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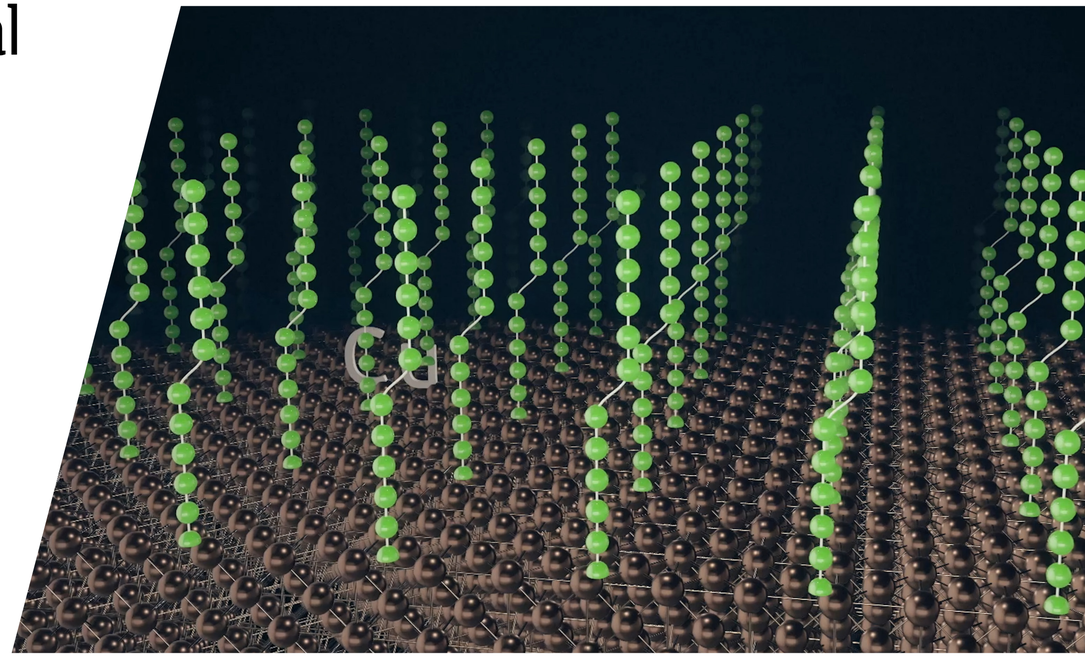
Development of fundamentals for new functional materials based on low-dimensional carbon modifications



The project is being implemented by the **StrAU** “Institute of Natural Sciences and Mathematics” within the framework of natural scientific aspects of development and study of new functional materials.

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Global task

Development of fundamentals and technologies for production of carbon nanomaterials with a given set of unique electronic and optical properties.

Key idea

Creating unique low-dimensional materials for the new branch of science and technology — the carbon nano-, micro- and optoelectronics.

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Research Supervisor of the project

Ernst Kurmaev

Scientific Advisor at the Institute of Metal Physics, Ural Division of the Russian Academy of Sciences, Professor, Doctor of Physics and Mathematics, State Prize winner, h-index: 30

Scientific activity: the world famous expert in the field of X-ray and photoelectron spectroscopy. He has extensive background in the study of low-dimensional carbon modifications, including graphene and graphene oxide, papers published in top international journals.

Role: determines the direction of the research in general, forms an ideology, and coordinates the work of the researchers and the project's partners. In addition, Dr. E. Kurmaev will lead the synchrotron research of the energy structure of low-dimensional carbon materials by means of X-ray emission, X-ray absorption and photoelectron spectroscopy.

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Director of the project

Vladimir Rychkov

Director of UrFU Institute of Physics and Technology

Doctor of Chemistry, Professor, Veteran of Nuclear Energy Industry

Scientific activity: Director of UrFU Institute of Physics and Technology with experience of managing large research programs.

"The development of industrial technology for associated extraction of rare earth metals and scandium from technological solutions at uranium mining by drillhole in-situ leaching with the purpose of increasing the efficiency of processing industrial products of uranium ores, and meeting the growing demand and import substitution for REM and scandium in radioelectronics, instrumentation, nuclear engineering, mechanical engineering, chemical industry, and metallurgy", 2014–2016, 360 m rubles.

Role: Coordinates the work of scientists and project partners, monitors the implementation of the key performance indicators, regulates the financial model of the project.

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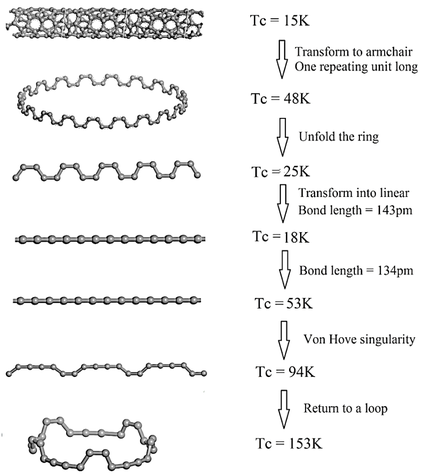
Scientific results before 2016



Ural Federal University created:

Interdepartmental laboratory of UrFU Institute of Physics and Technology "Advanced Carbon Materials" (headed by A. Zatsepin) and "Ural Center for Modern nanotechnologY" (headed by V. Shur).

Results obtained in the area of nano-carbon:

- Original mathematical models and algorithms – tools for predicting the unique properties of 2D and 1D carbon structures – have been created;
- New efficient methods for monitoring and identification of new nano-carbon metamaterials have been developed;
- Unique technologies for linear-chain carbon synthesis in the form of regular coatings have been tested, a number of unique properties investigated.
- The technologies were patented in the USA.
- A large series of scientific and technological research of low-dimensional carbon modifications has been performed. The results were published in leading journals: Nature Communications. Impact factor 11.470; Advanced Materials. Impact factor 15.409; Nature. Impact factor 38.138.

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Scientific results obtained by UrFU in the II half of 2016

Conferences:

- “European Material Research Society – Spring Meeting” 2016, Lille, France;
- International Conference “Diamond and Carbon Materials” 2016, Montpellier, France;
- “American Advanced Materials Congress” 2016, Miami, USA.

Awards:

- Medal of the American Congress (USA), "Advanced Materials — AAMC 2016"

Articles:

- Carbon, IF = 6.78. Simulation of chemical bond distributions and phase transformation in carbon chains .114 (2017) pp. 106-110;
- RSC Advances, IF = 3.84. Tuning the electronic structure of grapheme through nitrogen doping: experiment and theory. 6 (2016) 56721–56727;
- Nature Materials. IF = 38.8. A theoretical quest for high temperature superconductivity on the example of low-dimensional carbon structures, (2017);
- Nanoscale. IF = 7.76. Influence of dopants on the impermeability of grapheme, (2017);
- Carbon. IF = 6.78. 2D-ordered Kinked Carbyne Chains: DFT modeling and Raman characterization (2017);
- Carbon. IF = 6.78. Atomic and electronic structure of graphene oxide/Cu interface (2017);
- Advanced Materials Letters. IF = 1.46. Effect of symmetry on electronic DOS, Peierls transition and elastic modulus of carbon nanowires characterization, (2017).

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Scientific novelty

Studies of unique physical properties of new carbon nanomaterials constitutes one of the “hottest” topics of solid state physics, nanophysics and modern materials.

Analysis of the world's leading research groups’ activities and the dynamics of the publications in the field indicate that the direction of research corresponds to the global trend of development of transport research, spin-dependent quantum and wave phenomena in carbon nanomaterials.

One-dimensional carbon 1D-materials such as carbyne and LCC (an array of carbon chains with a hexagonal structure) have been predicted and experimentally proved to have outstanding characteristics: high strength (many times greater than that of diamond), low electron work function, excellent biocompatibility, etc., which generally provides the broadest possibilities of their use — from tiny micro devices, nanotechnology, optoelectronics, cold nanocathodes, to functional coatings, microsystem technology and special medical instruments.

Human resources and scientific expertise of the research team members in conjunction with the existing hardware and technological capabilities allow us to assume that all the tasks will be completed in full.

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Leading international partners

HKUST (Hong Kong) Top 100 THE, Top 200 ARWU
The program of high temperature superconductivity research of carbon structures (Prof. Dr. med. Rolf Lortz).

Kyoto University (Japan) Top 100 THE, Top 100 ARWU
Experimental investigations of the electronic structure of carbon nanoscale modifications using synchrotron radiation (Prof. Jun Kawai).

Hanyang University (South Korea) Top 200 QS
The mathematical modeling of the electronic structure of low-dimensional carbon materials (Prof. S. Kim, prof. D.V. Boukhvalov).

Universities of Palermo and Catania (Italy) Top 500 QS
Work on the study of photophysical processes in carbon materials and composites with quantum dots (Prof. Marco Cannas, prof. Luisa D'Urso).

Saskatchewan University (Canada) Top 500 THE
A study of carbon materials by inelastic scattering of x-rays at the synchrotron, Berkeley, US, and Canadian synchrotron source (Prof. Alex Moewes).

Zhejiang University (China) Top 500 THE
Development of intelligent ferromagnetic and piezoelectric systems based on graphene.

The research also involved the US universities (Clemson), Germany (Berlin, Rostock), Bulgaria (Sofia), Poland (Warsaw), and others.

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Academic partners

JINR Laboratory of Nuclear Reactions, Dubna
Synthesis and studies of radiation resistance of low-dimensional carbon modification (Prof. S.N. Dmitriev)

IPTM RAS, Chernogolovka
Element base for microsystem technology, including nanoelectronics and nano-optics, synthesis and analysis of new materials (Prof. Vyatkin A.F.)

Nizhny Novgorod State University
Design, prototyping and research of functional nanoelements, optoelectronics. (Prof. D.I. Tetelbaum)

Institute of Electrophysics UD RAS
Ion beam synthesis and modification of the properties of materials, the study of high-speed electronic processes. (Prof. Gavrilov N.V.)

Institute of Metal Physics, Ural Division of Russian Academy of Sciences
Production of metal-diamond nanoheterostructures for microwave applications, integrated research structure-energy states of objects. (Prof. Rinkevich A.B.)

Moscow State University, Faculty of Physics
Priority knowledge and expert analysis in the field of synthesis and properties of linear-chained carbon. (Prof. M.B. Guseva)

Research Institute for Technical Physics and Automation
Creating special objects for a new generation of radiation equipment. (Director S. Koloskov)

Chuvash State University
Linear-chain carbon coating technology for metal, semiconductor and dielectric substrates. (Prof. Kochakov V.D.)

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Practical significance

Creation of fundamental basis for a new branch of science and technology — the carbon nano-, micro- and optoelectronics.

Emphasis will be given to on one-dimensional carbon, development of methods for the synthesis of long linear carbon chains with a variable number of atoms, the study of their properties.

Development of fundamentals and creation of element base for a new branch of science and technology will radically change the approach to production of devices in virtually any field of human activity.

Применение наноуглерода

Elactronics

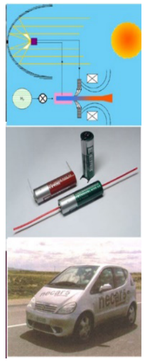
Flat screens

Light sources

X-ray tubes

Night vision devices

Energy

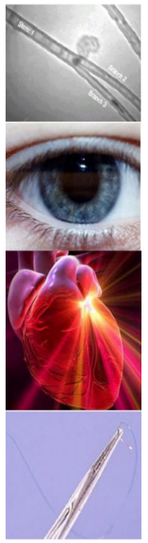


Thermoelectric power converters

Li current sources

Hydrogen engines

Medicine



Functional coatings

Industrial partners/consumers

Presently several companies are ready for joint implementation of the results of low-dimensional carbon research:

- "Carbon Technologies" (Moscow) — a wide range of applications of LCC;
- NGO "Geophysics-NV", NGO "Automation“, "RTI Systems" concern, "Samsung" — electronic components and microsystems technology;
- "Haldor Topsoe" Russia (Moscow) — catalysts and adsorbents with a specific surface area increased by several times;
- "Rosatom" Corp. — thermoelectric converters, molecular nuclear membrane, nuclear energy and superior batteries;
- Scientific Center for Cardiovascular Surgery — biocompatible implants and suture materials;
- Center for Advanced Studies (Moscow) — the latest items of special equipment;
- Military-industrial Complex of the Russian Federation — micro- and opto-electronic components for special purpose systems/

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Cofinancing sources

Project income	2017	2018	2019	2020	2021	TOTAL
Partners co-financing (m rubles)	25	100	50	50	25	250
University co-financing (m rubles)	0	10	20	10	10	50
Subsidy funds (m rubles)	100	200	150	50	0	500
Total:	125	310	220	110	35	800

LLC «Carbon technologies», Moscow: Transfer of equipment and intellectual property
UrFU (state assignment), grants from RFBR, RSCF
At the final stage – consumers of new materials and devices

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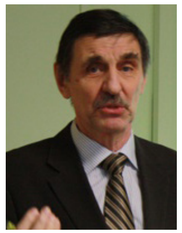
Leading project participants









V. N. Rychkov, UrFU
M. B. Guseva, MSU
V. Ya. Shur, UrFU
E. Z. Kurmaev, IMP UB RAS
A. F. Zatsepin, UrFU
A. Moewes, Canada
R. Lortz, Hong Kong
S. N. Dmitriev, JINR
A. L. Kholkin, UrFU