale Limited, Graphenea, Graphene Laboratories, Bluestone Global Tech, Angstron Material, Inc., ACS Material, LLC.

Today, prices for an aqueous emulsion of high quality graphene oxide are at 50 / g. In China, offer variable quality products for 20 / g. These prices are comparable to the price of platinum and some rare earth metals, which are widely used in modern technical devices. That is, graphene oxides have already overcome the price psychological barrier and can be used on an industrial scale.

The use of graphene and materials on its basis will provide the structures and instruments created with greater speed, lower power consumption and fundamentally new properties in comparison with existing devices.

#### **Project Summary**

The purpose of this applied scientific research and experimental development, the production of a new functioning nanocarbon material FR - Oxigraphenum is an analogue of graphite oxide and a precursor for the production of graphene.

The way of obtaining FR-Oxigrafen is an innovative high-tech, highly economical energysaving and environmentally friendly technology.

In this paper we present the results of an investigation of a carbon material synthesized by a low-temperature, catalytic, oxidative pyrolysis of structured polymeric substances containing heterocyclic carbon units and having a nano crystalline structure. Micro-fibrils of nano crystalline cellulose are used as a nano crystalline polymer.

It found that a synthetic material is a nanocrystalline carbon material consisting of carbon nanostructures of closed carbon nano tubes, oxigraphene fullerene-like particles.

The proposed method of carbonization is highly productive, forgive, cheap and effective. Synthesis is carried out by low-temperature SHS reaction (Self-propagating high-temperature synthesis method) is energy-saving and does not require special complex equipment.

#### **Product description**

FR - Oxigraphenes (Naming from English FR- OXIGRAPHENES Freely Radical Oxi Graphenes, naming on behalf of the mechanism of formation of nanocarbon). FR - Oksigrapheny a new kind of allotropic modifications of carbon, which is a carbon tube multisloynye filamentous forms of sostoschey oksigrafena (graphene oxide containing stable free radicals than is due to their unique properties specific).

Multilayer carbon nanotubes FR OXI-GRAPHENES are carbon quasi-one-dimensional nanoscale filamentous formations of polycrystalline graphite of cylindrical shape with an internal channel.

Carbon nano materials the FR - oxigraphenes are one-dimensional nano scale filamentary formations with a tube diameter of 2-10  $\mu$ m, up to 1000  $\mu$ m in length.

The basis of the super molecular structure of FR - oxigraphenes have - elementary highly ordered fibrils. The latter are associated in aggregates, micro fibrils - contain several hundred macromolecules; The dimensions in the transverse direction are from 4 to 10-20 nm, the average length of the crystallites is 7-10 nm. In the ultrasonic dispersion of FR- oxigraphenes in a liquid medium, it transforms into a low-layer graphene with a particle thickness of 0.34 to 4 nm.

The structure and dimensions of the FR tubes were studied by scanning electron microscopy, the two-dimensional graphene structure of the tube walls was confirmed by X-ray diffraction.

The morphology of the synthesized material is similar to the structure of the precursor of nano crystalline cellulose material, but differs from it by the carbon content, which can reach up to 100% in FR-oxigraphenes.

#### **Competitive advantages**

A new method for the preparation of nano conclusions FR-Oxigrraphenes is a cheap and high-tech way of obtaining the functioning oxide of graphene and graphene in tangible quantities by the method of available raw materials.

Advantages of the developed technology for the preparation of nano carbon FR - Oxigraphen compared to the known ones: availability, cheapness, expressiveness, reproducibility, manufacturability and scalability, the technique does not require the use of toxic and explosive reagents, severe synthesis conditions and expensive equipment. Development of environmentally safe mass production of oxygraphene.

# Innovative uniqueness of the project

A new functional material based on nano scale modifications of carbon FR - Oxigraphen has been developed. The technology of obtaining carbon nano materials FR - Oxigraphen with the given set of unique adsorption, energy storage, mechanical, electronic and optical properties is developed and mastered.

The uniqueness of FR - Oxigraphenes lies in the content in the carbon matrix of the nano material, free radicals, which gives it unique properties and can be used both in the traditional and in the new field of science and technology - carbon nano-, micro- and optoelectronics.

Depending on the synthesis conditions, FR - Oxigraphen may have the properties of both a semiconductor and a dielectric. This makes it possible to widely use graphite oxide in electroluminescent devices, super capacitors, electronics and other fields.

FR - Oxigraphenes is a super sorbent with the greatest absorption capacity among known materials. FR - The oxigene sorbent has a gigantic internal surface - more than 1000 sq.m. For 1 gram.

FR - Oxigraphenes are, nano fibrils, in the form of single-layer, meow-layered carbon structures of tubular structure.

In comparison with the known method of producing carbon microtubes by electric arc method, gas-phase catalytic hydrocarbon deposition and laser ablation, the proposed method has the advantage, both in terms of productivity, economic, technological expediency, and the ability to synthesize nanocarbon materials with specified parameters and properties.

#### Super composites based on carbon nanotubes FR - oxygene - technological breakthrough

Composite is a material created by a minimum of two components with essentially different properties that complement each other. For example, reinforced concrete consisting of concrete and steel reinforcement, or rubber, consisting of rubber and carbon black, fiberglass, carbon plastic - all these are composite materials. Their properties are determined by the properties of their components. And if the components are ideally conjugated, then the property of the final composite is the average between the properties of its components in proportion to their mass fraction.

If you intend to replace the material with 4 times stronger composite, then it should include the same mass of reinforcing component with strengths higher by 8 times. And if you want to increase the initial material by 4 times with a hardening additive of only 1%, then the strength of this additive should be stronger than the starting material 400 times. Conceptually, this approach is true for all properties - strength, thermal conductivity, electrical conductivity, etc.

Is it possible to radically strengthen the key properties of all basic materials (metals, cement, ceramics, polymers, electrode materials of batteries and solar cells, paints, coatings, glass, etc.) with an extremely small additive, turning them into similar supercomposites. And what properties should this super gift have. Will it be universal.

Let's list the properties under which super additive can become a universal additive for all basic materials:

- extreme strength,
- record electrical and thermal conductivity,
- low specific gravity,
- a huge specific surface area,
- chemical inertness,
- thermal stability,
- the ability to form chemical compounds with a huge range of substances,
- nontoxicity.

Of all the entities known to mankind, only two are suitable for the role of such a universal additive: single-walled carbon nanotubes and graphene.

Moreover, for a significant impact on world production, the super additive should be produced in millions of tons. Therefore, the requirements for the technology of its production can also be determined

- nontoxicity of components,
- economic and physical availability of raw materials,
- safety of the technological process,
- Scalability of technology,
- Minimal energy intensity,
- non-toxic waste.

A huge number of scientific studies have confirmed the most important thing for civilization: single-walled carbon nanotubes are a truly universal additive that improves properties.

Why are these opportunities still not used by civilization at full capacity.

The two main reasons are high cost and lack of scalable production technology. 100,000 per 1 kilogram of single-walled carbon nanotubes - beyond the limits of economic applicability (aluminum ~ 2 / kg), this is really very expensive. And the world production volume of 1 ton is too little.

Thanks to the production of FR - Oxigrains, very soon everything will change. Nanostructured materials and supercomposites will become really affordable. Algorithms for introducing carbon nanotubes into most materials will be invented, and thousands of tons of carbon nanotubes will be sent to thousands of plants to enhance properties.

FR - Oxigraphen allows the use of a wide range of functional paints, for many possible applications. They can be high adhesive properties, provided with high adhesion properties, antibacterial coating, solar paints that provide insulation of houses, anti-corrosion coatings, fog paints and UV-blockers, non-stick coatings for various household applications.

The developed methods and technologies of FR - Oxigraphenes can provide a significant expansion of the field of practical and scientific knowledge in dependence of the functional characteristics of carbon materials on the nature and degree of atomic order and disorder.

Development and mastering of the technology of production of single-layer and multilayer carbon nano tubes FR-Oxigraphen and composite materials on their basis in will make it possible to further enhance the complex of physic mechanical properties of carbon composites.

#### Examples of priority areas apply FR - Oxigraphen:

The use of the FR-Oxigraphen composite will enable the development of fundamentally new technologies for the production of electrode materials and electrodes using semiconductor technology.

The use of the composite FR-Oxigraphen vanadium oxide for lithium-ion, graphite batteries and super capacitors will enable the improvement of their capacitance and electrochemical characteristics

The use of FR-Oxigrafen composite using TiO2 / FR-Oxigraphen will enable the improvement of the photoelectric characteristics of inverted hybrid bulk hetero junctions of solar cells. The use of FR-Oxigraphen composite for the development of electrodes and other components of solar cells will reduce their cost.

The use of the FR-Oxigraphen composite, the development of new non-platinum catalytic systems and catalysts with a reduced content of precious metals, the development of new anion captions of conducting polymeric membranes based on FR-Oxigraphen can significantly increase the life of fuel cells while reducing their cost.

The use of the FR-Oxigraphen composite to create technology for high-temperature polymer matrices can increase their operating temperature to 400-450°C. The stability of polymers is enhanced by changing the kinetics of embryos and structuring and crystallization as well as the plasticizing effect of FR-Oxigraphen.

The use of the FR-Oxigrafen composite will make it possible to obtain radiation-resistant and radiation-absorbing ceramic composites together with an iron-phosphate binder for intermolecular immobilization for the neutralization of radioactive waste and protective structures in the construction of radiation facilities.

The use of the FR-Oxigraphen composite will make it possible to obtain hybrid nanoparticles with low toxicity and high fungicidal and bactericidal activity as well as the creation of biocompatible surgical materials.

**Project title:** 

"Development of a highly economical, environmentally friendly way of obtaining the nano carbon material FR - Oxigraphen"

The name of the organization within which the project is being implemented:

# CSTRE - Ararta Light (Center for Scientific and Technical Research and Expertise-Light Ararta, a special organization that is created to implement this project) RA, Yerevan.

**Purpose of the project:** 

The purpose of this work is to obtain high-quality functionalized graphene oxide FR - Oxigrafenes, which is a new kind of allotropic modification of carbon, possessing a unique composition and being a precursor for the production of graphenes

Main results of the project:

An innovative method for obtaining high-quality nano carbon FR-Oxigrafen, a unique method of pyrolysis of nano crystalline cellulose, is developed in which graphitization (graphitization) is carried out while maintaining the structure and morphology of the nano crystal cell of the carbon matrix of the starting material-nano crystalline cellulose.

Experimental samples of nano-crystalline carbon materials (carbon nano tubes, graphene) are made.

The reliability of the developed materials was confirmed by an analysis of the composition and morphology of the product being synthesized, as well as by the study of some of its physic-chemical properties (chemical stability, thermal stability, specific all, electrical conductivity, etc.).

## Appointment and scope of the project results:

The research is related to the field of nanotechnology and nano materials, the method for obtaining nano carbon materials - functioning graphene oxide FR - oxigraphenes and can be used in many branches of the nano industry in the manufacture of nano electric devices, chemical current sources, composites, catalysts, lubricants, protective coatings.

## Effects from the implementation of the project results:

Reducing the cost of production of single-layer and multilayer carbon nanotubes FR - Oxigraphen and graphene, increasing physical and mechanical properties of carbon composites.

## Forms and volumes of commercialization of project results:

The project will be implemented in 3 stages:

- 1. Laboratory research and development of synthesis technology and properties of FR-Oxigraphen;
- 2. Pilot small-scale production of FR Oxigraphen;
- 3. Commercialization of development results, organization of large-scale production of FR Oxigraphen.

Terms of the project (years of implementation)

# 2017-2022.

- 2017-2018. Laboratory research and development of technology of synthesis and properties of FR Oxigraphen, synthesis of 10-20 kg per month;
- 2019-2020. Pilot small-scale production of FR Oxigraphen with a capacity of 18 tons per year;
- 2020-2022. Planning and organization of production of FR Oxigraphen with a capacity of 200 tons per year;

## **Financial feasibility of the project**

The implementation of the project will require investment:

1. Laboratory research and development of technology of synthesis and properties of FR - Oxigraphen, synthesis of 10-20 kg per month; - **\$ 400 000** 

2. Pilot production of FR - Oxigraphen with a capacity of 18 tons per year; - \$ 2 million

3. Production of FR-Oxigraphen with a capacity of 200 tons per year; - \$ 12 million

## Total need for financial costs: - \$ 14.4 million US

# Payback period and the expected revenue from production

Annual productivity of FR-Oxigraphen 200T.

Cost of 1KG FR-Oxigraphen, 20 \$ USA

Selling price 1KG FR- Oxigraphen 80 \$ USA \*

Revenue from the sale of 1KG FR- Oxigrafen 60 \$ USA

## Expected annual income from the production of FR-Oxigrafen 12 000 000 \$ USA

The planned payback period of capital expenditures is  $\sim 2$  years (2 years after the commissioning of production).

Pilot production of FR - Oxigraphen with a capacity of 18 tons per year, after commissioning will be self-financing enterprise with a profitability of 1 000 000 \$ USA per year.

The planned payback period of capital expenditures of pilot production is  $\sim 2$  years (2 years after commissioning of pilot production).

\* The selling value of FR- Oxigraphen is 10 times lower compared to the market price of nanocrystalline cellulose and 100 times lower compared to the market price of graphene, which ensures a highly competitive product in the market.

### The proposed form of cooperation

Direct investments;

Participation in the project on a compensation basis in the form of deliveries of finished products, etc .;

Protecting the results of intellectual activity

The application for the invention "Development of a highly economical, environmentally friendly method for the preparation of the nano carbon material FR - Oxigraphen " was filed. As the development and research of new nano carbon composites based on FR- Oxigraphen are completed, a further 7 patents will be issued.

# **Project team (key employees):**

Name Family	Role in project	graduation degree	Comment
Khachatryan Vram	Scientific Founder	Engineer inventor	Author 25 Inventions, 110 scientific publications and monographs 8
Sekyan Hamlet	Lead researcher	PhD	Institute of Mechanics National Academy of Sciences ,Republic of Armenia
Nazaryan Ernest	Lead researcher	PhD	Yerevan State University
Suren Harutyunyan	Lead researcher	PhD	First National Laboratory. A.I. Alihanyan (EFI) Armenia
Varderesyan Gagik	Lead researcher	PhD	National Polytechnic University of Armenia
Oganesyan Arutyun	Lead researcher	Engineer	AT-METALS LLC Armenia

# Presence of asoispolnitelej:

Partners Project	Name partners
1	Institute for Basic Science (IBS), South Korea
2	Organization «MoRe Research» Sweden enterprises for the production of nano crystalline cellulose.
3	Department of Chemical Engineering and Department of Chemistry, Center for Electrochemistry, University of Texas at Austin,
4	University of Maryland Energy Research Center (UMERC) USA
5	University degli study di Palermo
6	LLC "Carbon Technologies", Moscow
7	Institute of Mechanics National Academy of Sciences ,Republic of Armenia
8	Institute of Physical Research of the National Academy of Sciences of Armenia

9	Institute of General and Inorganic Chemistry named after Academician Manvelyan (National Academy of Sciences of Armenia)
10	National Polytechnic University of Armenia

# **Project implementation condition:**

- 1. Research of the latest achievements in the field of nano carbon materials. A comparative analysis has been made between the known and novel production method, oxygrafen and graphene.
- 2. The technological process of synthesis of nano carbon pipes from FR-Oxigraphen by a special method of pyrolysis of nano crystalline cellulose was developed. The regimes and catalysts for the synthesis of FR-oxigraphene, the method of low-temperature pyrolysis, and SHS synthesis have been determined
- 3. The laboratory synthesis of FR-oxigraphen samples was carried out.
- 4. The composition and structure and some properties of the synthesized substance FR-Oxigraphen, scanning electron microscopy and X-ray diffraction were studied.
- 5. The composition of the structure and the expected property and technologies for obtaining nano composites based on FR-Oxigraphen are modeled, in priority directions.

# **Program Phase I implementation of the project:**

## Development of synthesis technology and study of the properties of FR - Oxigrafen:

- 1. Research of the latest achievements in the field of nano carbon materials, determination of priority directions of their application, to make a comparative analysis of the methods of production and properties of carbon-containing materials of various modifications:
  - Fullerenes
  - Graphene
  - Nano diamonds
  - Nano tubes
  - Nano graphite
  - Nano porous carbon
- 2. Development of technology for obtaining FR- Oxigraphen by low-temperature catalytic pyrolysis of nano cellulose. Determining modes of synthesis, the type of catalysts, the new hardware design method for producing FR Oxigraphen .
- 3. Investigation of the properties of the material FR -Oxigraphen
  - Electronic properties
  - Magnetic properties

- Optical properties
- Mechanical properties
- Adsorption properties
- Theory and computer modeling of carbon nano structures
- Characteristics of carbon nano structures
- Application of carbon nano structures
- 4. Development of the technology for modifying FR- Oxigraphen , to give them the desired properties. Investigation of the properties of modified FR- Oxigraphen material.
- 5. Development of a technology for the preparation of composites based on FR- Oxigraphen
  - for graphene batteries.
  - for solar cells.
  - for new non-platinum catalytic systems and catalysts with a reduced content of precious metals.
  - for high-temperature polymer materials with an operating temperature of 400-450°C.
  - for radiation-resistant and radiation-absorbing ceramic materials.
  - for materials with low toxicity and high fungicidal and bactericidal activity as well as composites of biocompatible surgical materials.
  - for catalytic composite catalysts.
  - for magnetic membranes.
  - for electrically conductive compositions
  - for high-strength polymeric materials
- 6. Investigation of the material of composites based on FR-Oxigraphen
  - Electronic properties
  - Magnetic properties
  - Optical properties
  - Mechanical properties
  - Characteristics of carbon nanostructures
  - Application of carbon

7. To make planning, technological, organizational work for the pilot production of FR- Oxigraphen.

# **Program event**

Conducting research works in conjunction with foreign scientific organizations.