SERIES
"SOURCES OF NEW INDUSTRIES"

ISSUE 1

Advanced Chemistry

SAINT PETERSBURG

2022

SOURCES OF NEW INDUSTRIES. ISSUE 1. ADVANCED CHEMISTRY

Expert report

Authors: V. N. Knyaginin, M. S. Lipetskaya, D. V. Sanatov, L. V. Sklyar,
A. V. Oleinik, M. O. Makov, M. S. Mulyukin, S. V. Salkutsan, E. M. Kholodnova
Scientific editor: E. V. Skorb
Interviewees: M. E. Trusova, P. S. Postnikov, K. G. Nikolaev, A. V. Vinogradov
Foresight participants, interviewees: D. S. Bolotin, E. A. Mostovich, A. S. Drozdov
Preparation of foresight results, analytics: A. A. Davydova, E. A. Mazilov

This report was prepared jointly by the Center for Strategic Research "North-West" and the Innovations and Youth Initiatives Support Fund of St. Petersburg with the support of the Government of St. Petersburg.

The report was based on the Foresight project "Frontiers in New Sciences". The aim of the project was to identify longterm trends and prospects for the development of new industrial and technological markets; to identify the most promising areas of research and development in the so-called "frontier" areas of R&D — advanced chemistry, synthetic biology, artificial intelligence and environmentally friendly industrial technologies.

The methodological basis of the project is based on the analysis of the results of the foresight session with the participation of leading and young scientists, the processing of scientific data, a series of interviews with researchers, the evaluation of strategies of large industrial concerns, the analysis of venture capital markets.

The report consists of eight sections, which consider:
— transition from a linear classical R&D model to a model of autonomous chemical research with reverse design;
— transformation of the laboratory into the AI-Driven Lab format and the emergence of a new type of researcher — chemist-administrator;
— frontier areas of chemistry that open up completely new technological markets of the future.

The report describes the main factors of the development of advanced chemical technologies:
— the change of technological tools provides faster, cheaper, safer and more efficient innovations in chemical science;
— laboratories where artificial intelligence is gradually becoming the subject of the research process have the greatest potential;
— integration of cross-industrial players into chemical market platforms to address the challenges of modern science.

The results of the project formed the basis of the experimental BlueSkyResearch competition "Artificial Intelligence in Science", held in 2022 jointly by "Center for Strategic Research "North-West" Foundation and the Innovations and Youth Initiatives Support Fund of St. Petersburg.

Series "Sources of new industries"

Report design by M. I. Petrova , commissioned by the Innovations and Youth Initiatives Support Fund of St. Petersburg

ISBN 978-5-9909736-5-7
Saint Petersburg 2022

The authors of the report express their special gratitude to to the Ministry of Science and Higher Education of the Russian Federation for supporting the foresight project "Frontiers in the New Sciences".

Table of contents

List of Figures, Tables and Cases

Introduction

The emergence of Industry 4.0 technologies in the past decade has changed industry markets forever. To ensure competitiveness, companies started gradual and, in some cases, total digitalal transformation (primarily of processes related to sales support), as well as the implementation of technologies to improve production efficiency.

In the next stage of digital transformation, which ensures economic growth, the research and development sector is being transformed. Digital technology has fundamentally changed the way research and development (R&D) is conducted. In the last 20 years, two Nobel Prizes have been awarded for research in computational chemistry, and the potential of this field is far from being exhausted [1,2]. The chemical industry has moved to new principles of engineering molecules and compounds, making research faster, more accurate, and more efficient. Moreover, there has been a shift in the perception of artificial intelligence, which has progressed from a partial introduction into research as a tool with a narrow set of functions to a full-fledged subject of scientific activity. The change in the nature of R&D allows us to talk about new chemistry - scientific knowledge, based on big data, formed with the use of digital tools of experimentation and modelling.

The introduction of artificial intelligence technologies into the research process prepares the ground for Industry 5.0, a new industrial concept based on the principles of cyber-physical cognitive systems, continuous personalization, distributed value chains, and characterized by human-centricity, flexibility and sustainability[3].

The development and diffusion of new chemistry is creating not only individual breakthrough technologies for a better quality of life, but also entire markets for green technology, electrical energy, medicine and nutrition, and new materials. Given the cross-industry nature of chemistry (all high-tech industries are based on chemical processes and materials), investment in the key actors of new chemistry - research laboratories - will help to make scientific, technological and commercial breakthroughs in several directions at once.

The advanced experience of using digital approaches in research tools can become a driver for the realization of Russia's high scientific potential in the field of chemistry. Artificial intelligence and machine learning technologies combined with a strong scientific base are a factor in the qualitative development of the chemical industry. In addition, the chemical industry is one of the industries that has been tasked with import substitution due to the economic sanctions imposed in 2014. The first action plan was adopted in 2015 and was subsequently adjusted several times. In general, the policy of import substitution in chemistry, according to experts, has become one of the most successful and can be continued to solve new ambitious tasks. The issue of supplying low- and medium-tonnage chemistry products remains particularly acute. Taking into account the trend for digitalization and green technologies, it is the advanced chemistry that can provide the development of new technologies in the conditions of import substitution development.

The Government of St. Petersburg initiated the project "Frontiers in the New Sciences" in order to determine the prospects of development of new fields of science, including the direction of "New Chemistry". The foresight "Frontiers in the New Sciences" was conducted jointly by Foundation for Support of Innovation and Youth Initiatives of St. Petersburg and the Center for Strategic Research "North-West" with the support of the Ministry of Education and Science of the Russian Federation in November 2021. For each of the topics considered, ideas for breakthrough research were formulated, trends in the development of the direction and the necessary competencies for future work were identified.

1 Noble Prize. URL: nobelprize.org/prizes/chemistry/1998/summary/ (date of reference: 14.02.2022).

2 Noble Prize. URL: nobelprize.org/prizes/chemistry/2013/summary (date of reference: 14.02.2022).

3 Industry 5.0, a transformative vision for Europe // European Comission. URL: op.europa.eu/en/web/eu-law-and-publications/publication-detail/-/publication/38a2fa08-728e-11ec-9136-01aa75ed71a1 (date of reference: 14.02.2022).

The outcome of the foresight session (with an additional foresight study, including interviews with scientists) was the report "Advanced chemistry", dedicated to the long-term aspects of research development in the field of chemistry.

Chapter one of the report describes the features of the transformation of the chemical R&D process as a result of the total implementation of digital technologies.

Chapter two presents key digital tools for conducting research.

Chapter three describes the transformation of laboratories, which are the source of chemical innovation, and defines the infrastructure model of the future AI-driven Lab.

Chapter four focuses on current and future changes in the competency profile of the researcher. Bridging the gaps between the quality supply and demand for new chemistry competencies can contribute to the development of the chemical industry.

Chapter five introduces current chemical research topics in which the greatest scientific breakthroughs are expected.

Chapter six gives an overview of the chemical R&D market and identifies key trends in its development.

Chapter seven looks at new technology markets that are becoming available through industry innovation.

Hapter eight outlines the prospects for cooperation and government support in the field of new chemistry.

The report is intended to help chemical companies to determine the focus of technological development and the trajectory of innovative growth. Existing laboratories of educational, scientific and production organizations will be interested in promising requirements for infrastructure and research competencies. Authorities and management bodies can use the report materials to select promising areas for support of research topics and R&D infrastructure.

1 TRANSFORMATION OF CHEMICAL R&D

Research in chemistry is undergoing radical transformation. Real laboratory experiments are replaced by autonomous robotic processes and virtual simulations. Construction of hypothesis for finding solutionsis acquires new character with artificial intelligence (hereafter, AI), which is capable of designing molecules and selecting synthesis methods independently, drawing information from databases.

At present, not only the model of scientific knowledge development in general, but also the system of research methods and the nature of research activity organization is changing. The following factors may influence the transformation.

1

The increase in the complexity of scientific knowledge, caused by the increase in the volume and speed of scientific data, as well as the subtleties of the topology of research. This leads to a decrease in the number of significant discoveries and radical innovations (Figure 1). The challenge of the increasing complexity of scientific discovery can be overcome by the spread of advanced digital tools due to the digitalization of science, the growth of computing power, the decreasing cost of high-performance computing, the development of algorithms and methods for AI problem solving, and machine learning.

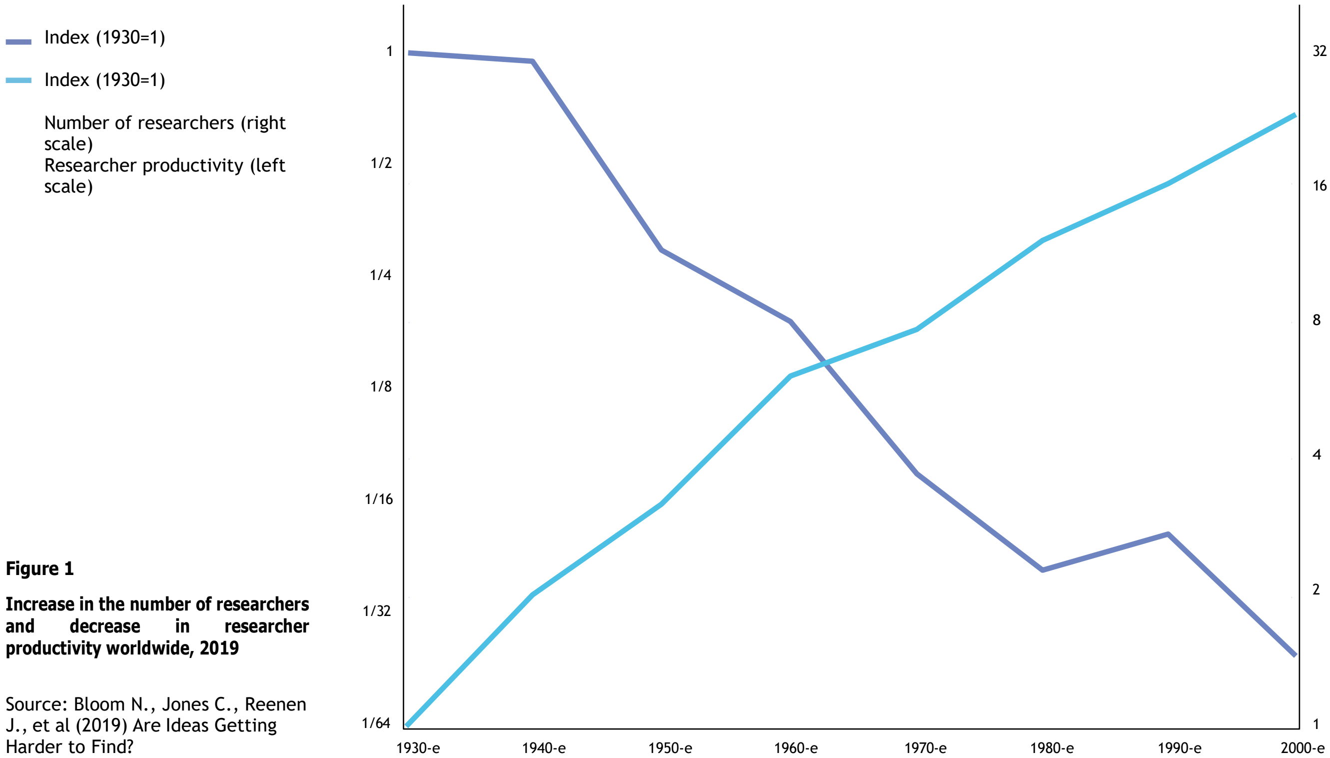


Figure 1

Increase in the number of researchers and decrease in researcher productivity worldwide, 2019

Source: Bloom N., Jones C., Reenen J., et al (2019) Are Ideas Getting Harder to Find?

Technological power has accelerated the transition to polyparadigmacy. The fields of scientific knowledge that were able to use AI for their own reorganization have changed radically. This especially applies to chemistry, biology, sociology, medical sciences, climatology, some engineering sciences.

2 **New stage of the scientific-rechnological revolution.** The scientific revolution of the 1970's-1980's was caused by the active introduction of computer technology, genetic engineering, simulated materials, the development of new ways of energy conversion, which led to the emergence of advanced production technologies. The modern economic paradigm (2010-2020) - Industry 4.0 - continues to be largely shaped by the influence of the field of deep tech. Consistent movement in this direction could lead to the next technological revolution at the turn of the 2020s and 2030s, which will open up ways to solve global challenges using nature-like technologies, super- and AI metamaterials in the context of a post-carbon economy and total robotization.

3 **New global challenges.** The transformation of chemistry research is taking place in the context of approaching "wicked "[4] and "super wicked "[5] problems, which include such global challenges as pandemic new infections, increasing bacterial resistance to common antibiotics, the negative effects of climate change, and the depletion of available resources.

4 **Knowledge cycle compression.** The modern scientific revolution is accompanied by a reduction in the time to move from a scientific hypothesis to a useful product from the traditional 15-20+ years to 5-8 years, and in some cases 3-6 years.

5 **Transition to research ecosystems.** The speed of advancement in R&D largely depends on the ecosystem in which the leadership team works, the package of services and tools available to it, the proximity of professional communities, allied partners, and suppliers. R&D development is determined by network effects (Metcalfe's law: a network's value is proportional to the square of the number of nodes) in the network and the Matthew effect: the core grows faster than the periphery. The core is always able to get more out of the cooperation and to spread the resources in its favor. Only the core can cope with the growing complexity of R&D.

4 Churchman C. West Wicked Problems // Management Science. — 1967. — № 14 (4). — С. 141-142.

5 Levin K., Cashore B., Bernstein S. et al. Overcoming the tragedy of super wicked problems: constraining our future selves to ameliorate global climate change // Policy Sci. — 2012. — № 45. — С. 123-152.

The above factors have influenced the transformation of research activities in chemistry. The middle of the last century was one of the most fruitful periods for chemical innovation, but then the rate of creation of new molecules and materials slowed down. With the exception of innovative plant protection chemicals, the chemical industry has not developed any disruptor products in the last decade[6]. However, the introduction of digital technologies is radically changing the architecture of research and increasing its efficiency, which could lead to new breakthrough discoveries in the future.

Previously, the R&D process was a consistent chain of actions, from setting a goal to obtaining a result (not always positive). To test hypotheses, real experiments with reagents were conducted, and by "trial and error" method a researcher could conclude that the hypothesis was untenable, correct it, and repeat the experiments (Figure 2). With the introduction of digital research tools, the intermediate stage of hypothesis testing is reduced due to modeling or partial automation of the process, as well as already accumulated databases of chemical data. The process differs from the research of the previous stage digital R&D environment and access to a virtually unlimited amount of known data.

6 Innovation in chemicals // Deloitte. URL: www2.deloitte.com/us/en/insights/industry/oil-and-gas/chemical-innovation.html (date of reference: 11.02.2022).

In the next step in the transformation of chemical research, a reverse design paradigm will become available, where artificial intelligence can not only process a researcher's request for the necessary characteristics of a molecule, material or substance, but also shape their design and synthesis method based on big data. There is a transition to a model of autonomous chemical research with inverse design.

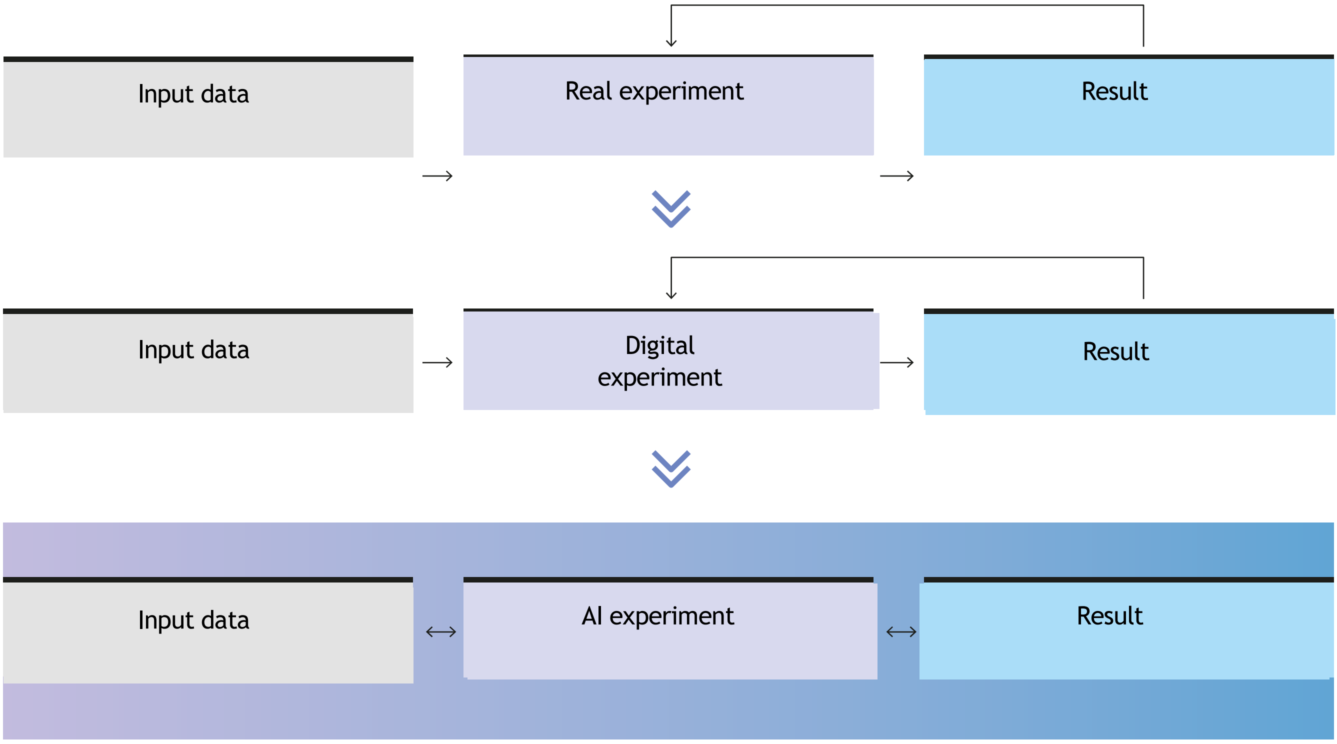


Figure 2.
Transformation of the Principles of Chemical Research
Source: Foundation "Center for Strategic Research "Northwest"

The transition to an autonomous chemical research model implies a transformation of the role of artificial intelligence - from a research tool (as a machine learning algorithm for analyzing big data) to a research subject.

Thanks to its computational capabilities, AI is able to select the most energy- and resource-efficient reactions, such as cascade reactions, which are arranged according to the domino principle: instead of conducting a series of reactions in stages, one can obtain the desired result by adding reagents once and running the reaction, whose first derivatives will become the basis for the next stage, and so on down the chain[7].

With the use of digital tools, the focus in the chemical industry has shifted from research at the molecular level to materials, functions, and complex systems. High-performance computing, artificial intelligence, and other capabilities allow us to work with more complex problems and systems (including updatable ones in which we have to deal with large amounts of data, their diversity, and the speed of connections between multiple variables). New tools make it possible to study structure at the nanoscale, to determine the organization of the genome or the structure of a molecule, and to trigger complex reaction cascades, which should provide breakthrough results in completely new and, moreover, unexpected areas.

7 Nowak G., Fic G. Machine Learning Approach to Discovering Cascade Reaction Patterns. Application to Reaction Pathways Prediction // Journal of Chemical Information and Modeling. — 2009. — № 49 (6). — C. 1321-1329.

Whereas earlier R&D stages could be disconnected from each other in time and space, the digital environment makes the passage of research stages virtually seamless, increasing their connectivity and thereby accelerating their execution.

The shift to digital technologies in R&D in the global chemical sector is largely supported by global trends.

1 Sustainability

Sustainability, like digitalization, is a megatrend of modern development. In the early 1990s, even before the formation of the UN Sustainable Development Goals, the concept of preventing the generation of hazardous waste at the stage of technology development instead of solving future disposal problems was formulated. In 1998, 12 principles of green chemistry were developed, which later became the basis for the idea of the essence of sustainable chemistry.

The adoption of the Green Deal by the European Union was followed by the approval of the EU Chemicals Strategy for Sustainable Development. The Strategy fully recognizes the key role of chemicals for the transition of the European economy and society to green and digital technologies.

Chemical products have a detrimental impact on the environment, especially petrochemicals, fertilizers and pesticides. The application of digital technologies will make it possible to move towards a green chemistry that reduces or eliminates the use and formation of hazardous substances (this is the basis of the concept of Industry 5.0 [8]).

8.Industry 5.0 // European Commission. URL: ec.europa.eu/info/research-and-innovation/research-area/industrial-research-and-innovation/industry-50_en (date of reference: 11.02.2022).

2 Prohibition of animal testing

41 countries around the world have passed laws restricting or completely banning animal testing of products[9]. Computer simulations can replace such experiments with a more humane approach.

9.These Countries Have Banned Animal Testing (2021) // Cruelty Free Soul. URL: crueltyfreesoul.com/animal-testing-banned-countries/ (date of reference: 11.02.2022).

3 Increased cost of research

In the pharmaceutical sector, increased requirements for research conditions lead to higher R&D costs. For example, the average cost of developing a new drug can be as high as $2.51 billion. (Figure 3).

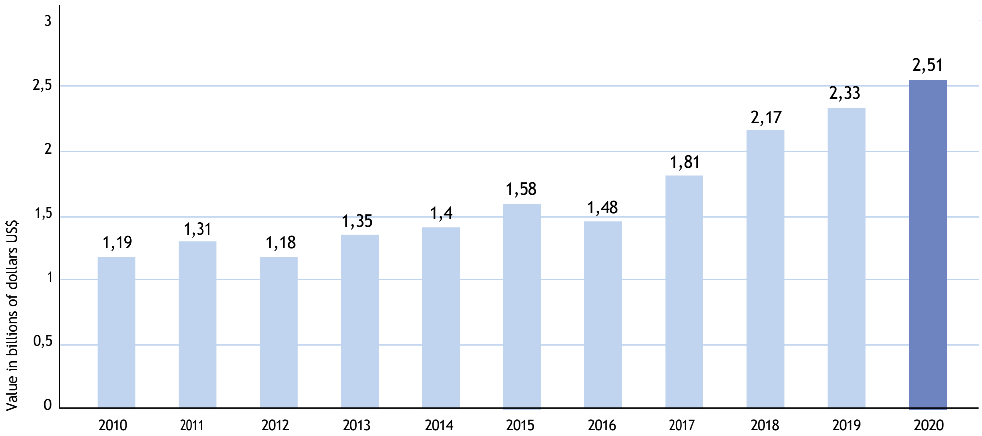


Figure 3.
Average cost of R&D for a new drug by the world's 12 largest pharmaceutical companies, 2010-2020
Source: Statista

4 Increased competition from technology companies

Another driver of the transition to digital chemical R&D is the diversification of the business of technology companies, which are starting to work not only in related sectors, but also in completely new areas (Figure 4).

In the original business sectors
In new business sectors

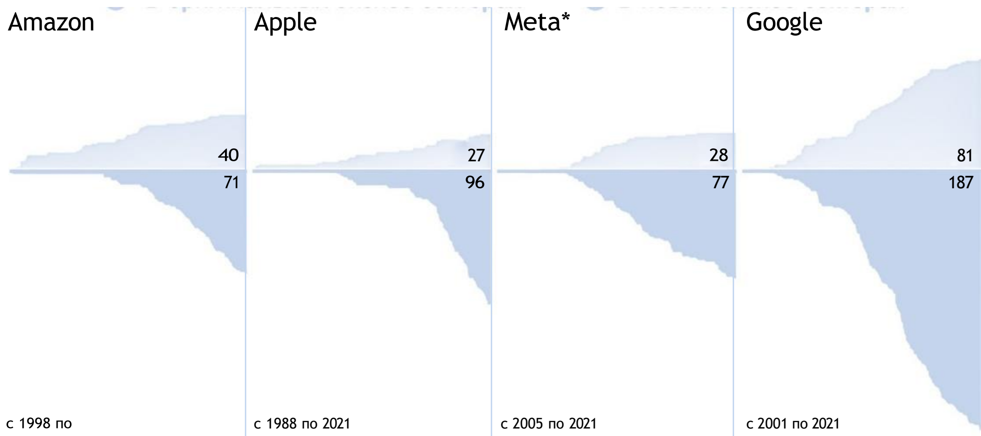


Figure 4.
Number of takeovers of major technology companies, units, from the date of the first takeover by a company to 2021
Source: Washington Post

* the organization is recognized as extremist in the Russian Federation

These trends only accelerate the transition of players in the chemical market to conduct research and development in a virtual format and intensify the use of digital tools and artificial intelligence.

2 DIGITAL TOOLS FOR CHEMICAL R&D

Digital technologies increase the efficiency of chemical R&D and are already being implemented in Russian laboratories. The integration of automation elements, computer modeling and other hardware solutions into a single system thanks to artificial intelligence leads to the formation of cyber-physical cognitive systems.

The level of use of digital tools in chemical R&D distinguishes Industry 3.0 from Industry 4.0 and the nascent Industry 5.0. If, in the realities of Industry 3.0, chemical R&D was characterized by human work using "analog" tools, 4.0 research is provided by cyber-physical systems - using digital tools. As digital technology develops and artificial intelligence penetrates into research tasks, there is a transition to cyber-physical cognitive systems - Industry 5.0.

The use of digital technology in chemical research and development provides:
- faster, cheaper, safer and more efficient innovation;
- more effective diagnosis, prevention and treatment of diseases;
- new sustainable technologies - from better batteries and solar cells to next generation plastics and resource-saving industrial processes;
- better environmental management and regulation, based on high quality data and big data analysis;
- breakthroughs and new knowledge in the physical, natural and digital sciences.

Automation

Improvement of instrumentation, robotization and technologization of the research process make it possible to:
- reduce the time and labor costs of research, primarily routine operations;
- increase researchers' productivity;
- increase research accuracy by eliminating the "human factor";
- simplify the reproducibility of chemical experiments;
- increase the safety of technological processes, including due to the autonomy of operations.

Automated systems are designed to perform simple steps of synthesis. The transition to the next stage of development of automation of chemical research in the field of synthesis should solve the problem of providing the connected automation between different stages of synthesis, automation of more complex stages and synthesis of complex molecules.

Dmitry Bolotin, Doctor of Chemistry, Associate Professor, Department of Physical Organic Chemistry, Institute of Chemistry, SPbSU:

> *«The equipment of modern laboratories makes it possible to carry out reactions hundreds of times faster. If earlier ten people were working sumultineously on obtaining forty compounds, now one person can do it: to load substances into a special apparatus and obtain up to a hundred compounds»*[10]

10 From an interview with D. S. Bolotin (01.12.2021).

Computer simulations and experiments

Precision simulation of operations is accomplished through high-performance mathematical computations, which make it possible:
- predict the parameters (i.e., structure and properties) of synthesized materials;
- conduct large-scale tests under safe conditions;
- shorter research periods, avoiding lengthy laboratory tests.

Ekaterina Skorb, Candidate of Chemical Sciences, Director and Leading Professor of the Scientific and Educational Center of Infochemistry, ITMO University:

> *«No one invests today to synthesize millions of structures. Initially you model the properties of these structures and only then you start synthesizing, which makes the technology and everything else cheaper. For crystalline substances, Artyom Oganov's Uspex program is very popular - it is good at predicting many properties. The new AlphaFold program makes it possible to avoid having to grow large proteins. We are currently testing it.»* [11]

11 From an interview with E.V.Skorb (17.10.2021).

Advanced measurement techniques

Advanced measurement techniques (various types of spectroscopy, spectrometry and microscopy, distributed sensor networks, etc.) provide new insights into the structure, properties and interactions of systems at the atomic and molecular levels, to study materials and surfaces, organisms and ecosystems. Such methods include:

— smart microscopy based on the integration of light and electron microscopy with automation and machine learning;
— a combination of several research methods (e.g., studying protein structure and function through x-ray diffraction, cryogenic electron microscopy, and mass spectrometry);
— distributed network of sensors;
— real-time measurement of parameters.

Andrey Drozdov,
Cand.Sc. Chemistry, Senior Researcher at the Laboratory of Nanobiotechnology, MIPT:

> *«Just 10 years ago we did not have access to many research methods. Skolkovo has an electron transmission microscope with tomography and elemental analysis capabilities. It can show the location of atoms in space. This device is the only one in Russia, and there aren't very many of them in the world.»* [12]

12 From an interview with A.S.Drozdov (30.10.2021).

Imaging and visualization

By harnessing the power of automation, statistics, and machine learning, it is possible to improve work with imaging and visualization tools, among them:
- image analysis (extracting data from images with high accuracy, processing and identifying them);
- medical diagnostics (interpretation of image data for making medical decisions);
- presentation of research data in an accessible form.

Artificial Intelligence and Machine Learning

Researchers use artificial intelligence and machine learning in conjunction with other digital technologies. As an end-to-end technology, AI opens up a whole new perspective for researchers. It allows:
- finding the best solution with minimal human involvement (artificial intelligence analyzes a large volume of data, identifies promising properties and patterns, and eliminates less promising areas);
- improving imaging and diagnostics;
- filtering a large amount of data;
- mining of chemical data (automatic analysis of scientific literature to identify physical and chemical patterns);
- automation of routine laboratory work (use of machine learning methods to accelerate the workflow, optimization of chemical synthesis);
- optimization of measurement systems, predictive and prescriptive analytics, multi-parameter signal analysis;
- more accurate prediction of properties, especially when quantum chemistry and artificial intelligence technologies are used together.

The introduction of artificial intelligence technologies is expected to have the greatest effect on R&D and discoveries. For example, four new materials have already been discovered, including a family of solid-state materials that conduct lithium, thanks to the AI algorithm developed at the University of Liverpool. Solid electrolytes stimulate the development of solid-state batteries that improve the life and safety of electric vehicles [13,14].

13 Vasylenko A., Gamon J., Duff B. B. Element selection for crystalline inorganic solid discovery guided by unsupervised machine learning of experimentally explored chemistry // Nature Communications. — 2021. — № 12.

14 New AI tool developed by University of Liverpool researchers accelerates discovery of truly new materials // Eurek Alert. URL: eurekalert.org/news-releases/929009 (date of reference: 11.02.2022).

Evgeny Mostovich, Candidate of Chemical Sciences, Head of the Laboratory of Low-Carbon Chemical Technologies at FNS NSU:

«There is, for example, a big challenge, Total synthesis, when you synthesize natural compounds not in nature, but in the laboratory. It is very close to art, where you select the optimal synthetic sequence - from the most basic compounds to the big structure. Artificial intelligence is most likely to make a big breakthrough in chemistry, if it can synthesize natural compounds on its own and make optimal synthesis schemes» [15]

15 From an interview with E A. Mostovich (03.12.2021).

Hardware Solutions

The development of computer equipment not only speeds up the research process, but also makes it possible to solve more complicated tasks. There are high hopes associated with the development of computer computing power.
First of all, these are:
- peripheral computing of distributed infra-structures;
- streaming computing for continuous processing of large data sets and real-time analytics (in microscopy streaming computing can be used to overcome problems of transmission, storage and processing of large volumes of data);
- quantum computing;
- specialized processors (optimized for specific tasks).

Dmitry Bolotin, Doctor of Chemistry, Associate Professor, Department of Physical Organic Chemistry, Institute of Chemistry, SPbSU:

> *«If we have a computer one billion times faster, we can count a thousand times more atoms in the same time. The more productive computers are, the larger are the systems the computers can calculate in the same amount of time, or the more accurate calculations we can do with the same number of atoms»*[16]

16 From the interview with D. S. Bolotin (01.12.2021).

The prospects for the application of digital technologies in chemical R&D depend on how well existing barriers can be overcome, among which we should mention:
- computational capacity limitations (experts primarily associate overcoming this challenge with the development of quantum technologies);
- the accuracy of digital experiments, i.e., the correspondence of the results in simulations to the results of real experiments;
- the low quality of the data sets, as there is currently a disconnection between data holders (real sector organizations and researchers) and a lack of data standardization (increasing complexity of access and decreasing transparency);
- the need for additional digital competencies of chemical researchers, the need for digital experts (machine learning specialists, AI developers, etc.).

The solution of these problems will make it possible to move digital chemistry tools from the category of "not for everyone" to the category of basic technologies.

3 THE TRANSFORMATION OF CHEMICAL LABORATORIES

Chemical laboratories are undergoing a transformation from automation and the introduction of research software to the use of artificial intelligence as a subject of research activities. Russia has some examples of modern laboratories of international level, but the country's potential in the infrastructure of advanced chemistry has not yet been realized enough.

The chemical industry is highly science-intensive. Companies are turning to advanced technologies to accelerate the creation of new products with higher added value and, as a result, to increase profits and take additional market share. The most dynamic sectors rely heavily on the research and development process, because successful research can lead to new products and improve existing products. Consequently, the design of laboratories as a key actor in R&D is of paramount importance.

Research laboratories are currently undergoing a transition from the physical model to a fully virtual form. The former model - lab 3.0 - used internal resources and classical research methods without reliance on digital solutions. The lab of the future, or 5.0, is a digital platform driven by artificial intelligence - **an AI-driven lab model** where AI becomes the subject of research. Modern lab 4.0 refers to a hybrid version - as a transition from the infrastructure elements of the previous stage of development to the 5.0 version. The above-mentioned elements include *personnel skills, methods of idea generation and hypothesis building, data search methods, equipment provision, cooperation with other R&D subject*s (Figure 5). When all the described mechanisms are integrated, laboratories controlled by artificial intelligence will emerge.

In the previous stage, researchers had to turn to articles, books, and reference books in printed media as the only source of data. The first phase of the digital transition allowed many materials to be converted into electronic form, and in the following years more and more databases, including scientific publications, began to emerge. Nevertheless, today such datasets (datasets) are still fragmented and unstructured "islands" of data. Further processing and the creation of a single data lake will simplify the process of retrieving the necessary information and thus accelerate the pace of research.

With the development of science and manufacturing, society came to an open innovation model. This approach allowed researchers to draw ideas from a common intellectual space. The next stage should lead to the fact that the chemical laboratory, having collected the necessary datasets, will send them to an artificial intelligence, capable of generating its own hypotheses within the framework of the outlined task. Moreover, it seems promising to create "AI factories" that can draw the necessary information from the data lake in accordance with the outlined objectives, and then, after conducting a cycle of construction and hypothesis testing, will autonomously create new products.

The "AI factories" scenario raises the question of the role of scientists in a state-of-the-art laboratory system. Most likely, it is impossible to completely exclude humans from the R&D process. A symbiosis of a chemical scientist, who defines the rules and goals of research, and an algorithm could be a breakthrough

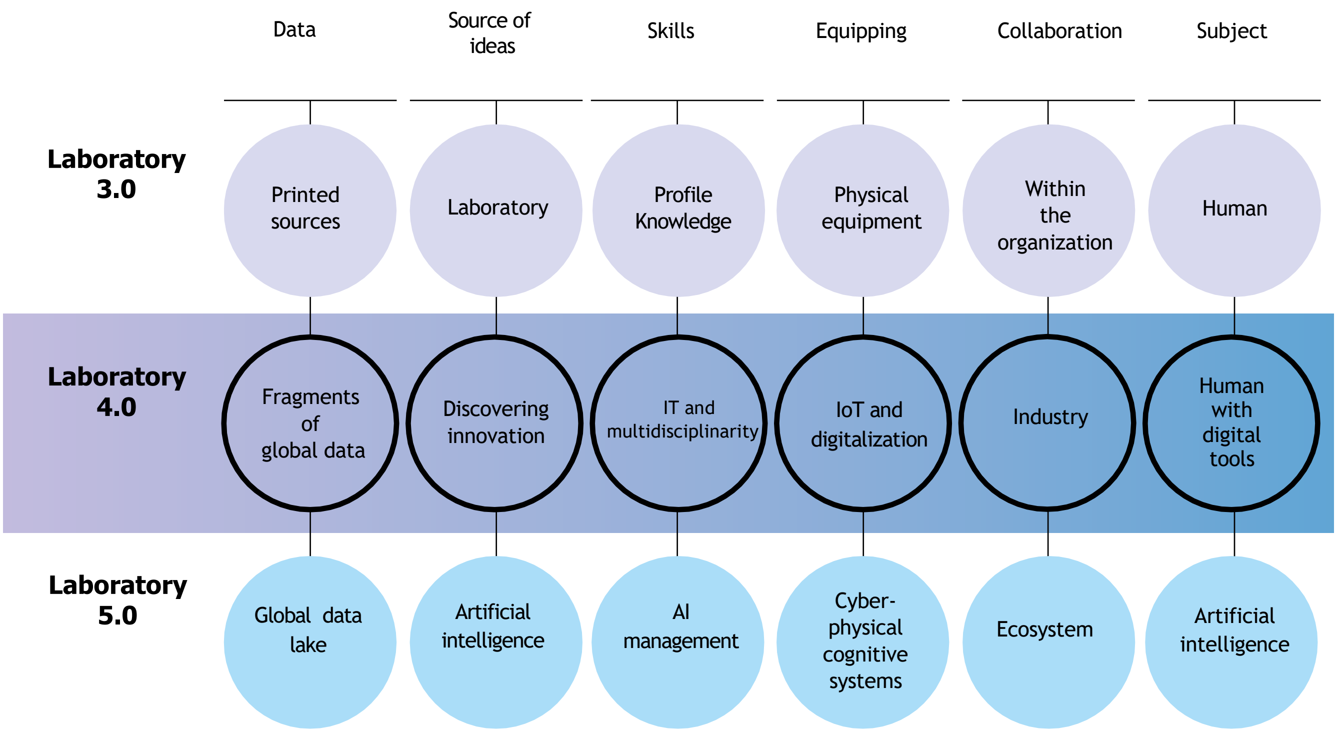


Figure 5.
Elements of the chemical laboratory of the future
Source: Foundation "Center for Strategic Research "Northwest"

capable of performing operations in a short period of time. We can already see that the boundaries of traditional requirements, which prioritized knowledge in a particular field, are shifted, and digital skills are given more and more prominence. And the emergence of affordable quantum computing technologies will only reinforce this trend.

Computer modeling technologies existed before, but because of their rapid improvement, along with the growing availability of computing equipment and multipurpose algorithms, there will be no need to turn to classical laboratory equipment at many stages of research. This approach will overcome some of the barriers to R&D. The time it takes to conduct research is only one of these barriers The cost of reagents and the long waiting time to obtain them is a significant barrier to research activities in chemistry. Today, elements of simulation are partially implemented in the first stages of research, but full-cycle simulation similar to the in silico approach will open new horizons for the chemistry industry.

In chemistry of the previous stage, R&D could be carried out by laboratories of individual institutes or organizations in a closed format. The growing complexity of the chemical industry leaves no room for isolation from the global scientific and industrial community. Industry 4.0 players are joining industry unions for individual projects. Further increasing complexity will require closer cooperation, and the benefits of working together within the ecosystem (e.g., in the form of consortia) may outweigh organizations' desire to keep their research solely for their own use.

Advanded laboratories are already integrating some elements of the latest approaches into their research activities, approaching the lab 5.0 model, although even the most technologically advanced ones are in a transitional phase where the application of AI is intermittent.

Global experience demonstrates a smooth evolutionary transition from classical laboratories to the 5.0 model.

Case 1. Examples of leading chemical laboratories abroad

Pande Group, Stanford University, USA

A group of scientists specializing in the application of artificial intelligence and machine learning to chemical research is led by Vijay Pande, professor of structural biology and computer science[17]. Advanced digital approaches are used to solve scientifically challenging problems in chemical biology, biophysics, and biomedicine [18].

Scientists publish unique algorithms to make them available for other researchers to use[19]. Dr. Pande was able to successfully launch Genesis Therapeutics, a drug discovery startup, with $52 million in private funding and a partnership with Genetech, a major biotech company, thanks to the algorithm he created[20].

Hong Kong Quantum AI Laboratory, University of Hong Kong

The lab has brought together data chemists and computational scientists in a research group to develop an R&D platform based on machine learning and big data. The ultimate goal of the lab is to discover next-generation materials and develop new devices. This symbiosis is unique and is one of the first examples for the industry. The developed platform is designed specifically for research in OLEDs and solid-state lithium-ion batteries. This makes it possible to accurately predict the properties of materials used for lithium-ion batteries and OLED displays, and the research results can easily be used to develop solar cells, fuel cells and related catalysts. The uniqueness of the approach has led to the involvement of the California Institute of Technology and such major industrial partners as Samsung [21].

Computer Science and Artificial Intelligence Laboratory, Massachusetts Institute of Technology, USA

A group of MIT scientists is adapting AI and machine learning technologies for chemical research. Researchers found some applications of artificial intelligence for drug discovery [22], and technological solutions using AI to automate a chemistry laboratory [23]. This led to creation of an autonomous system for conducting experiments that has creative potential: it is capable not just of repeating a predetermined set of actions, but of synthesizing molecules that did not exist before. Scientists hope that further advancement in this direction will allow them to get rid of routine and focus their time and efforts on creative tasks [24]. The approaches to R&D created by the laboratory are being adopted by dozens of companies. For example, the assistant vice president of Merck, a multibational science and technology company, claims that the laboratory's algorithms have been adopted to solve the company's current tasks [25].

17 Pande Lab at Stanford University // Pande Lab. URL: pandelab.org/about#bio (date of reference: 13.02.2022).

18 Pande Lab at Stanford University / Medium. URL: medium.com/@pandelab (date of reference: 13.02.2022).

19 Pandegroup // GitHub. URL: github.com/pandegroup (date of reference: 13.02.2022).

20 Genesis Therapeutics Secures $52M Series A to Further Accelerate AI Innovation and to Launch Drug Discovery & Development Pipeline // Businesswire. URL: https://www.businesswire.com/news/home/20201202005297/en/Genesis-Therapeutics-Secures-52M-Series-A-to-Further-Accelerate-AI-Innovation-and-to-Launch-Drug-Discovery-Development-Pipeline (date of reference: 15.01.2022).

21 Hong Kong Quantum AI Lab // Hong Kong Quantum AI Lab. URL: hkqai.com (date of reference: 14.02.2022).

22 Computer system predicts products of chemical reactions // MIT News. URL: news.mit.edu/2017/computer-system-pre - dicts-products-chemical-reactions-0627 (date of reference 13.02.2022).

23 Guided by AI, robotic platform automates molecule manufacture // MIT News. URL: news.mit.edu/2019/automate-molecule-production-ai-0808 (date of reference: 13.02.2022).

24 Guided by AI, robotic platform automates molecule manufacture // MIT News. URL: news.mit.edu/2019/automate-molecule-production-ai-0808 (date of reference: 13.02.2022).

25 Scientists make digital breakthrough in chemistry that could revolutionize the drug industry // CNBC. URL: cnbc.com/2020/10/24/how-a-digital-breakthrough-could-revolutionize-drug-industry.html (date of reference: 15.01.2022).

Sources: official website of Pande Lab at Stanford University, Zeng Laboratory, MIT

It is worth noting that major research organizations, whose chemistry laboratories apply AI, are often also strong in such fields of knowledge as computer science, engineering, and ecology (Figure 6). It is probable that access to a strong IT school contributes to unlocking additional researchers' potential.l

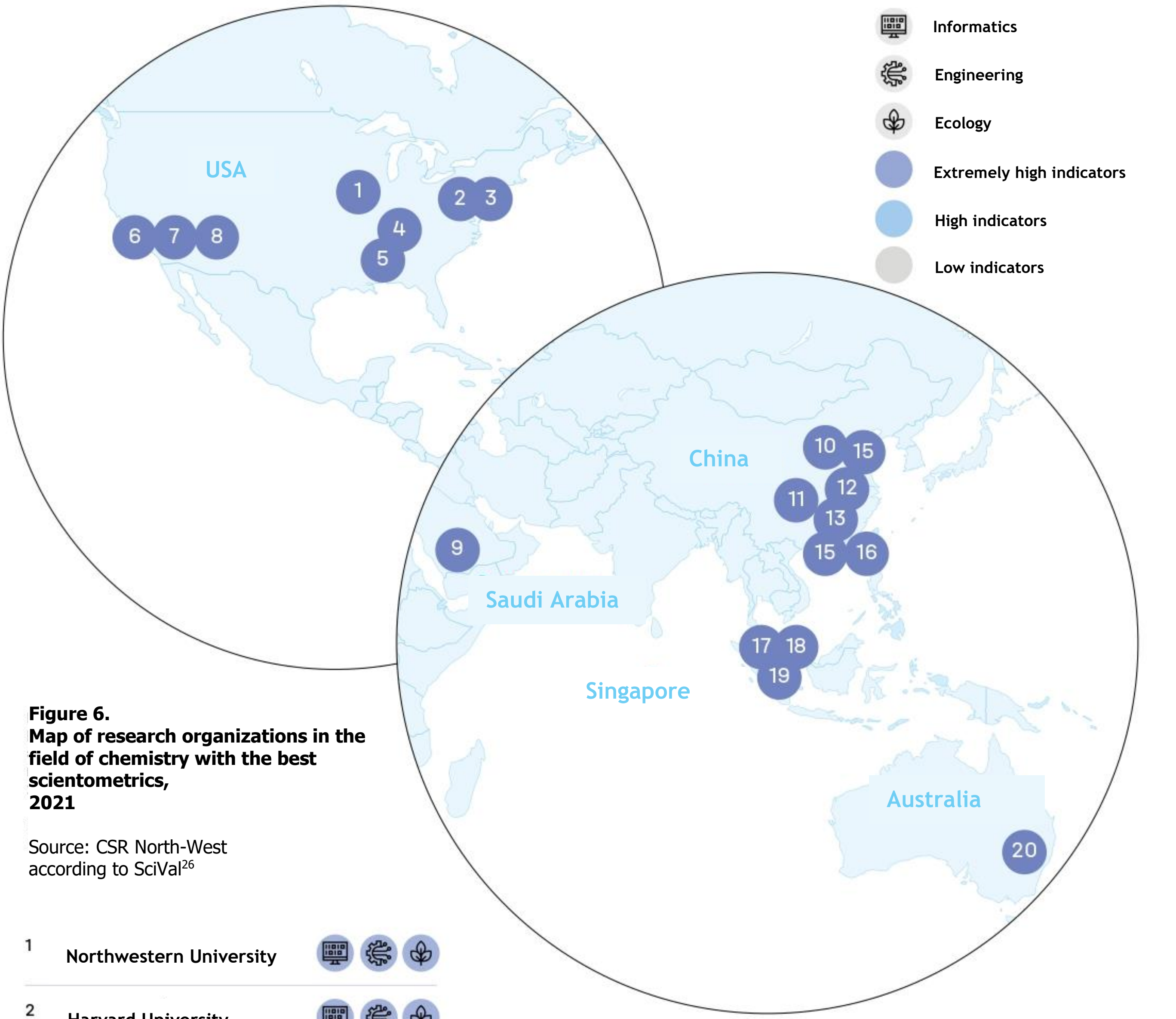
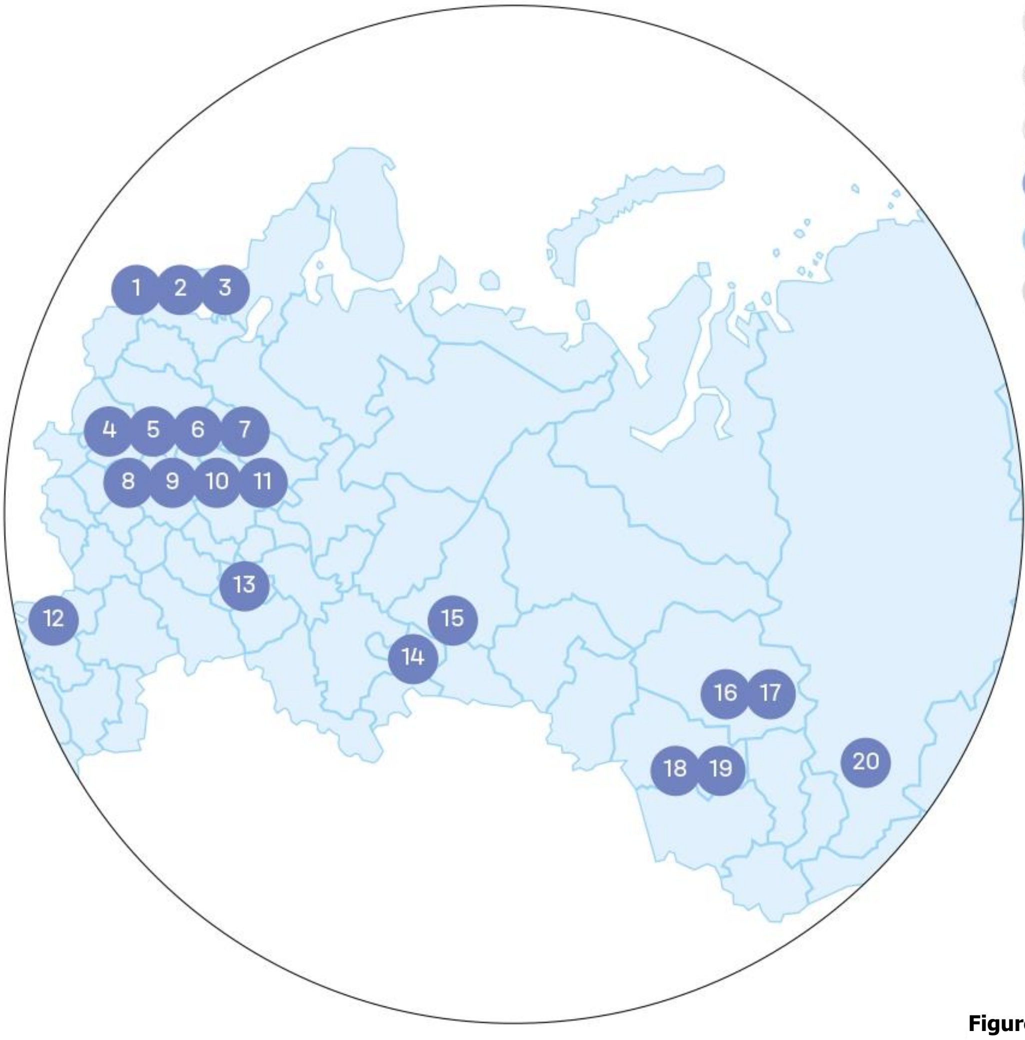


Figure 6.
Map of research organizations in the field of chemistry with the best scientometrics, 2021

Source: CSR North-West according to SciVal[26]

1	Northwestern University
2	Harvard University
3	Massachusetts Institute of Technology
4	University of Tennessee
5	Georgia Institute of Technology
6	Stanford University
7	Lawrence Berkeley National Laboratory
8	University of California at Berkeley
9	King Abdullah University of Science and Technology
10	Institute of Chemistry, Chinese Academy of Sciences
11	University of Electronic Science and Technology of China
12	Wuhan University
13	Hunan University
16	Shandong University of Science and Technology
14	City University of Hong Kong
15	The University of Hong Kong
17	National University of Singapore
18	Nanyang Technological
19	The Agency for Science, Technology and Research
20	University of Wollongong

26 The map shows the 20 research organizations in the world with the highest average citation rates for chemistry publications and the number of chemistry publications is more than 1,500 between 2018 and 2021. The level of indicators of additional competencies is based on two criteria: more than 500 publications in the period under consideration and an above-average citation rate in the respective scientific field (computer science, engineering, ecology). "Extremely high scores" of scientometrics imply exceeding the threshold of 2,000 publications on the topic for ecology, 4,000 for computer science, and 6,000 for engineering. The sample did not include major research organizations such as Cambridge or the Max Planck Institute, because of the relatively low average citation rate of articles when compared to similar ones in the U.S. or China, etc.



Informatics

Engineering

Ecology

Extremely high indicators

High indicators

Low indicators

1	ITMO (St. Petersburg)	11	MIPT (Moscow)
2	Peter the Great St. Petersburg Polytechnic University	12	SFedU (Rostov-on-Don)
3	SPbU (St. Petersburg)	13	KFU (Kazan)
4	Skoltech (Moscow)	14	SUSU (Chelyabinsk)
5	RUDN (Moscow)	15	UrFU (Yekaterinburg)
6	Sechenov University (Moscow)	16	TSU (Tomsk)
7	MEPhI (Moscow)	17	TPU (Tomsk)
8	National University of Science and Technology "MISIS"(Moscow)	18	BIC RAS (Novosibirsk)
9	INEOS RAS (Moscow)	19	NSU (Novosibirsk)
10	N.D. Zelinsky Institute of Organic Chemistry (Moscow)	20	SibFU (Krasnoyarsk)

Figure 7.
Map of the capacity of higher education institutions and scientific organizations to
Creation of breakthrough laboratories in advanced chemistry, 2021

Source: CSR North-West according to SciVal[27]

27 The map shows 20 research organizations of the Russian Federation with the highest average citation rates for chemistry publications from 2018 to 2021. The level of indicators of additional competencies is based on two criteria: more than 500 publications during the period under consideration and a citation level above the average in the corresponding scientific field in Russia (informatics, engineering, ecology). "Extremely high indicators" of scientometrics imply a significant excess of the average level of the number of publications and the citation rate of articles. Such large research organizations as MSU, for example, were not included in the sample due to the relatively low average citation rate of articles, which may be caused by the size of the organization and the negative effect on the quality indicators of scientometrics

Domestic scientists also use digital approaches, but (unlike the advanced laboratories of the world, which have a long history) in Russia the greenfield scenario is often implemented - MIPT, ITMO, Skoltech (Figure 7). As a result, we see private examples of research structures that integrate individual elements of the lab 5.0 paradigm rather than reproduce it completely. It is noteworthy that the flagship laboratories appeared just in the universities with a strong IT direction.

As a result of the established competencies of research organizations and the specifics of frontier areas of research, potential centers of new chemistry can be predicted. A serious scientific base in IT, engineering (due to the application of engineering approaches - design, assembly, testing, data analysis - in solving problems in chemistry) and ecology (as a foundation for the development of sustainable chemistry) in combination with classical chemistry is able to provide a scientific breakthrough. This means that universities such as SPbSU, SPbPU, TSU, TPU, and SUSU can become leaders in this area.

Case 2: Examples of Leading Chemical Laboratories in Russia

Laboratory of Programmable Functional Materials, MIPT

In early 2021, the MIPT project to create a laboratory of programmable functional materials, headed by Nobel laureate Professor Konstantin Novoselov, was announced. The initiative received funding of 500 million rubles from a private public investor for the first five years of work - a unique example of attracting private capital to form a research unit thanks to a significant name and relevant subject matter. Scientists are researching substances with non-standard conditions for second-order phase transitions (the same topic is handled by Novoselov's laboratory in Singapore).
This is a potentially breakthrough area of science that will open the way to creating nanorobots. The applied ideas born in the laboratory are valuable, for example, for the pharmaceutical industry due to the methods developed to predict the properties of macromolecules. Applications for programmable materials can be found in the chemical industry, electronics and energy [28].

28 Konstantin Novoselov Creates Laboratory of Smart Materials at MIPT // Kommersant. URL: kommersant.ru/ doc/4683651 (date of reference: 11.02.2022).

Scientific and Educational Center of Infochemistry, ITMO University

The Center of Infochemistry emerged as a result of the actualization of interdisciplinary directions in this field of knowledge. Professor Ekaterina Skorb became the director (and head of one of the scientific groups). ITMO is home to the Artificial Intelligence Laboratory for Smart and Functional Materials, with which Konstantin Novoselov (see above) and Daria Andreeva-Beumler, professor at the National University of Singapore, collaborate. The university's laboratories actively apply advanced digital approaches to a wide range of scientific problems requiring advanced solutions and international cooperation. The Infochemistry Research Center brings together other scientific groups in advanced areas: infochemistry, computational chemistry, biomimetic materials, chemoinformatics, chemometrics, digitalization of food technology, bioelmentology, digital trans- formation, structured and dynamic soft matter, robotization of chemical technology, and triboinformatics. An example of development of the ITMO Infochemistry Center is a universal electrochemical test platform.
A tool of advanced chemistry, the technpology has great commercial potential due to the wide range of possible applications: in healthcare, food production, and sports.

Sources: Kommersant, Skolkovo, ITMO University

Case 2: Examples of Leading Chemical Laboratories in Russia

Laboratory for Computer-Aided Design of New Materials, Skoltech

In 2019, the Russian Science Foundation and Gazpromneft STC launched a joint project: a laboratory for computer-aided design of new materials started operating at Skoltech. A model of the neural network, created under the guidance, allows calculating superhard materials. These materials are used in many fields, from microelectronics to oil production. Professor Oganov also created a computational method for predicting crystal structures USPEX, which made it possible to discover new materials and substances and was actively used in the USA. The relevance of knowledge about materials with superproperties was one of the main reasons for creating the new laboratory. The industrial industry is also interested in stimulating research and development, as advanced composites are becoming more and more attractive in the sense of application[29].

International Scientific Institute of Solution Chemistry of Advanced Materials and Technologies (SCAMT), ITMO University

In 2014, Alexander and Vladimir Vinogradov founded the International Scientific Laboratory of Solution Chemistry of Advanced Materials and Technologies (SCAMT) at ITMO University. Later on, several scientific groups were formed, engaged in advance research topics, like sol-gel processes and ink-jet printing. The laboratory was transformed into an institute, on the basis of which a chemical-biological cluster was built, where both applied and fundamental research is carried out[30]. A center of artificial intelligence in chemistry was established within the institute. It focused on research, using machine learning. Its creation contributed to the use of high-performance and automated methods of data generation and prediction of material properties, as well as test-platforms for validation of potentially new materials.

29 A laboratory for computer-aided design of new materials opened in Skolkovo // Skolkovo. URL: old.sk.ru/news/b/press/archive/2019/09/09/v-skoltehe-otkrylas-laboratoriya-kompyuternogo-dizayna-novyh-materialov.aspx (date of reference: 11.02.2022).

30 International Science Center SCAMT // ITMO University. URL: scamt.ifmo.ru/ru/ (date of reference:11.02.2022).

Sources: Kommersant, Skolkovo, ITMO University

Modern laboratories are effective not only as a source of scientific discoveries: they can be in demand in the research and development market, and large companies that apply high-tech technologies should be interested in collaborations with such teams.

4 TRANSFORMATION OF RESEARCH COMPETENCIES

Key researchers in today's environment must possess a broad set of skills beyond their scientific profile. The ability of scientists to interact with artificial intelligence and integrate it into the R&D process becomes dominant.

The transition to the AI-driven lab model 5.0 and the trend toward sustainability are leading to a transformation of the competencies of chemistry researchers. This transformation is taking place by building new expertise and information on the already existing scientific base. Researcher toolkit is changing significantly at every stage of scientific and technological progress (Figure 8).

In Chemistry 3.0, all of the scientist's knowledge, skills, and tools were used within the laboratory. Globalization, the emergence of digital technologies, and the transformation of the nature of scientific activity were catalysts for the transformation of the research chemist into a Principal Investigator (PI). The next stage, Chemistry 5.0, will bring to life the Chemist-Laboratory Administrator 5.0 model, which will require new human-machine knowledge, skills, and tools.

	Knowledge	Skills	Tools
Chemistry 3.0	— General knowledge in all traditional areas of chemistry with a key specialization in one area — Knowledge of and adherence to instructions in the workplace — Knowledge of methods for the analysis of chemical compounds — Natural science background — Knowledge of research tools	— Conducting manual experiments, experiments, analyses — Determining the quality and chemical composition of substances by analog methods	— Physical equipment for experiments, tests, analyses — Printed sources of scientific information ↓
Chemistry 4.0	— Knowledge of the mechanisms of innovation economics — Knowledge of human resources management — Scientific ethics — Knowledge of digital technologies and their application in chemistry	— Possession of modern synthesis methods — Organizational planning, preparation of grant applications — Skills in intellectual property — Steady networking for collaboration — Skills in carrying out chemical science activities according to SDG principles — Presentation and writing skills, advanced literary research, time management	— Working with databases, with references/bibliographies in foreign languages — Online platforms for collaborative formula writing, modeling — Digital technologies for working with research data — Interdisciplinary tool methods ↓
Chemistry 5.0	— Knowledge in frontier science topics - biophotonics, new types of energy storage, etc. — Basic knowledge base in the field of digital technology, particularly, in the field of machine learning and working with large data volumes. — A thorough knowledge of the SDGs and the principles of Closed Loop Economics — Understanding of the basic principles of sybersecurity	— Professional administration of lab 5.0 — Creating a flexible network of interdisciplinary and interdisciplinary networking. — Yet unknown skills of the future	— Intelligent control systems based on machine learning — (Industrial) Internet of Things — Development of blockchain-based solutions technologies — Service robots — Additive manufacturing (reverse engineering)

Figure 8.
Transformation of research competencies in chemistry

Source: CSR North-West Foresight-session data, Accenture[31], Report "National Technological Initiative: 7 years on the move".

31 The evolution of digital R&D in chemicals // Accenture. URL: accenture.com/_acnmedia/PDF-158/Accenture-Digital-Research-And-Development-Chemicals.pdf (date of reference: 11.02.2022).

The current trend toward interdisciplinary knowledge and digital competencies is confirmed by Russian researchers. They also speak about filling the competence gap through the involvement of subject matter experts.

Ekaterina Skorb, Ph.D. in Chemistry, Leading Professor and Director of the Scientific and Educational Center (SEC) of Infochemistry at ITMO University:

«In is hard to progress in the field of chemistry at the interface with IT everywhere, simply because chemists with traditional education make little effort to learn computer science. People either "catch up" on the knowledge on their own, or we (the staff of the Research Center of Infochemistry. - Author's note) have to develop new directions.

New chemistry is developing at ITMO University because it has the ground where programmers and mathematicians can be involved in solving important problems in chemistry and materials science, robotization of chemistry and chemical technologies.» [32]

32 From the interview with E. V. Skorb (17.10.2021).

Marina Trusova, Ph.D., professor, director of TPU Research School of Chemical and Biomedical Technologies:

«A researcher must be prepared not only with knowledge in different fields, but also trained to search for, read, and interpret already existing research.

Research is becoming so interdisciplinary that we also have optometrists, mechanical engineers, biomedical scientists, material scientists…»[33].

33 From the interview with M.E. Trusova (28.10.2021).

The current changes in competencies for experts are already reflected in the list of job requirements. If previously chemical R&D required skills solely in chemistry, now employees with IT knowledge and competencies are needed. The largest online job search platforms publish vacancies with an emphasis on digital skills (Table 1).

34 Machine-learning Atomistic Modeling of Corrosion Postdoctoral Researcher // C&EN. URL: chemistryjobs.acs.org/job/36059/machine- learning-atomistic-modeling-of-corrosion-postdoctoral- researcher/ (date of reference: 11.02.2022).

35 Principal Investigators in Machine Learning in Biomedicine (f/m/x) // New Scientist Jobs. URL: jobs.newscientist.com/en-gb/job/1401737580/principal-investigators-in-machine-learning-in-biomedicine-f-m-x-/ (date of reference: 11.02.2022).

36 Master's student or intern: Artificial Intelligence in Chemistry and Material Science // IBM Research Europe. URL: zurich.ibm.com/careers/2021_009.html (date of reference: 11.02.2022).

37 PhD or post-doctoral researcher: Organic Chemistry for Autonomous Lab Development and Operation // IBM Research Europe. URL: zurich.ibm.com/careers/2021_054.html (date of reference: 11.02.2022).

38 Jobs, personnel search and publishing vacancies // HeadHunter. URL: hh.ru (date of reference: 11.02.2022).

Job title	Requirements
Postdoctoral Fellow in machine learning approaches to modeling corrosion of actinide metals and metal-oxide materials at Lawrence Livermore National Laboratory [34]	— PhD in physics, chemistry, materials science, or a related field — experience with first principles of condensed phase modeling — high level programming experience in C++, Fortran 95 or equivalent. Knowledge of scripting language will be an advantage
Key researcher in machine learning in biomedicine at the Helmholtz Center [35]	— PhD degree — application of machine learning to biomedical data — innovative thinking
Research Intern in Artificial Intelligence Applications in Chemistry and Materials Science at IBM Research Zurich [36]	— received or is pursuing a master's degree in computer science, physics, chemistry, or engineering with a sincere interest in chemistry, chemical synthesis, or materials science — experience in machine learning and data modeling — excellent Python programming skills — experience with TensorFlow/ PyTorch libraries, Python scientific stack
PhD or postdoctoral researcher Researcher at the Autonomous Laboratory for Organic Chemistry at IBM Research Zurich [37]	— Master's or PhD degree in organic chemistry with a sincere interest in automation, machine learning, data science, computer science — experience with automation platforms in chemistry — experience in machine learning and data modeling — programming skills in Python
Medical chemist at Insilico Medicine (Skolkovo) [38]	— university degree in chemistry (medicinal chemistry, organic chemistry, bioorganic chemistry) — PH degree / PhD; — experience in development of low molecular weight bioactive compounds — proficiency in molecular modeling software packages (Schrodinger, MOE,Dock, etc.) — programming skills on the level of writing scripts for automated analysis of experimental data is a plus

Table 1.
Current vacancies for researchers, 2021

Источник: CSR North-West,
data from open sources

Thus, artificial intelligence skills are becoming a key skill in scientific activities, and there is an increased demand for appropriate personnel.

Actual digital skills are used in the most cited areas of advanced chemistry (Figure 9). Talented Russian chemists are applying state-of-the-art tools to frontline topics.

Valentin Ananikov heads the laboratory of metal complex and nano-sized catalysts at the N. D. Zelinsky Institute of Organic Chemistry of the Russian Academy of Sciences. His research focuses on improving 3D printing technology for chemical synthesis of biologically active molecules and design of flow reactors. A methodology developed with his participation to determine the safety of chemical processes in green chemistry was published in 2021[39]. As part of groups of scientists, V. Ananikov forms new sustainable approaches in chemistry, allowing to observe the principle of atom-economy in the synthesis of substances[40].

Artem Abakumov works in the advanced field of energy storage technologies in metal-ion batteries (based at the Skoltech Center for Energy Science and Technology)[41]. In 2021, together with his colleagues from Skoltech, he patented a technology that will help improve the next generation of environmentally friendly batteries and make them commercially viable. The nano-tube anode created by the scientists will accelerate the mass market penetration of such potassium-ion batteries. As a counterpart to lithium-ion batteries, Abakumov's development will reduce the consumption of lithium, whose reserves are limited.[42].

Maxim Molokeev from Siberian Federal University and Kirensky Institute of Physics, one of the most cited scientists in the world, conducts research at the intersection of physics, chemistry, and materials science[43]. In the process of cooperation with Chinese specialists, he determined the structure of a promising phosphor, a substance on the basis of which new white LEDs can be brought to the market[44]. And in 2021 as a member of the international scientific team M. Molokeev developed a unique luminophore, which due to its versatility is suitable for use in sensors of a wide range of areas - in medicine (to monitor the condition of patients), agriculture and biosensor technology[45].

As part of Russia's international cooperation program, Yuri Kivshar was one of the first recipients of a megagrant to create a laboratory of metamaterials at ITMO University (which later became the basis for an entire department)[46]. The researcher participated in the creation of metasurfaces that change the structure of light, which shifted the paradigm of nonlinear optics [47]. Yu. Kivshar is a co-director of the ITMO University project to improve fiber optics for data transmission. It is now possible to use this fiber optic to improve images in endoscopy and laparoscopy, for quantum technologies and fiber optic sensors [48].

In Russia, however, even the best members of the scientific community do not always have knowledge in the field of AI or do not integrate it in their work. Moreover: amid the smooth generatioinal change of researchers, widespread application of AI by young promising scientists has not been noted(Figure 10).

39 Egorova K., Galushko A., Dzhemileva L., D'yakonov, V., Ananikov V. Building bio-Profiles for common catalytic reactions // Green Chem. — 2021. — № 23.

40 Romashov L. V. et al. Atom-economic Approach to the Synthesis of α-(Hetero)aryl-substituted Furan Derivatives from Biomass// Chemistry — An Asian Journal. — 2022. — № 17 (1).

41 Artem Abakumov // Skoltech Faculty. URL: faculty.skoltech.ru/people/artemabakumov (date of reference: 11.02.2022).

42 New Skoltech patent: Nanotube anode to improve potassium-ion battery efficiency// Skoltech. URL: skoltech.ru/2021/03/novyj-patent-skolteha-an-od-iz-nanotrubok-povysit-effe-ktivnost-kalij-ionnyh-akkumu-lyatorov/ (date of reference: 11.02.2022).

43 Physicists from Krasnoyarsk are in the top of the world's best scientific reviewers// Our Krasnoyarsk Krai. URL: gnkk.ru/news/fiziki-iz-krasnoyars-ka-voshli-v-top-luchsh/?utm_source=yxnews&utm_medi-um=desktop&utm_refer-rer=https%3A%2F%2Fyandex.ru%2Fnews%2Fsearch%3F-text%3D (date of reference: 11.02.2022).

44 The Structure of a New Type of Material Determined // Nauchnaya Rossiya. URL: scienti-ficrussia.ru/articles/opredele-no-stroenie-novoj-struktury (date of reference: 11.02.2022).

45 Scientists created universal substance-base for broad-spectrum sensors // RIA Novosti. URL: ria.ru/20211018/ sfu-1754972217.html (date of reference: 11.02.2022).

46 The air of unfreedom. What motivates Russian scientists go abroad // BBC Rusian Service. URL: bbc.com/ russian/features-57028917 (date of reference: 11.02.2022).

47 Wang L., Kruk S., Koshelev K., Kravchenko I., Luther-Davies B., Kivshar Y. Nonlinear Wavefront Control with All-Dielectric Metasurfaces // Nano Letters. — 2018. — № 18 (6).

48 «Shedding light» from the right angle// Kommersant. URL: kommersant.ru/ doc/4540238 (date of reference: 11.02.2022).

Among foreign researchers with the highest citation rates, this practice is not widespread either (Figure 11). It turns out that in terms of using the capabilities of AI, the best domestic scientists are at a comparable level with foreign ones. It can be assumed that the active introduction of artificial intelligence in chemical research can bring Russia to the leading position due to the technological equipment of laboratories.

Digitalization and new technologies lead to personnel transformation not only in science, but also in industry. The consulting company Deloitte[49], predicts that new professions to emerge in chemical industry by 2030 include:

- computational materials scientist (discovering new materials by analyzing data and predicting the relationships of structures and properties of new materials);
- nano-chemical engineer (studying nanoscale structures, modeling new materials);
- fuel cell engineer (designing fuel cells that produce electricity through a chemical reaction involving hydrogen);
- predictive supply analyst (evaluating AI recommendations and making final decisions in securing supplies of materials, customer service, etc.)
- digital twin engineer (digital twin management).

The transition to new competency profiles of the chemical industry, while maintaining the existing approaches to training specialists, may soon cause a shortage of research and production personnel with the necessary qualifications to work in a changing industry. The Federal State Educational Standards for Chemistry training contain only framework requirements for computer literacy in solving problems of professional activity. There are no requirements for new competencies and digital tools in the professional standards either. The introduction by universities of disciplines of other natural science disciplines into the educational courses for chemists-researchers, as well as training in the use of digital tools, including artificial intelligence management and machine learning, will help to meet the increasing demand for future competences.

49 The future of work in chemicals // Deloitte. URL: www2.deloitte.com/content/dam/Deloitte/us/Documents/energy-resources/us-the-future-of-work-in-chemicals-pov.pdf (date of reference: 11.02.2022).

TC.30 SECONDARY BATTERIES

Sergey V. Savilov (h-index: 26)

Moscow State University, laboratory of catalysis and gas electrochemistry	Research: sodium-ion accumulators; ion storage

Artem M. Abakumov (h-index: 43)

Skolkovo Institute of Science and Technology, Center for Energy Science and Technology	Research: solid state chemistry, electrocatalysis, materials for metal-ion batteries

TC.8 PHOTOCATALYSIS

Pavel A.Troshin (h-index: 41)

Institute of Chemical Physics Problems of the Russian Academy of Sciences, Laboratory of Functional Materials for Electronics and Medicine	Research: organic semiconductors, organic material science, solar batteries

Maxim S. Molokeev (h-index: 56)

Institute of Chemical Physics Problems of the Russian Academy of Sciences, Laboratory of Functional Materials for Electronics and Medicine	Research: organic semiconductors, organi materials science, sola batteries

TC.22 GRAPHENE; CARBON NANOTUBES

Mikhail M. Glazov (h-index: 43)

The Ioffe Physical-Technical Institute of the Russian Academy of Sciences, Center for physics of nanoheterostructures, sector theory of quantum coherent phenomena	Research: spin dynamics charge carriers, optical spectroscopy

Albert G. Nasibulin (h-index: 50)

Skolkovo Institute of Science and Technology, Photonics and Engineering Center	Research: nanoparticles, nano-tube films, quadruped-saturable absorbers

TC.47 PLASMONS; METAMATERIALS

Yuri S. Kivshar (h-index: 121)

St. Petersburg National Research University of Information Technologies, Laboratory of Metamaterials	Research: nanophotonics, nanoantennas

Nikolai L. Kazansky (h-index: 50)

Samara University, laboratory of automated research systems	Research: diffraction nanophotonics; computer optics

TC.4 CATALYSIS; SYNTHESIS; CATALYSTS

Valentin P. Ananikov (h-index: 56)

N.D. Zelinsky Institute of Organic Chemistry, Laboratory of Metallocomplex and nano-sized catalysts	Research: catalysis; organic synthesis; molecular complexity and transformations

Irina P. Beletskaya (h-index: 63)

The Institute of Physical Chemistry and Electrochemistry RAS (IPCE RAS), laboratory of new physicochemical problems	Research: arylation; cross-linking reactions; Iodobenzenes

TC.7 CATALYSTS; ZEOLITES; HYDROGENATION

Evgeny Y. Gerasimov (h-index: 26)

The Boreskov Institute of Catalysis of the Siberian Branch of Russian Academy of Sciences	Researches: hydrodesulphurization; dibenzothiophene; hydrogen generation

Anton L. Maksimov (h-index: 25)

A.V.Topchiev Institute of Petrochemical Synthesis, RAS (TIPS RAS)	Research: hydrodesulphurization; dibenzothiophene; catalysts

TC.71 ORGANOMETALLICS

Denis G. Samsonenko (h-index: 29)

Nikolaev Institute of Inorganic Chemistry of the Siberian Branch of the RAS, laboratory of organometallic coordination polymers	Research: organometallic structures

Vladimir P. Fedin (h-index: 47)

Nikolaev Institute of Inorganic Chemistry of the Siberian Branch of the RAS, laboratory of organometallic coordination polymers	Research: organic semiconductors, organic material science, solar batteries

TC.61 OLED; SOLAR CELLS

Sergey A.Ponomarenko (h-index: 33)

The Institute of Synthetic Polymeric Materials (ISPM), laboratory of metal-organic coordination polymers	Research: organic solar cells, organic electronics

Dmitriy Y.Parashchuk (h-index: 22)

MSU, Organic Electronics Group	Research: organic electronics, organic semiconductors, semiconductor polymers, organic solar batteries

TC.128 BIOSENSORS; ELECTRODES; VOLTAMMETRY

Tatiana G. Volova (h-index: 29)

Federal Research Center "Krasnoyarsk Science Center of the Siberian Branch of the Russian Academy of Sciences, laboratory of chemoautotrophic biosynthesis	Research: biomedical materials science and polymer applications

Ekaterina I. Shishatskaya (h-index: 23)

Federal Research Center "Krasnoyarsk Science Center of the Siberian Branch of the Russian Academy of Sciences, Laboratory of chemoautotrophic biosynthesis	Research: polymers

TC.128 BIOSENSORS; ELECTRODES

Arkady A. Karyakin (h-index: 46)

Moscow State University, electrochemical methods laboratory, chemistry department	Research: physicochemistry of enzymes, biosensors based on nanostructures electro- and biocatalysts

Maria A. Komkova (h-index: 10)

Moscow State University, electrochemical methods laboratory, chemistry department	Research: flow biosensors, electrochemical analyzers, hexacyanoferrates

TC.609 ADDITIVES; MANUFACTURE; PRINTING

Vadim S. Sufiyarov (h-index: 18)

St. Petersburg Peter the Great Polytechnic University, laboratory of synthesis of new materials and designs	Research: 3D printing, selective laser melting

Anatoly A. Popovich (h-index: 20)

Peter the Great St.Petersburg Polytechnic University, the laboratory of synthesis of new materials and designs	Research: 3D printing, selective laser melting

TC.191 ADSORPTION; ADSORBENTS

Alexei G. Tkachev (h-index: 16)

Tambov State Technical university, department "Technologies of nanoproducts manufacturing"	Research: adsorbents; graphene oxide; biosorbents

Yevgeny V. Galunin (h-index: 13)

Tambov State Technical university, department " Technologies of nanoproducts manufacturing""	Research: adsorbents; graphene oxide; biosorbents

TC.248 FLUORESCENCE; SUPRAMOLECULAR CHEMISTRY

Ivan I. Stoykov (h-index: 25)

Kazan Federal University	Research: organic, elementorganic, supramolecular and medicinal chemistry of macrocyclic compounds

Violeta K. Voronkova (h-index: 14)

Zavoisky Physical-Technical Institute, FRC Kazan Scientific Center, Russian Academy of Sciences, laboratory of spin physics and spin chemistry	Research: spectroscopy; spin properties of new materials

TC.223 MEMBRANES; DESALINATION

Viktor V. Nikonenko (h-index: 41)

Kuban State University, Natural Polymers Laboratory	Research: electrodialysis; ion-exchange membranes;ionic transport

Natalia D. Pismenskaya (h-index: 31)

Kuban State University, Laboratory of electromembrane phenomena	Research: membranes; membrane processes

TC.82 PHARMACEUTICAL PREPARATIONS

Yuri A. Skorik (h-index: 21)

RAS Institute of High Molecular Compounds , Natural Polymers Laboratory	Research: analytical and coordination chemistry, chemistry and physicochemistry polysaccharides, polymeric drug delivery systems

Lucia Ya. Zakharova (h-index: 28)

A.E. Arbuzov Institute of Organic and Physical Chemistry, Laboratory of Highly Organized Structures	Research: self-organization, amphiphiles, cyclophanes, polymers, supramolecular catalysis, nanocontainers

Figure 9.
Leading researchers in advanced chemistry in Russia, 2021

Source: CSR North-West according to SciVal [50]

AI applications in scientific research

The list of researchers was formed from the two representatives with the highest volume of citations in each area of breakthrough chemistry research for the period of 2016-2020.

TC.30 SECONDARY BATTERIES

Roman R. Kapaev (h-index: 11)

Skolkovo Institute of Science and Technology, Laboratory of Photocatalysis and Electrocatalysis	Research: high-capacity batteries with organic anodes and cathodes, Na-ion batteries

TC.8 PHOTOCATALYSIS

Dmitry S. Selischev (h-index: 14)

Institute of Catalysis SB RAS, Laboratory photo- and electrocatalysis	Research: photocatalytic oxidation, photocatalytic air purification, composite photocatalysts

TC.22 GRAPHENE; CARBON NANOTUBES

Artem V. Kuklin (h-index: 10)

Siberian Federal University, international Research Center for Spectroscopy and Quantum Chemistry	Research: ferromagnetism and semimetallicity at the nanoscale, magnetic tunnel junctions

TC.47 PLASMONS; METAMATERIALS

Kirill L. Koshelev (h-index: 17)

University of Information Technologies, Mechanics and Optics, physics and technology department	Research: nonlinear metasurfaces, nonlinear nanophotonics

TC.4 CATALYSIS; SYNTHESIS; CATALYSTS

Vladimir A. Larionov (h-index: 13)

A.N.Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, Laboratory of asymmetric catalysis	Research: synthesis of non-natural α-amino acids, asymmetric synthesis

TC.7 CATALYSTS; ZEOLITES; HYDROGENATION

Alexander P. Glotov (h-index: 14)

Gubkin Russian State University of Oil and Gas laboratory of physical and colloidal chemistry	Research: catalysis with nanotubes, nanoclay, hydrodesulfurization

TC.71 ORGANOMETALLICS

Yekaterina N. Zorina-Tikhonova (h-index: 10)

Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Laboratory of Chemistry of coordinated polynuclear entities	Research: coordination polymers, magnetic relaxation, magnetocaloric effects

TC.61 OLED; SOLAR CELLS

Andrey Yu. Sosorev (h-index: 10)

Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry, Laboratory of Modelling of Biomolecular Systems	Research: organic nanoelectronics, organic semiconductor crystals

TC.69 POLYPROPYLENES; LACTIC ACID; BLENDING

Nikita V. Minaev (h-index: 12)

Federal Research Center "Crystallography and Photonics", Russian Academy of Sciences, laboratory of spin physics and spin chemistry	Research: quasi-isothermal foaming, foaming for polylactides, plasticized SCFs

TC.128 BIOSENSORS; ELECTRODES

Maria A. Komkova (h-index: 10)

Moscow State University, Electrochemical Methods Laboratory Chemistry Department	Research: flow biosensors, electrochemical analyzers, hexacyanoferrates

TC.609 ADDITIVES; MANUFACTURE; PRINTING

Roman A. Surmenev (h-index: 29)

Tomsk Polytechnic University, research center "Physical Material Science and Composite Materials"	Research: sprayed coatings; plasma spray; bioceramics

TC.191 ADSORPTION; ADSORBENTS

Vladimir S. Semenischev (h-index: 24)

Ural Federal University, Department of Radiochemistry and Applied Ecology	Research: nanostructured inorganic materials for sorption, adsorbent on magnetic metalorganic basis

TC.248 FLUORESCENCE; SUPRAMOLECULAR CHEMISTRY

Alexander A. Ksenofontov (h-index: 11)

G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, the Laboratory "Physical Chemistry of Solutions of Macrocyclic Compounds"	Research: fluorescence, photoinduced electron transfer electrons

TC.223 MEMBRANES; DESALINATION

Anton N. Petukhov (h-index: 13)

Mendeleev University of Chemical Technology of Russia, Laboratory of Smart Materials and Technologies	Research: membrane hybrid process of adsorption

TC.82 PHARMACEUTICAL PREPARATIONS

Aleksandr V. Gerasimov (h-index: 12)

Kazan Federal University, Laboratory of physicochemical research	Research: antimicrobial salt activity, smart thermal behavior of tripeptides, rapidly crystallizing drugs

Figure 10.
Young researchers are the stars of advanced chemistry in Russia, 2021
Source: CSR North-West according to SciVal [51]

Using of AI in scientific work

51 The list of researchers is compiled of two representatives with the highest growth rates of the number of citations in each area of research in the field of advanced chemistry for the period 2016-2020 and the Hirsch index of over 10 under the age of 40.

TC.30 SECONDARY BATTERIES

Yuri Gogotsi
(h-index: 167)

Drexel University, USA	Research: ion storage, electrochemical capacitors, sodium-ion batteries

TC.8 PHOTOCATALYSIS

Wang Zhonglin
(h-index: 243)

Georgia Institute of Technology, USA	Research: Nanogenerators, energy storage

TC.22 GRAPHENE; CARBON NANOTUBES

Taniguchi Takashi
(h-index: 137)

National Institute of Materials Science, Japan	Research: superlattices, graphene, van der Waals hetero-structures

TC.47 PLASMONS; METAMATERIALS

Chen Xiaoyuan
(h-index: 167)

National University of Singapore, Singapore	Research: photothermotherapy, photoacoustics, theranostic nanomedicine

TC.4 CATALYSIS; SYNTHESIS; CATALYSTS

Lutz Ackerman
(h-index: 116)

University of Göttingen,Germany	Research: alkenylation, activation of C-H-transition metals

TC.7 CATALYSTS; ZEOLITES; HYDROGENATION

Tao Zhang
(h-index: 96)

Dalian Institute of Chemical Physics Chinese Academy of of Sciences, China	Research: catalysis, heterogeneous monatomic catalysis, olefins

TC.71 ORGANOMETALLICS

Omar Farha
(h-index: 123)

Northwestern University, USA	Research: metal-organic frameworks

TC.61 OLED; SOLAR CELLS

Ho Jienhui
(h-index: 111)

Institute of Chemistry, Chinese Academy of Sciences, China	Research: organic solar cells; organic photovoltaics; bulk heterojunction

TC.69 POLYPROPYLENES; LACTIC ACID; BLENDING

Zare Yassir
(h-index: 50)

Iranian Academic Center for Education, Culture and Research, Iran	Research: interphase, polymeric nanocomposites, percolation threshold

TC.128 BIOSENSORS; ELECTRODES

Wei Keen
(h-index: 73)

Jinan University, China

Research: electrochemiluminescence, luminol, immunosensors, biosensing based on nanomaterials

TC.609 ADDITIVES; MANUFACTURE; PRINTING

Debroy Tarasankar
(h-index: 65)

University of Pennsylvania, USA

Research: selective laser melting; additive manufacturing of metals

TC.191 ADSORPTION; ADSORBENTS

Ван Ксианке
(h-index: 131)

North China Electric Power University,China

Research: nanomaterials based on hydroxide-based, organometallic framework materials

TC.248 SUPRAMOLECULAR CHEMISTRY

Rabiul Aual
(h-index: 98)

Curtin University, Australia

Research: adsorbents; wastewater treatment, adsorption isotherms

TC.223 MEMBRANES; DESALINATION

Ahmad Ismail Fauzi
(h-index: 91)

University of Technology Malaysia, Malaysia

Research: ultrafiltration, membranes for water purification

TC.82 PHARMACEUTICAL PREPARATIONS

Abdul Basit Faseh
(h-index: 63)

University College London, United Kingdom

Research: 3D printing of personalized targeted drugs

Figure 11.
Most Cited Advanced Chemistry Researchers in the World, 2021

Source: CSR North-West according to SciVal[52]

Using AI in scientific work

52 The list is formed of the researches with the highest number of citations in each research area in the field of breakthrough chemistry in the period 2016-2020 and Hirsch index of at least 50

5 FRONTIERS OF ADVANCED CHEMISTRY

The analysis conducted by the authors of the report showed that the following topics are on the research frontier of chemistry: the process of catalysis, the development of new batteries, drug delivery systems, materials based on graphene and nanopesticides. R&D using the tools of new chemistry will be relevant here in the coming decade.

The products of industry provide for all spheres of human activity to the maximum extent possible. Due to its global and fundamental nature, chemistry is influenced and challenged not only by economic and scientific reasons, but also by the political demands of society.

A decade ago the main challenges for the chemical industry were the state of the environment and natural resources, the growth of the global population, globalization, political regulation and civic activism (Paris Agreement, CO2 emission quotas, restrictions on the use of diesel cars in Europe, etc.), innovative technologies and consumption patterns (demand for recyclable and more durable products, the growing popularity of veganism and conscious consumption).

The COVID-19 pandemic has changed priorities. Processes in chemistry, both industrial and scientific, are now subordinated to the tasks of preserving and developing a comfortable and safe life on Earth. The chemical industry has to confront new challenges[53]:

- active transition to sustainable consumption;
- a slowdown in globalization and even de-globalization;
- structural changes in key industries;
- temporary suspension of restructuring of chemical companies' business portfolios;
- disruption of supply chains and a change in the type of communication;
- forced introduction of remote work models.

"Green transition" and the environmental agenda dictate courses of action for chemical scientists. Research and theory are currently focused on the development of materials for energy storage to support the widespread use of renewable energies, the production of hydrogen as a clean energy vector, the direct use of carbon dioxide for the introduction of man-made carbon circulation, and the creation of infinitely recyclable synthetic polymers[54].

Technological priorities for chemistry are driven by digitalization, the green transition, and the COVID-19 pandemic. A qualitative breakthrough in technology is needed to meet the challenges facing the industry.

In order to identify frontier topics of advanced chemistry that will be relevant in the coming decades, the authors of the report combined data from:

— scientometric analysis (SciVal, Scopus): the most cited topics by information for 2019-2021;
— foresight results (Foresight "Frontiers in New Sciences", November 9-10, 2021): themes addressed in the presentations in the context of promising research for the periods up to 2030 and 2050;
— analysis of other sources (international profile organizations, consulting agencies, technology transfer networks): information on promising topics according to 2019-2021, Table 2.

53 COVID-19 is challenging the way we think of chemical industry trends. This is how // World Economic Forum. URL: weforum.org/agenda/2021/03/chemical-industry-trends-forecasting-resilience/ (date of reference: 11.02.2022).

54 Fantke P., Cinquemani C., Yaseneva P., De Mello J., Schwabe H., Ebeling B., Lapkin A. Transition to sustainable chemistry through digitalization // Chem. — 2021. — № 7 (11). — C. 2866-2882.

Direction	SciVal	Foresight	Analytics
Ecology	Perovskites Nanocellulose Adsorbents Lignin Carbon capture	Fast degradable materials Unified recyclable materials Inert long-life materials Harmless plasticizers	Macromonomers for plastic recycling Air and water quality control Biological and renewable raw materials Urban mining (collection and recycling of rare metals from municipal solid waste) Sustainable ammonia production Metal-free synthesis of aryl compounds
Energy	Electrochemical capacitors Organic photovoltaics Bioelectricity Flow battery	Energy storage based on organic hydrogen compounds	Solid state accumulators Dual-ion batteries
Medicine	Theranostics Photodynamic therapy Gold and Silver Nanoparticles Smart drug delivery systems	Nanobiomedicine Sensitivity and selectivity of sensors Cosmetics based on biocomponents	Metal organic frameworks 3D bioprinting Microbiome and bioactive compounds Rapid diagnostic testing RNA vaccines Chemiluminescence for Biological Applications Chemical synthesis of RNA and DNA Semi-synthetic life form Targeted protein degradation Direct fluorination Single cell metabolomics

Direction	SciVal	Foresight	Analytics
Electronics	Flexible electronics Sensors	Organic electronics Bioelectronics	Organic electronics Nanosensors
Agriculture	Nanopesticides	Agrochemicals	Nanopesticides
Materials	Two-dimensional materials Nanocomposite materials Natural Fiber Composites Organometallic compounds Coordination polymers Self-Restoring Materials	Smart materials Biodegradable materials Graphene Coatings, adhesives, pigments Structural engineering plastics Nanodiamonds Carbon fiber Thermoplastic composites Carbon materials Polymeric materials Organofluorine polymers, compounds and materials Biomaterials for 3D-printing	Conversion of plastics into monomers Artificial humic substance derived from biomass Aggregation induced radiation Sonochemical coatings Superwettability Nanomaterials and functional textiles "Light" materials and new insulation products Chemical IoT systems
General	Photocatalysis Electrocatalysis Advanced oxidation technologies Cross-combination reactions Nanocatalysts 3D printing	Non-covalent organocatalysis Chemistry of natural compounds Chemical vapor deposition Plasma-chemical selective etching	Flux chemistry Reactive extrusion Directed evolution of selective enzymes Reversible deactivation of radical polymerization High-pressure inorganic chemistry Liquid gating technology

Table 2.
Perspective topics of chemistry development until 2030 / 2050
Source: CSR North-West according to open sources

Based on scientometric data, expert evaluations of foresight, and analysis of other materials, we can identify topics identified in all of the sources. First of all, this is the topic of catalysis. There is an extensive promising technology tree for this area of research, including photocatalysis (related, in particular, to the search for environmentally friendly power generation), electrocatalysis, and nanocatalysts. Another important topic is the development of new generations of batteries, including the creation of alternative types of cathodes and anodes and the use of previously unused materials. In the medical field, research into smart drug delivery systems seems promising. Great expectations of the scientific community are related to two-dimensional materials, for example, based on graphene. Finally, the importance of the topic of nanopesticides for the agricultural technology industry is emphasized.

The performance of R&D on these topics can provide breakthrough results and high economic effect for new technological markets. At the same time, the tools of new chemistry, in particular artificial intelligence, being an end-to-end technology, will increase the efficiency of research.

6 ADVANCED CHEMISTRY MARKET

Changes in the research process have brought new players to the market. New chemistry start-ups are attracting the most investment, primarily from sources outside the industry. Chemical laboratories can be a source of innovation and startups.

The R&D market in chemistry, in response to qualitative changes in the research format, is also undergoing transformation and new business models are emerging. Intellectualization of the chemical research process is caused by the creation of special software necessary to perform R&D: process analysis and modeling, calculations, visualization, resource management, which, in turn, brings a new type of companies to the market (Table 3).

Software	Headquarters country	Purpose
Chemstations	USA	Modeling of chemical processes
NEXTMOL	Spain	Design of new materials and molecules (atomic modeling and data analysis tools)
ChemADVISOR Inc.	USA	Databases, tutorials, and services for hazardous materials
Alchemy	USA	Flexible formulation development in specialized chemistry
SustAnalyze	Netherlands	Data-driven tools for developing sustainable chemical processes
chembid.com	Germany	Chemical market analysis
ChemAlive	Switzerland and predictive analytics	Molecular design, drug discovery, reaction modeling, advanced analytics

Table 3.
Software (SaaS) for Chemical R&D, 2022

Source: CSR North-West according to open sources

Another tool is platforms - hardware and software solutions that combine the capabilities to perform a wide range of analyses in various fields of application. The platform combines new automation capabilities (use of electrochemical sensors), research tools, machine learning and data analytics, databases, and software and applications (Figure 12).

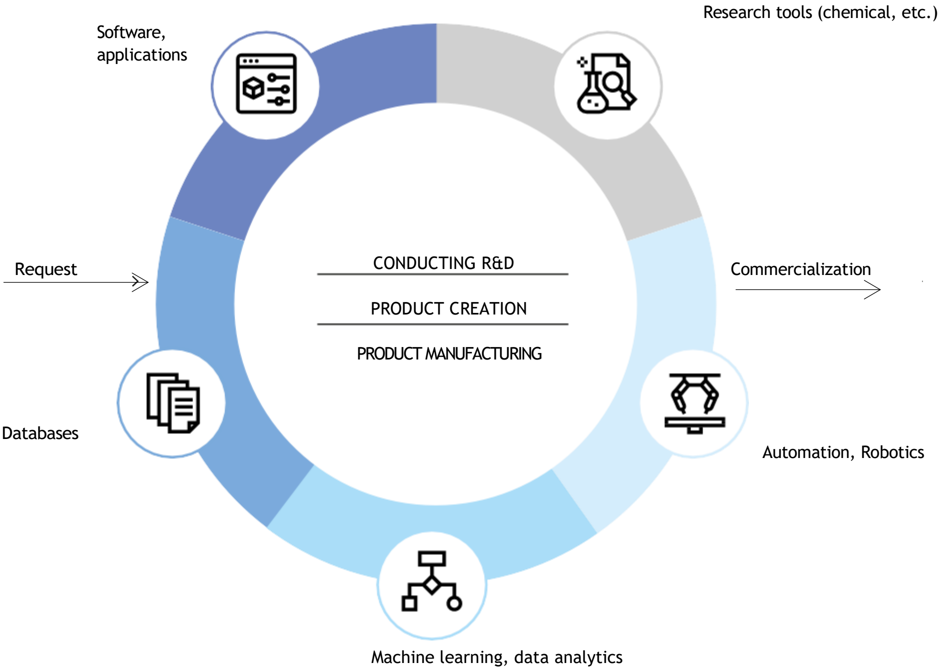


Figure 12.
Diagram of a universal hardware platform used in chemistry

Source: CSR North-West

Companies are entering the market with research platforms such as:

— DNA synthesis platform Twist Bioscience: semiconductor-based production of synthetic DNA using a high-performance silicon platform that makes it possible to miniaturize the chemistry required for DNA synthesis. The results are used in medicine, agriculture, and industrial chemistry[55];

— Zymergen biomanufacturing platform: creation of molecules using genomics, machine learning and automation[56]. The company's activity with the help of this platform includes three elements:

— product development. From a database of biomolecules, a molecule suitable for the client's problem is selected. Then microbes which can make it with the help of genomic libraries are created;

— microbe development. Using machine learning algorithms, billions of designs are created and tested, and molecules are fermented;

— large-scale manufacturing;

— ITMO electrochemical test platform - designed to analyze and test the specified chemical properties of an object. Based on the universal electrochemical test platform, it is possible to create devices that determine the content of various particles in the body - metal ions, viruses and antibodies to viruses, DNA or RNA fragments, antibiotic traces, etc.[57]

55 Technology // Twist Bioscience. URL: http://twistbioscience.com/technology (date of reference: 11.02.2022).

56 What We Do // Zymergen. URL: zymergen.com/what-we-do/ (date of reference: 11.02.2022).

57 Report by E.V. Scorb at the Forsight-session «Frontiers in the New Sciences», December 9-10, 2021

At the same time the chemical industry is a highly fragmented market, because the areas of application (pharmaceuticals, food production, agriculture, electronic devices, etc.) have specific requirements and rules, which often make the business processes complex and confusing. Companies cooperate with each other, looking for partners to reduce R&D costs and share risks. Online sales platforms of individual companies or B2B marketplaces where suppliers and buyers of chemical products meet are emerging in the market (Figure 13).

Online sales	B2B Marketplaces			
XIAMETER	e-Chemicals	ECHEMI	LookChem	chembid
SINOPEC	CHEMOCART	ChemNet ZAGENO	CHEMPOINT eMolecules	MOLBASE
Epoxy.com	Omnexus	knowde	OKCHEM	chemberry
Asellion	Elemica	CHEMARC	WuXi LabNetwork	WuXi AppTec

Figure 13.
Chemical sales platforms

Source: CSR North-West according to open sources

In the last five years, there has been a growing interest in chemical start-ups: investments in them have increased significantly, especially from sources outside the industry (Figure 14).

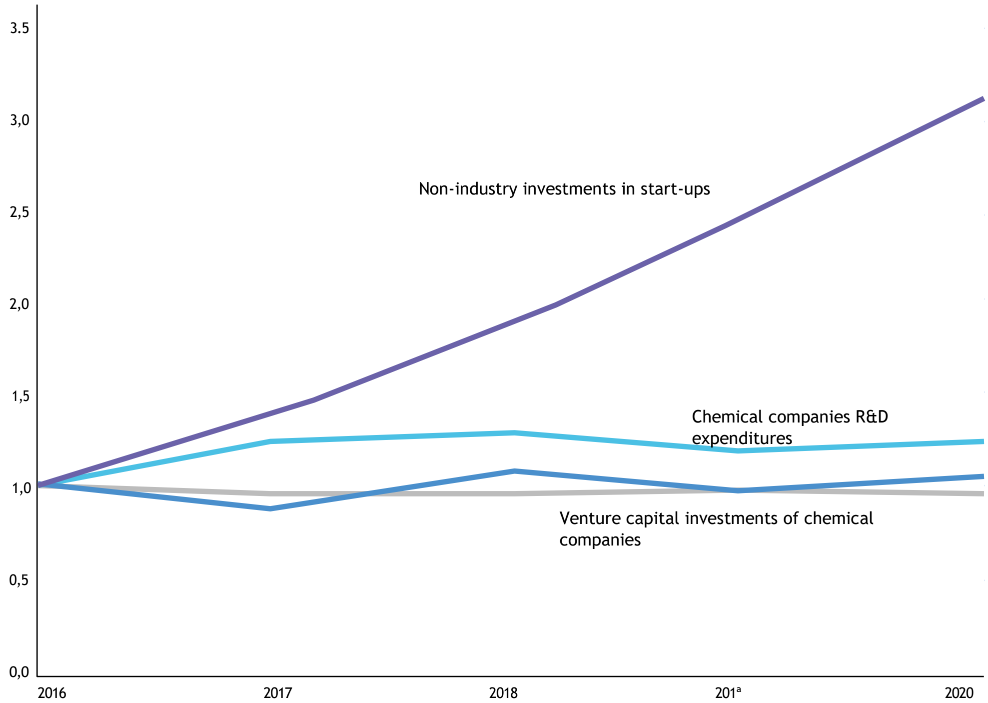


Figure 14.
Growth rate of investments in chemical companies, up to 2016
Source: Accenture: Growth and innovation in the chemicals

Venture financing of chemistry in recent years has been focused on solving problems related to current big challenges and development of new markets: sustainability, development of new drugs, food products, materials and energy (examples of global start-ups attracting capital from leading investors are given in Appendix 1). There has been a multiplication of investments related to chemistry, defined as new by the authors of the report (Figure 15).

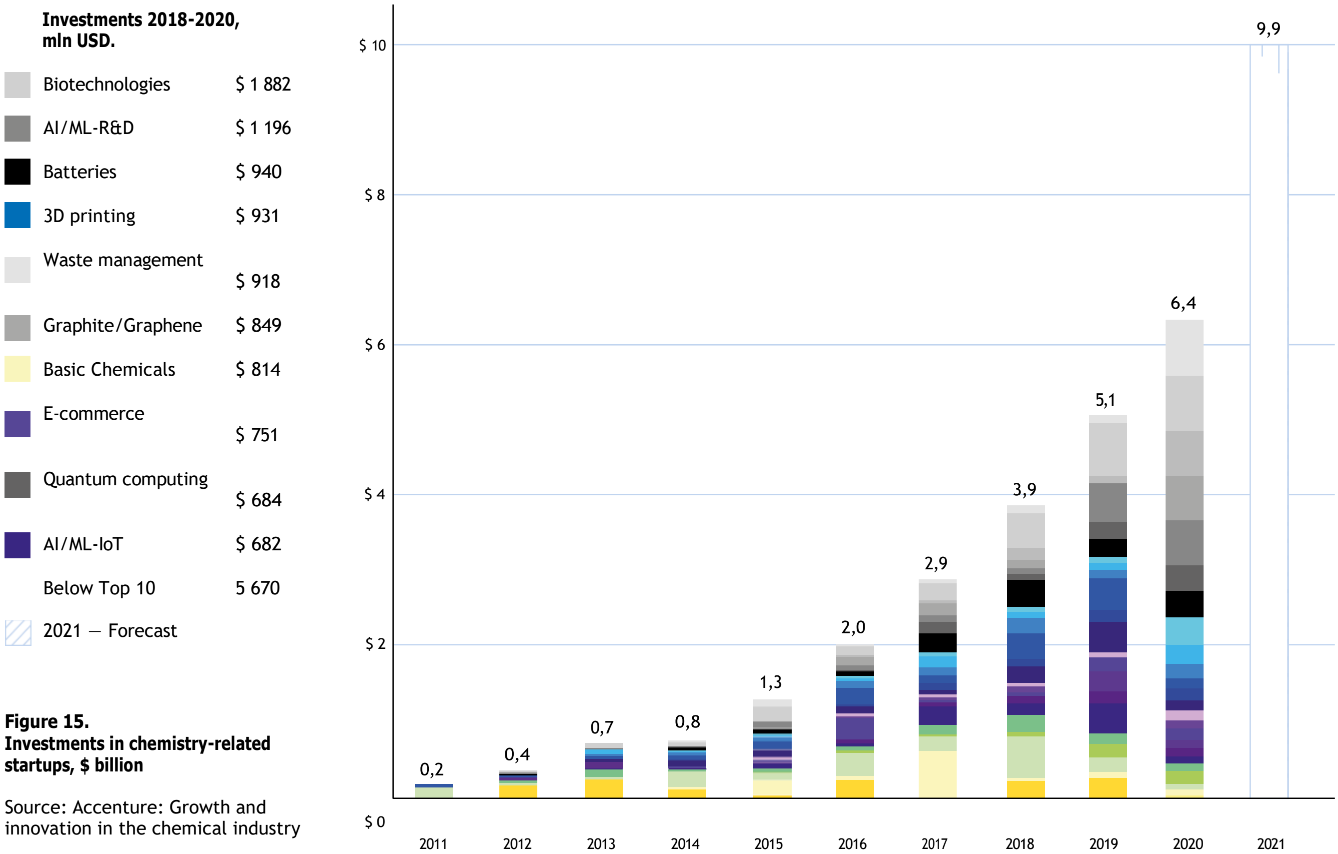


Figure 15.
Investments in chemistry-related startups, $ billion

Source: Accenture: Growth and innovation in the chemical industry

Almost 20% of investments were aimed at digital solutions, such as artificial intelligence or machine learning for molecule discovery, quantum computing for modeling, or work in e-commerce and business-to-business interactions. Start-ups exploring materials that contribute to reducing CO2 emissions and developing a circular economy account for 10% of investments. In 2021, total investment in chemical startups is projected to be in the range of $10 billion, which represents an increase of 54% over 2020[58].

In Russia, the trend of rapid growth of investment in new areas of chemistry has not yet been confirmed. Domestic science has developed a specialization in basic chemicals, including petrochemicals, while the segments that attract the largest volume of investment in the world are specialty chemistry, biotechnology and digital chemical instruments. The class of Russian start-ups in the field of new chemical technologies is still forming, however, there are some examples:

— Prometey RD LLC (batteries) - highly effective platinum containing catalysts for low temperature fuel cells and electrolysers;
— Hitlab LLC (batteries) - fuel cell energy source with chemical hydrogen generator;
— Zdravprint LLC (3D printing) - printing of limb orthoses;
— Chemexsol (e-commerce) - platform for search of contractors in the oil and gas sphere for purchase of chemicals.

58 Growth and innovation in the chemical industry // Accenture. URL: accenture.com/us-en/insights/chemicals/chemical-growth-and-innovation (date of reference: 11.02.2022).

Many startups of Russian origin have emerged, but they are successfully developing in foreign markets:

- Insilico Medicine (biotechnology + artificial intelligence / machine learning in R&D) - drug development using artificial intelligence technologies;
- OCSiAl (graphite/graphene) - production of graphene (single-walled) nanotubes;
- Renca (3D printing) - geopolymer inks for 3D construction printers.

Investments in advanced chemistry start-ups, as well as their capitalization, will grow in the near future. One of the key sources for the emergence of technological start-ups in the world is research laboratories. Funding and transition to new laboratory models can be a factor in the emergence of breakthrough technologies with high commercial potential, which are the basis for the growth of new knowledge-intensive companies.

7 NEW MARKETS BASED ON CHEMICAL INNOVATIONS

The synthesis of worldwide global trends with advanced solutions in chemical R&D has led to emergence of new sectors across the economy. A strong chemistry base coupled with best practices in applying technologies such as artificial intelligence and machine learning can provide a breakthrough in these sectors.

New approaches to R&D in chemistry are drivers of the development of new markets. The considered examples of emerging markets, can be attributed to such sectors as energy, agriculture and food industry, ecology, materials, biotechnology and medicine, etc. (Figure 16). They overlap with each other and have a significant impact on each other. In many ways, they are united by an approach to R&D that is highly integrated with digital technologies. Although in some cases the factors leading to rapid market growth are not primarily related to digital technologies and AI, it is advanced digital solutions that ensure the realization of positive scenarios for markets. For example, in the air transport sector, the UN International Civil Aviation Organization's "Carbon Offset and Reduction Scheme for International Aviation" played a key role for the growth of the biofuel market [59]. However, achieving this goal depends on integrating digital approaches, including AI, into chemical R&D [60].

One of the fastest growing markets for advanced chemistry is the battery and recycling segments, as well as the related area of solar electric power. Demand for new materials on these markets that can be developed using artificial intelligence, together with the trend towards sustainability, opens up the prospect of directing R&D resources to this area. The markets of synthetic biology and personalized medicine are also on the rise and will get an additional impetus to growth due to application of AI. Most growing markets of new chemistry (organic electronics, smart materials, nanopesticides) are based on materials science, which, in its turn, is a key beneficiary of development of predictive capabilities of AI, capabilities to conduct virtual experiments and smart database analysis (description of markets and their connection with the tools of new chemistry are given in Appendix 2).

In general, the markets under consideration have high growth rates compared to traditional and long-established markets, and will become dominant in the future due to digital solutions introduced during the chemical R&D phase, which are fundamental in these fields. Advanced chemistry can guide Russia's transition to promising markets. They are characterized by high growth rates and heavy reliance on R&D. Growing markets have a lot to do with materials science, and research by Russian scientists in this area accounts for a significant share of the country's R&D structure when compared to the research profiles of other countries. Russia can realize its high scientific potential by complementing its research tools with best practices in digital approaches, thus providing access to new fast-growing technology markets.

59 CORSIA Implementation Elements // ICAO. URL: icao.int/environmental-protection/CORSIA/Pages/implementation-elements.aspx (date of reference: 11.02.2022).

60 Barradas A. O., Amorim I. M. Applications of Artificial Neural Networks in Biofuels // Advanced Applications for Artificial Neural Networks. IntechOpen, 2018.

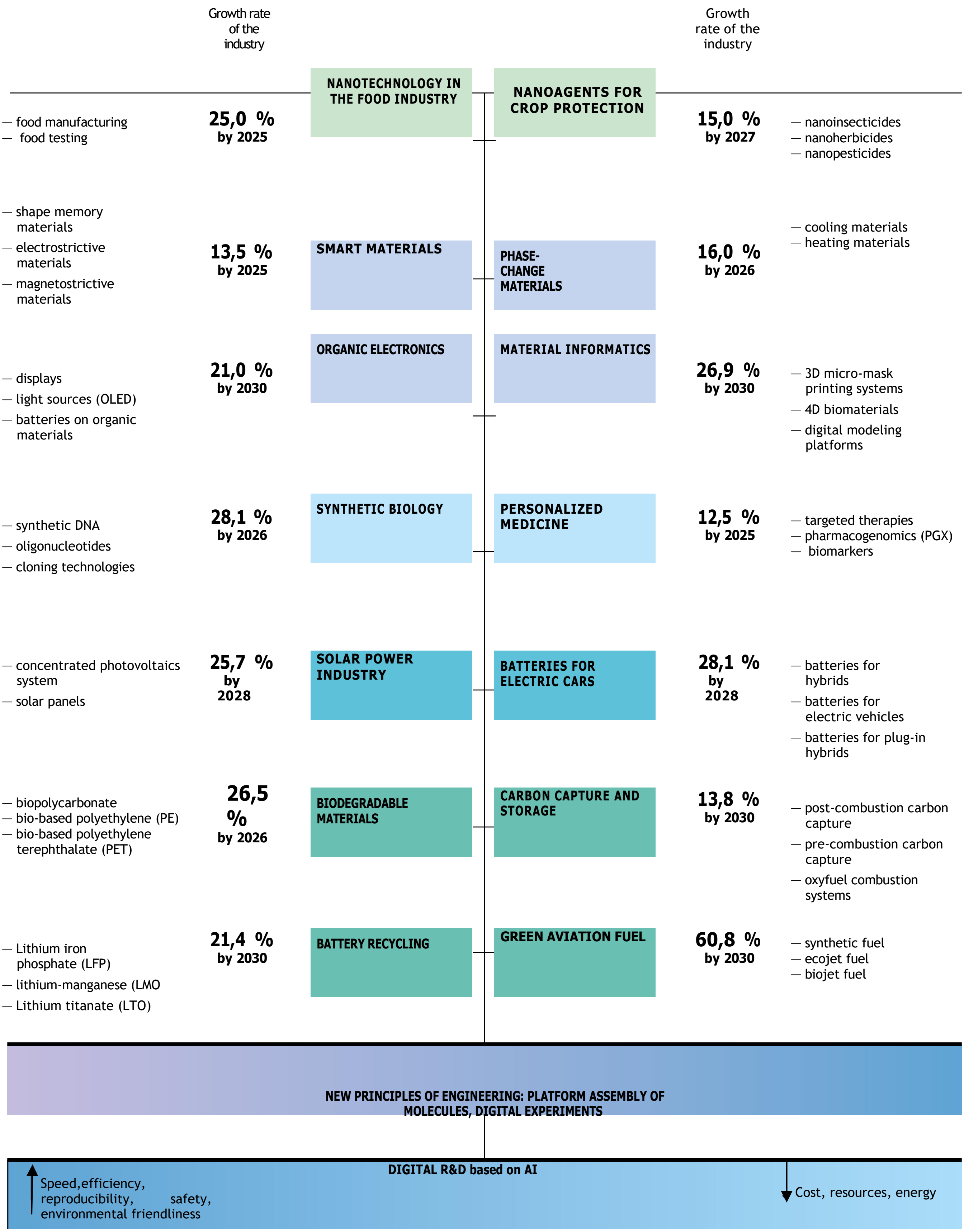


Figure 16
Fast Growing Markets for Advanced Chemicals, 2021

Source: CSR North-West according to open sources

Agriculture and food processing

Materials

Biotechnology and medicine

Energetics

Ecology

8 DEVELOPMENT OF COOPERATION AND SUPPORT

International experience proves that collaboration of the participants of the chemical industry is vital to tackle contemporary challenges. The state can help create conditions for the development of advanced chemistry.

Today's challenges are complex and cannot be overcome alone. To this end, companies in the chemical industry are increasingly interacting with universities, research organizations, consumers and often their competitors by forming collaborations.

Universities have laboratory facilities allowing to conduct advanced R&D. That is why companies, as a rule, face the choice: to create their own laboratories or outsource R&D in universities. In some cases, combinations of these options are possible, including flexible research ecosystems.

Case 3. Examples of Collaborations between Universities and Global Companies in Chemical Research

Aalto University (Finland)

Cooperation with **Nokia** in development and launching of doctoral program in the field of quantum technologies. Funding - 150,000 euro [61].

Collaboration with **Bayer** to develop AI to improve safety and effectiveness of clinical trials of medicines [62].

Cooperation with **Neste**. Joint research programs and financing by the chemical concern [63].

BASF

Global research network of the company on the basis of universities around the world [64]. The map shows the extensive network of the company's university laboratories.

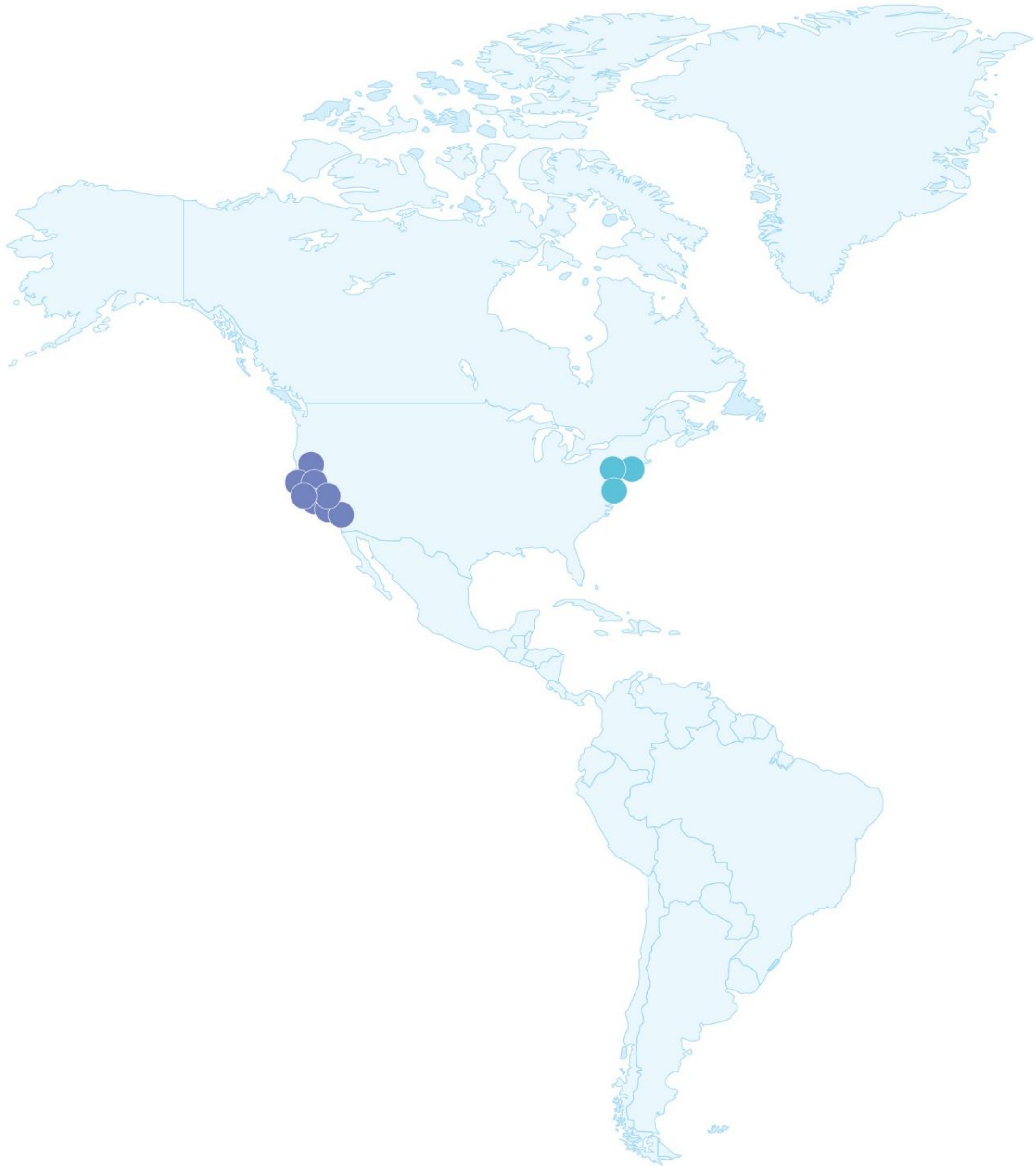
61 Nokia donates seed funding to Aalto University for launching an industrial PhD program on quantum technology // Aalto University. URL: aalto.fi/en/news/nokia-donates-seed-funding-to-aalto-university-for-launching-an-industrial-phd-program-on (date of reference: 11.02.2022).

62 Bayer, Aalto and HUS expand collaboration — artificial intelligence to support clinical drug trials // Aalto University. URL: aalto.fi/en/news/bayer-aalto-and-hus-expand-collaboration-artificial-intelligence-to-support-clinical-drug (date of reference: 11.02.2022).

63 Neste donates 750 000 euros to Aalto University // Aalto University. URL: aalto.fi/en/news/neste-donates-750-000-euros-to-aalto-university (date of reference: 11.02.2022).

64 Innovation // BASF. URL: report.basf.com/2020/en/managements-report/our-strategy/innovation.html (date of reference: 11.02.2022).

Sources: Aalto University official website, BASF, Exxon Mobil, 2020-2022



CARA
California Research Alliance, USA

University of California, Davis

University of California, Berkeley

Stanford University

University of California, Santa Barbara

California Institute of Technology

University of California, Los Angeles

University of Southern California

University of California, Irvine

University of California at River Side

University of California, San Diego

NORA
Northwest Research Alliance, USA

Harvard University

Massachusetts Institute of Technology

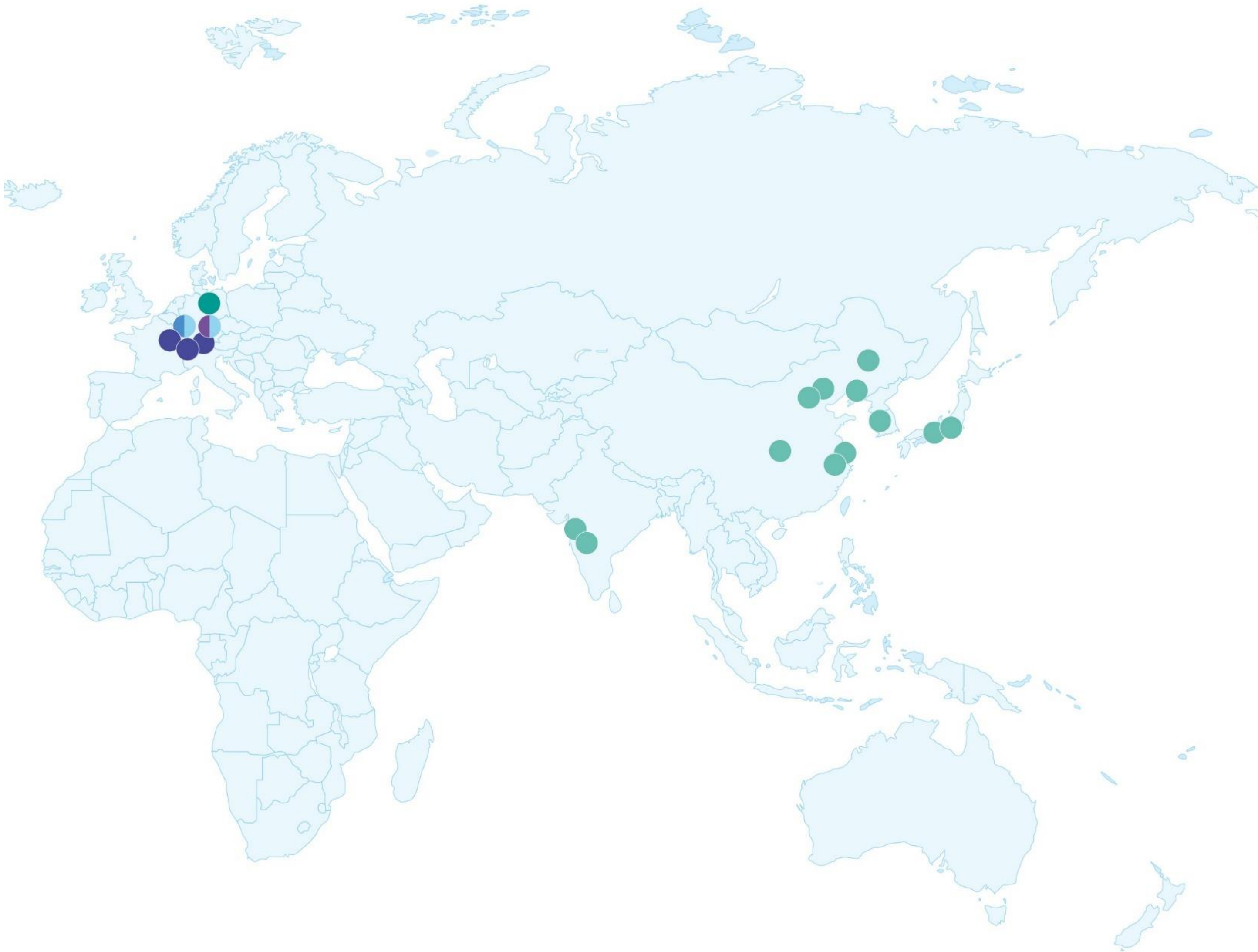
University of Massachusetts

JONAS
Joint Research Network on Advanced Materials and Systems, USA

University of Strasbourg, France

University of Freiburg, Germany

Swiss Federal Institute of Technology Zurich, Switzerland



BasCat
BASF Joint Lab, Germany

Technical University of Berlin

iL
Innovation Lab, Germany

Karlsruhe Institute of Technology

University of Heidelberg

NAO
Network of laboratories conducting open research in Asia

Changchun Institute of Applied Chemistry, China

Tsinghua University, China

Beijing Institute of Technology, China

Sichuan University, China

Zhejiang University, China

Fudan University, China

Tokyo Institute of Technology, Japan

Kyoto University, Japan

Seoul University, South Korea

National Chemical Laboratory, India

Indian Institute of Technology Bombay, India

CaRLa
Catalysis Research Laboratory, Germany

University of Heidelberg

BELLA
Battery and electrochemistry laboratory, Germany

Karlsruhe Institute of Technology

Case 3. Examples of Collaborations between Universities and Global Companies in Chemical Research

Exxon Mobil [65]

MIT
Cooperation in improving the efficiency of conventional energy and the development of new energy technologies.

Princeton University
Collaborative research in sustainable energy and eco-logical solutions.

University of Texas at Austin
Development of sustainable energy technologies.

Georgia Institute of Technology
The collaboration has existed for over 15 years. Developed many innovative technologies, including a new carbon-based molecular sieve membrane.

Stanford University
Organization and financing of a wide range of research programs on topics such as large-scale carbon storage, flow-through battery power storage, efficient hydrogen production, informatics/ machine learning, the fundamentals of high efficiency/low carbon intensity natural gas combustion, life-cycle studies of polymer composites for new building materials, and a new program to study the stability and efficiency limits of perovskite-based solar materials.

Singapore Energy Centre
Development of technologies that improve the efficiency of fuel and chemical production and expand the use of low-carbon hydrogen and stable polymers.

In total, Exxon Mobil cooperates with more than 80 universities worldwide.

65 Collaborating with leading universities to meet global energy demand // ExxonMobil. URL: corporate.exxonmobil.com/Climate-solutions/University-and-National-Labs-partnerships/Collaborating-with-leading-universities-to-meet-global-energy-demand#MassachusettsInstituteofTechnology (date of reference: 11.02.2022).

Sources: Official website of Aalto University, BASF, Exxon Mobil, 2020-2022

Another source of innovation in chemistry, as mentioned above, is interdisciplinary consortia involving science, IT, and industry. Business can generate a large amount of digital data, and science can analyze them, so consortia help to overcome the barriers of lack of data or poor data quality.

Case 4. Examples of advanced chemistry consortia

NFDI4Chem [66]

An open infrastructure consortium for the management of chemistry R&D data through the application of digitalization at all key stages of research. NFDI4Chem focuses on molecular data, experimental and theoretical reactions. TThe consortium consists of the Friedrich Schiller University Jena, the German Chemical Society (GDCh), the German Bunsen Physical Chemistry Society (DBG) and the German Pharmaceutical Society (DPhG), representing around 40,000 members and active partners in the development of data acquisition tools, data management systems and data analysis solutions (GNWI, BASF, ETH, Novartis (Switzerland), Sanofi (France) and more).

Open Reaction Database [67]

An open chemical reaction database community to support machine learning, reaction prediction development, chemical synthesis planning, and experimental design. The steering and advisory committees include representatives from MIT, C-CAS, Merck, Pfizer, SynTech, Google, AstraZeneca, Caltech, etc.

66 Chemistry Consortium in the NFDI // NFDI4Chem. URL: nfdi4chem.de/ (date of reference: 11.02.2022)

67 Welcome to the Open Reaction Database! // Open Reaction Database. URL: docs.open-reaction-database.org/en/latest/ (date of reference: 11.02.2022).

Sources: NFDI4Chem official website, Open Reaction Database

To stimulate the emergence of start-ups, a number of countries support advanced chemistry initiatives at the state level and create special ecosystems for the cultivation of new technological businesses.

Case 5. Examples of incentives for the development of advanced chemistry

UMI Foundation for the Development of New Chemicals and Materials was established to strengthen Japan's technological capabilities[68]. Key areas for investment are new chemistry technologies for targeted therapies and sustainable materials. One of the projects invested is the Citrine software platform, which includes AI and intelligent data management infrastructure for the development and implementation of more efficient and environmentally friendly materials, chemicals, and manufactured goods and allows:

— use off-the-shelf data sets (eliminating additional experiments);
— predict material performance based on processing, composition and synthesis data;
— identify the experiments that need to be performed

68 Universal Materials Incubator // UMI. URL: umi.co.jp/en/ (date of reference: 14.02.2022).

5-HT Digital Hub Chemistry & Health

An initiative (one of 12 digital hubs) has been deployed in Germany, through an established ecosystem that supports companies in the chemical and medical industries in the implementation of digital innovations[69]. The digital platform brings together industry giants, universities and promising startups. In addition to the digital ecosystem, 5-HT Digital Hub Chemistry & Health offers participation in special programs:

— 5-HT X-Linker - presentations by digital chemistry and digital health startups to potential investors;
— 5-HT Digital Qualifier - setting real market challenges for university students from startups and large companies;
— 5-HT Softlanding - supporting foreign startups to enter the German market (with a guide, free office for four weeks);
— Chem-Match - networking event between start-ups and the chemical industry;
— online seminars, etc.

69 5-HT Digital Hub Chemistry & Health // 5-HT. URL: https://www.5-ht.com/en (date of reference: 14.02.2022).

Sources: official website of Universal Materials Incubator, 5-HT Digital Hub Chemistry & Health

In Russia, there is no systematic specialized support for R&D in the field of digital technologies in chemistry. Research in advanced chemistry can be financed by existing scientific foundations and development institutions (Russian Science Foundation, Foundation for Assistance to Innovations, Skolkovo Foundation, etc.) only within the framework of standard support programs.

A positive example is the launch at the end of 2021 of a joint project of the Skolkovo Foundation and Mendeleev accelerator with the support of the Russian Ministry of Industry and Trade and with the expert support of the Russian Chemical Technology University – the contest "Chemistry of Innovation", where the areas of new chemistry: digital modeling, additive technologies, bioinformatics, etc. were identified as the project topics.

Another promising support institution is the INTC "Mendeleev Valley". "This project is aimed at creation of infrastructure ecosystem for cultivation of new technological companies with tax and non-tax deductions.

Taking into account the global trends of growth in the volume of investments into technologies and startups of advanced chemistry, as well as the critical importance of these technologies for ensuring the development of the chemical industry as a whole, especially in those science-intensive sectors where Russia is not a leader, it is advisable to provide conditions at the state level for the creation and development of the market of advanced chemistry. It makes sense to start special programs to support R&D in the field of new chemistry in scientific foundations and development institutes. On the basis of INTC "Mendeleev Valley" a digital platform similar to the 5-HT hub could be deployed, launching programs to support technological start-ups and fast-growing companies of advanced chemistry. The partnerships formed on the platform will help overcome the common challenges of chemical companies and provide a contribution to Russian science.

Conclusion

Development of the industry, and especially of the knowledge-intensive sectors, depends on the technological base formed as a result of R&D. Digital technologies, which had a serious impact on the R&D sector, have led to the emergence of a new chemistry - the science of synthesizing new substances and developing new materials using new digital and sustainable interdisciplinary tools, where artificial intelligence technologies are becoming drivers of development.

AI-driven Labs - the main source of innovation in chemistry in the future - are performing research faster, more efficiently and cheaper than traditional ones. Creating and developing new labs on a model close to the AI-driven Lab will provide critical competitive advantages to universities, research organizations and business companies.

To solve complex scientific problems and generate the data necessary for the development of science, special consortiums should be created that bring together all stakeholders - universities, scientific organizations, and commercial companies of various levels of development and forms of ownership. Such partnerships need state support to form a common ecosystem of advanced chemistry, capable of generating new technologies and businesses.

Considering that the results of chemistry development are reflected in all branches of science and technology, the formation of the advanced chemistry sector is designed to provide significant economic and social benefits. First, advanced chemistry can bridge the gap between R&D and the chemical industry of Russian companies. Second, new business models of chemical R&D will emerge. Third, it can ensure the transition to completely new markets of prospective specialization of Russia as a whole and its subjects in particular

Bibliography

In Russian

1. Act of the Government of the Russian Federation "On measures to attract leading scientists to the Russian educational institutions of higher education, scientific institutions and state scientific centers of the Russian Federation" from 09.04.2010 № 220 // Garant. — 2010 (with amendments and additions in edition from 04.05.2021).
2. Artem Oganov about Russia, Science, God and Artificial Intelligence // Skolkovo. URL: old.sk.ru/news/b/press/archive/2020/09/29/artem-oganov-about-rossii-nauke-boge-i-iskusstvennom-intellekte.aspx (date of reference: 11.02.2022).
3. The Laboratory of New Materials Computational Design opened in Skolkovo // Skolkovo. URL: old.sk.ru/news/b/press/archive/2019/09/09/v-skoltehe-otkrylas-laboratoriya-kompyuternogo-dizayna- novyh-materialov.aspx (date of reference: 11.02.2022).
4. The Air of Unfreedom. What Makes Russian Scientists Go Abroad? // BBC Russian Service. URL: bbc.com/ russian/features-57028917 (date of reference: 11.02.2022).
5. Konstantin Novoselov creates a laboratory of "smart" materials in MIPT // Kommersant. URL: Kommersant.ru/doc/4683651 (date of reference: 11.02.2022).
6. International Scientific Center SCAMT // ITMO University. URL: scamt.ifmo.ru/ru/ (date of reference: 11.02.2022).
7. New Skoltech patent: nanotube anode will improve efficiency of potassium-ion batteries // Skoltech. URL: skoltech.ru/2021/03/novyj-patent-skolteha-anod-iz-nanotrubok-povysit-effektivnost-kalij-ionnyh-akkumulyatorov/ (date of reference: 11.02.2021).
8. Structure of a new type of material is determined // Scientific Russia. URL: scientificrussia.ru/articles/opredeleno-stroenie-novoj-struktury (date of reference: 11.02.2022).
9. «Пролить свет» под правильным углом // Коммерсантъ. URL: kommersant.ru/doc/4540238 (date of reference: 11.02.2022).
10. Work, personnel search and publication of vacancies // HeadHunter. URL: hh.ru/ (date of reference: 11.02.2022).
11. SIBUR Digital // SIBUR. URL: sibur.digital/ (the date of reference: 11.02.2022).
12. Scientists have created a universal base substance for a wide range of sensors // RIA Novosti. URL: ria.ru/20211018/ sfu-1754972217.html (date of reference: 11.02.2022).
13. Scientists of ITMO University have developed a way to create elements of plasmonics // RSCF. URL: rscf.ru/news/presidential-program/sposob-sozdaniya-elementov-plazmoniki/ (date of reference: 11.02.2022).
14. Physicists from Krasnoyarsk are in the top of best scientific reviewers of the world // Our Krasnoyarsk krai. URL: gnkk.ru/ news/fiziki-iz-krasnoyarska-voshli-v- top-luchsh/?utm_source=yxnews&utm_medium=desktop&utm_referrer=https%3A%2F%2Fyandex.ru%2Fnews%2Fsearch%3Ftext%3D ((date of reference: 11.02.2022).
15. This is a breakthrough: ten most important technologies of 2021 // RBC. URL: trends.rbc.ru/trends/innovation/606ecf18 9a79470e6428 5ce2 (date of reference: 11.02.2022).

In English

Scientific articles

16. Artemii S. Ivanov, Konstantin G. Nikolaev, Alexander S. Novikov, Stanislav O. Yurchenko, Kostya S. Novoselov, Daria V. Andreeva, and Ekaterina V. Skorb. The Journal of Physical Chemistry Letters 2021 12 (7). 2017-2022. DOI: 10.1021/acs.jpclett.1c00007
17. Artemii S. Ivanov, Konstantin G. Nikolaev, Anna A. Stekolshchikova, Weini T. Tesfatsion, Stanislav O. Yurchenko, Kostya S. Novoselov, Daria V. Andreeva, Maya Yu. Rubtsova, Mikhail F. Vorovitch, Aydar A. Ishmukhametov, Alex M. Egorov, and Ekaterina V. Skorb ACS Applied Bio Materials 2020 3 (11), DOI: 10.1021/acsabm.0c00954.
18. Barradas A. O., Amorim I. M. Applications of Artificial Neural Networks in Biofuels // Advanced Applications for Artificial Neural Networks. — Риека: IntechOpen, 2018.
19. Burger B., Maffettone P. M., Gusev V. V. et al. A mobile robotic chemist // Nature. — 2020. — № 583.
20. Churchman C. West Wicked Problems // Management Science. — 1967. — №14 (4). — С. 141-142.
21. Duncan Timothy V. Applications of nanotechnology in food packaging and food safety: Barrier materials, antimicrobials and sensors // Journal of Colloid and Interface Science. — 2011. — № 363 (1).
22. Egorova K., Galushko A., Dzhemileva L., D'yakonov, V., Ananikov V. Building bio-Profiles for common catalytic reactions // Green Chem. — 2021. — № 23.
23. Esfahani M., Sadegh Aghapour A., Zoheir D., Mostafa Dadashi F., Ahmad R., Joyner E., Isabel C. E., Mojtaba A., Lauren F. G., Amirsalar R. E., Anwar S., Negin K. Nanocomposite membranes for water separation and purification: Fabrication, modification, and applications // Separation and Purification Technology. — 2019. — № 213.
24. Fantke P., Cinquemani C., Yaseneva P., De Mello J., Schwabe H., Ebeling B., Lapkin A. Transition to sustainable chemistry through digitalization // Chem. — 2021. — № 7 (11).
25. Ganesh K., Deqing Z., Scott J.M., Rossen K., Chirik P., Kozlowski M., Zimmerman J., Brooks B., Savage P., Allen D., Voutchkova-Kostal A. Green Chemistry: A Framework for a Sustainable Future // Organometallics. — 2021. — № 40 (12).
26. Graham N., Lee R. J., Darren A. W., Bing Joe H., Hongxian H. Sustainability of Battery Technologies: Today and Tomorrow // ACS Sustainable Chemistry & Engineering. — 2021. — № 9 (19).
27. Joshi R. P., Kumar N. Artificial Intelligence for Autonomous Molecular Design: A Perspective // Molecules. — 2021. — № 26 (22)
28. Levin K., Cashore B., Bernstein S. et al. Overcoming the tragedy of super wicked problems: constraining our future selves to ameliorate global climate change // Policy Sci. — 2012. — № 45. — С. 123-152.
29. Lifset R. 3D Printing and Industrial Ecology // Journal of Industrial Ecology. — 2017. — №21 (S1)
30. MacLeod B. P., Parlane F. G. L., Morrissey T. D., Häse F., Roch L. M., Dettelbach K. E., Moreira R., et al. Self-driving laboratory for accelerated discovery of thin-film materials // Science Advances. — 2020. — №6 (20).
31. Nikolay V. Ryzhkov, Konstantin G. Nikolaev, Artemii S. Ivanov, and Ekaterina V. Skorb (2021) Infochemistry and the Future of Chemical Information Processing Annual Review of Chemical And Biomolecular Engineering, Vol. 12:63-95. DOI: doi.org/10.1146/annurev-chembioeng-122120-023514
32. Nowak G., Fic G. Machine Learning Approach to Discovering Cascade Reaction Patterns. Application to Reaction Pathways Prediction // Journal of Chemical Information and Modeling. — 2009. — № 49 (6).
33. Ong M. Y., Nomanbhay S., Kusumo F., Raja Shahruzzaman R. M. H., Shamsuddin A. H. Modeling and Optimization of Microwave-Based Bio-Jet Fuel from Coconut Oil: Investigation of Response Surface Methodology (RSM) and Artificial Neural Network Methodology (ANN) // Energies. — 2021. — № 14 (2).
34. Orbay K., Miranda R., Orbay M. INVITED ARTICLE: Building Journal Impact Factor Quartile into the Assessment of Academic Performance: A Case Study // Participatory Educational Research. — 2020. — № 7 (2).
35. P. R. Yaashikaa, P. Senthil Kumar, A. Saravanan, Dai-Viet N. Vo. Advances in biosorbents for removal of environmental pollutants: A review on pretreatment, removal mechanism and future outlook // Journal of Hazardous Materials. — 2021. — № 420.

36. Putra R., Maulana A., Saputro A. Study on building machine learning model to predict biodegradable-ready materials // AIP Conference Proceedings. — 2019. —№ 2088 (1).

37. Romashov L. V. et al. Atom-economic Approach to the Synthesis of α-(Hetero) aryl-substituted Furan Derivatives from Biomass // Chemistry — An Asian Journal. — 2022. — № 17 (1).

38. Sang-Won P., Andrew D. D., Nilesh R. D., Youngseon S., Hyung J. K., YounJoon J. Computer Simulation Study of Graphene Oxide Supercapacitors: Charge Screening Mechanism // The Journal of Physical Chemistry Letters. — 2016. — №7 (7).

39. Sha W., Guo Y., Yuan Q., Tang S., Zhang X., Lu S., Guo X., Cao Y., Cheng S. Artificial Intelligence to Power the Future of Materials Science and Engineering // Advanced Intelligent Systems. — 2020. — № 2 (4)

40. Shekhar S., Sharma S., Kumar A., Taneja A., Sharma B. The framework of nanopesticides: a paradigm in biodiversity // Material Advances. — 2021. — № 2 (20).

41. Smith M. J., Weinberger C., Bruna E. M., Allesina S. The Scientific Impact of Nations: Journal Placement and Citation Performances // PLoS ONE. — 2014. —№ 9 (10)

42. Thakur A., Mishra A. P., Panda B., Rodríguez D. C. S., Gaurav I., Majhi B. Application of Artificial Intelligence in Pharmaceutical and Biomedical Studies // Curr Pharm Des.. — 2020. — № 26 (29).

43. Tietze T., Szulc P., Smykowski D., Sitka A., Redzicki R. Application of Phase Change Material and Artificial Neural Networks for Smoothing of Heat Flux Fluctuations // Energies. — 2021. — № 14 (12).

44. Vasylenko A., Gamon J., Duff B. B. Element selection for crystalline inorganic solid discovery guided by unsupervised machine learning of experimentally explored chemistry // Nature Communications. — 2021. — № 12

45. Wang L., Kruk S., Koshelev K., Kravchenko I., Luther-Davies B., Kivshar Y. Nonlinear Wavefront Control with All-Dielectric Metasurfaces // Nano Letters. — 2018. —№ 18 (6).

46. Wenhong Y., Timothy T. F., Wen-Hua S. Machine Learning in Catalysis, From Proposal to Practicing // ACS Omega. — 2020. — №5 (1).

47. Xiaofeng J., Conghui L., Tailin X., Lei S., Xueji Z. Artificial intelligence biosensors: Challenges and prospects // Biosensors and Bioelectronics. — 2020. — № 165

48. Zimmerman J., Anastas P., Erythropel H., Leitner W. Designing for a green chemistry future // Science. — 2020. — № 367 (6476).

Internet sources

49. 5-HT Digital Hub Chemistry & Health // 5-HT. URL: https://www.5-ht.com/en (date of reference: 14.02.2022).

50. ABOUT THE MODEL: Chemical Leasing at Glance // Chemical leasing. URL: chemicalleasing.com/chemicalleasing-at- glance/ (date of reference: 11.02.2022).

51. AI & Blockchain: Chemical industry insights and actions // Accenture. URL: accenture. com/us-en/insights/chemicals/ai-blockchain-chemical-industry (date of reference: 11.02.2022).

52. AI Is Throwing Battery Development Into Overdrive // Wired. URL: wired.com/story/ ai-is-throwing-battery-development-into- overdrive/ (date of reference: 11.02.2022).

53. Artem Abakumov // Skoltech. URL: faculty. skoltech.ru/people/artemabakumov (date of reference: 11.02.2022).

54. Artificial Intelligence: A Game Changer for the Chemical Manufacturing Industry // NC State University. URL: cnr.ncsu.edu/news/2020/03/artificial-intelligence-chemical-industry/ (date of reference: 11.02.2022).

55. At 25.7% CAGR, Solar Panels Market Size Expected to Reach USD 902.55 Bn, Globally by 2028, says Brandessence Market Research // PR Newswire. URL: prnewswire. com/news-releases/at-25-7-cagr-solar- panels-market-size-expected-to-reach-usd-902-55-bn-globally-by-2028-says-brandessence-market-research-301460328.html (date of reference: 11.02.2022).

56. At 28.1% CAGR, EV Battery Market Size is Projected to Grow from USD 27.30 Billion in 2021 to USD 154.90 Billion in 2028 // Globe Newswire. URL: globenewswire.com/news-release/2021/10/27/2321353/0/en/At-28-1-CAGR-EV-Battery-Market-Size-is-Projected-to-Grow-from-USD-27-30-Billion-in-2021-to-USD-154-90-Billion-in-2028.html (date of reference: 11.02.2022).

57. Average R&D cost to develop a pharmaceutical compound from discovery to launch from 2010 to 2020, by study cohort // Statista. URL: statista.com/statistics/825727/ randd-cost-for-new-pharma-compounds-by-cohort/ (date of reference: 11.02.2022).

58. Bayer, Aalto and HUS expand collaboration — artificial intelligence to support clinical drug trials // Aalto University. URL: aalto. fi/en/news/bayer-aalto-and-hus-expand-collaboration-artificial-intelligence-to-support-clinical-drug (date of reference: 11.02.2022).

59. BP Energy Outlook 2018 edition // BP. URL: bp.com/content/dam/bp/business-sites/en/global/corporate/pdfs/energy-economics/energy-outlook/bp-energy-outlook-2018.pdf?_x_tr_sl=en&_x_tr_tl=ru&_x_tr_hl=ru&_x_tr_pto=sc (date of reference: 11.02.2022).

60. Building the Best Battery // QuantumScape. URL: quantumscape.com/ (date of reference: 11.02.2022).

61. C&EN's 2021 10 Start-Ups to Watch // C&EN. URL: cen.acs.org/business/start-ups/CENs-2021-10-Start-Ups-to-Watch-cleantech/99/i42?utm_source=mostread&utm_medium=mostread&utm_campaign=CEN (date of reference: 11.02.2022).

62. C&EN's Global Top 50 chemical firms for 2021 // C&EN. URL: cen.acs.org/business/ finance/CENs-Global-Top-50-2021/99/i27 (date of reference): 11.02.2022).

63. Carbon Capture, Utilization, and Storage (CCUS) Market 2022 // Allied Market Research. URL: alliedmarketresearch. com/carbon-capture-and-utilization-market-A12116 (date of reference: 11.02.2022).

64. Chemical (Re)action: Growth in a circular economy // Accenture. URL: accenture. com/us-en/insights/chemicals/chemical-reaction-circular-economy (date of reference: 11.02.2022).

65. Chemical Industry — Surviving or Thriving in the Next Normal? // CHEManager. URL: chemanager-online.com/en/news/chemical-industry-surviving-or-thriving-next-normal (date of reference: 11.02.2022).

66. Chemical Industry Vision 2030: A European Perspective // AT Kearney. URL: kearney. com/chemicals/article?/a/chemical-industry-vision-2030-a-european-perspective (date of reference: 11.02.2022).

67. Chemistry Consortium in the NFDI // NFDI4Chem. URL: nfdi4chem.de/ (date of reference: 11.02.2022).

68. Circular Economy // INEOS. URL: ineos.com/sustainability/circular-economy/ (date of reference: 11.02.2022).

69. Circular Economy // LG Chem. URL: lgchem. com/sustainability/esh-management/strategy/circular-economy (date of reference: 11.02.2022).

70. Circular Economy at BASF // BASF. URL: basf.com/global/en/who-we-are/ sustainability/we-drive-sustainable- solutions/circular-economy.html (date of reference 11.02.2022).

71. Citrine Informatics // Citrine. URL: citrine. io/ (date of reference: 11.02.2022).

72. Collaborating with leading universities to meet global energy demand // ExxonMobil. URL: corporate.exxonmobil.com/Climate-solutions/University-and-National-Labs-partnerships/Collaborating-with-leading-universities-to-meet-global-energy-demand#MassachusettsInstituteofTechnology (date of reference: 11.02.2022).

73. Companies // European Startups. URL: app.europeanstartups.co/companies (date of reference: 11.02.2022).

74. Computer system predicts products of chemical reactions // MIT News. URL: news. mit.edu/2017/computer-system-predicts- products-chemical-reactions-0627 (date of reference: 13.02.2022).

75. CORSIA Implementation Elements // ICAO. URL: icao.int/environmental-protection/CORSIA/Pages/implementation-elements.aspx (date of reference: 11.02.2022).

76. COVID-19 is challenging the way we think of chemical industry trends. This is how // World Economic Forum. URL: weforum.org/agenda/2021/03/chemical-industry-trends-forecasting-resilience/ (data of reference: 11.02.2022).

77. Digitalization // BASF. URL: basf.com/global/en/who-we-are/digitalization.html (date of reference: 11.02.2022).

78. Disruptive forces in the industrial sectors Global executive survey // McKinsey & Company. URL: mckinsey.com/~/media/mckinsey/industries/automotive%20and%20assembly/our%20insights/how%20industrial%20companies%20can%20respond%20to%20disruptive%20forces/disruptive-forces-in-the-industrial-sectors.ashx (date of reference: 11.02.2022).

79. ETC/WMGE Report 2/2021: Business Models in a Circular Economy // Eionet Portal. URL: eionet.europa.eu/etcs/etc-wmge/products/etc-wmge-reports/business-models-in-a-circular-economy (date of reference: 11.02.2022).

80. Food Nanotechnology Market to record a CAGR of 25.32% by 2025 // PR Newswire. URL: prnewswire.com/news-releases/food-nanotechnology-market-to-record-a-cagr-of-25-32-by-2025-technavio-301474651.html (date of reference: 11.02.2022).

81. Genesis Therapeutics Secures $52M Series A to Further Accelerate AI Innovation and to Launch Drug Discovery & Development Pipeline // Businesswire. URL: https://www.businesswire.com/news/home/20201202005297/en/Genesis-Therapeutics-Secures-52M-Series-A-to-Further-Accelerate-AI-Innovation-and-to-Launch-Drug-Discovery-Development-Pipeline (date of reference: 15.01.2022).

82. Global Bio-Based Materials Market Size Is Expected To Reach About USD 87 Billion by 2026, at a CAGR of 26.5%: Facts & Factors // Globe Newswire. URL: globenewswire.com/news-release/2021/12/17/2354362/0/en/Global-Bio-Based-Materials-Market-Size-Is-Expected-To-Reach-About-USD-87-Billion-by-2026-at-a-CAGR-of-26-5-Facts-Factors.html (date of reference: 11.02.2022).

83. Global Synthetic Biology Market Report 2021: Market to Reach $28.8 Billion by 2026 — Oligonucleotides & Synthetic DNA is Projected to Account for $16.1 Billion // Globe Newswire. URL: globenewswire.com/news-release/2022/01/21/2370810/28124/en/Global-Synthetic-Biology-Market-Report-2021-Market-to-Reach-28-8-Billion-by-2026-Oligonucleotides-Synthetic-DNA-is-Projected-to-Account-for-16-1-Billion.html (date of reference: 11.02.2022).

84. GREEN AND SUSTAINABLE CHEMISTRY: FRAMEWORK MANUAL // UNEP. URL: wedocs.unep.org/handle/20.500.11822/34338 (date of reference: 11.02.2022).

85. Growth and innovation in the chemical industry // Accenture. URL: accenture.com/us-en/insights/chemicals/chemical-growth-and-innovation (date of reference: 11.02.2022).

86. Guided by AI, robotic platform automates molecule manufacture // MIT News. URL: news.mit.edu/2019/automate-molecule-production-ai-0808 (date of reference: 13.02.2022).

87. How Big Tech got so big: Hundreds of acquisitions // The Washington Post. URL: washingtonpost.com/technology/interactive/2021/amazon-apple-facebook-google-acquisitions/ (date of reference: 11.02.2022).

88. How Quantum Computing can benefit chemistry // Covestro. URL: covestro.com/press/how-quantum-computing-can-benefit-chemistry/ (date of reference: 11.02.2022).

89. If you're into efficiency, COMPLEASE™ is for you // SAFECHEM. URL: safechem.com/en/ metal-cleaning/complease (date of reference: 11.02.2022).

90. Industry 5.0 // European Commission. URL: ec.europa.eu/info/research-and-innovation/research-area/industrial-research-and-innovation/industry-50_en (date of reference: 11.02.2022).

91. Innovation // BASF. URL: report.basf.com/2020/en/managements-report/our-strategy/innovation.html (date of reference: 11.02.2022).

92. Innovation in chemicals // Deloitte. URL: www2.deloitte.com/us/en/insights/industry/oil-and-gas/chemical-innovation.html (date of reference: 11.02.2022).

93. Let's drive sustainable chemistry together // SusChem. URL: suschem.org/ (date of reference: 11.02.2022).

94. Lithium-ion Battery Recycling Market to rise at CAGR of 21.43 % through 2030 — Report by Market Research Future (MRFR) // Globe Newswire. URL: globenewswire.com/news-release/2021/12/06/2346181/0/en/Lithium-ion-Battery-Recycling-Market-to-rise-at-CAGR-of-21-43-through-2030-Report-by-Market-Research-Future-MRFR.html (date of reference: 11.02.2022).

95. Machine-learning Atomistic Modeling of Corrosion Postdoctoral Researcher // C&EN. URL: chemistryjobs.acs.org/job/36059/machine-learning-atomistic-modeling-of-corrosion-postdoctoral-researcher/ (date of reference: 11.02.2022).

96. Making Smart Materials Smarter With Multiphysics Simulation // Digital Engineering 247. URL: digitalengineering247. com/article/making-smart-materials- smarter-multiphysics-simulation/ (date of reference: 11.02.2022).

97. Market share of chemical industry's sales worldwide from 2009 to 2020, by region // Statista. URL: statista.com/statistics/263136/global-market-share-in-the-chemical-industry-by-region/ (date of reference: 11.02.2022).

98. Master's student or intern: Artificial Intelligence in Chemistry and Material Science // IBM Research Europe. URL: zurich.ibm.com/careers/2021_009.html (date of reference: 11.02.2022).

99. Material Informatics Market Size to Surpass US$ 782.2 Mn by 2030 // GlobeNewswire. URL: globenewswire.com/en/news-release/2022/01/24/2372050/0/en/Material-Informatics-Market-Size-to-Surpass-US-782-2-Mn-by-2030.html (date of reference: 11.02.2022).

100. Nanopesticide Market By Type (Insecticides, Herbicides, Fungicides, Others), By Application (Production, Protection, Harvesting, Packaging, Others)- Growth, Share, Opportunities & Competitive Analysis, 2019-2027 // Credence Research. URL: credenceresearch.com/report/nanopesticide-market (date of reference: 11.02.2022).

101. Neste donates 750 000 euros to Aalto University // Aalto University. URL: aalto.fi/en/news/neste-donates-750-000-euros-to-aalto-university (date of reference: 11.02.2022).

102. New AI tool developed by University of Liverpool researchers accelerates discovery of truly new materials // EurekAlert. URL: eurekalert.org/news-releases/929009 (date of reference: 11.02.2022).

103. Nokia donates seed funding to Aalto University for launching an industrial PhD program on quantum technology // Aalto University. URL: aalto.fi/en/news/nokia-donates-seed-funding-to-aalto-university-for-launching-an-industrial-phd-program-on (date of reference: 11.02.2022).

104. Oganov, Artem R. // Scopus. URL: scopus.com/authid/detail.uri?authorId=6701334785 (date of reference: 11.02.2022).

105. On the look for new renewable raw materials // Nokian Tyres. URL: nokiantyres.com/company/sustainability/products/tires-and-renewable-raw-materials-/ (date of reference: 11.02.2022).

106. Optimizing the chemicals value chain with AI // IBM. URL: ibm.com/downloads/cas/Y4ZD7MVD (date of reference: 11.02.2022).

107. Organic Electronic Market 2022 // Allied Market Research. URL: alliedmarketresearch.com/printed-organic-and-flexible-electronics-market (date of reference: 11.02.2022).

108. Pande Lab at Stanford University // Medium. URL: medium.com/@pandelab (date of reference: 13.02.2022).

109. Pande Lab at Stanford University // Pande Lab. URL: pandelab.org/about#bio (date of reference: 13.02.2022).

110. pandegroup // GitHub. URL: github.com/pandegroup (date of reference: 13.02.2022).

111. Personalized medicine // National Cancer Institute. URL: cancer.gov/publications/dictionaries/cancer-terms/def/personalized-medicine (date of reference: 11.02.2022).

112. Phase Change Material Market by type (Inorganic, Organic), Application (Building & Construction, HVAC, Cold Chain & Packaging, Electronics, Textile) and Region (North America, Europe, APAC,Rest of World) — Global Forecasts to 2026 // MarketsandMarkets. URL:marketsandmarkets.com/Market-Reports/advanced-phase-change-material-pcm- market-1087.html (date of reference: 11.02.2022).

113. PhD or post-doctoral researcher: Organic Chemistry for Autonomous Lab Development and Operation // IBM Research Europe.URL: zurich.ibm.com/careers/2021_054. html (date of reference: 11.02.2022).

114. Precision Medicine Market Size Worth USD 26.14 Billion by 2025 at 12.48% CAGR — Report by Market Research Future (MRFR) // Globe Newswire. URL: globenewswire.com/ en/news-release/2021/07/12/2261393/0/ en/Precision-Medicine-Market-Size-Worth- USD-126-14-Billion-by-2025-at-12-48-CAGR-Report-by-Market-Research-Future-MRFR. html (date of reference: 11.02.2022).

115. Principal Investigators in Machine Learning in Biomedicine (f/m/x) // New Scientist Jobs. URL: jobs.newscientist.com/en-gb/job/1401737580/principal-investigators-in-machine-learning-in-biomedicine-f-m-x-/ (date of reference: 11.02.2022).

116. Publications // Zeng Laboratory. URL: zenggroup.org/publications/ (date of reference: 13.02.2022).

117. RoboRXN: Automating Chemical Synthesis // IBM. URL: ibm.com/blogs/ research/2020/08/roborxn-automating- chemical-synthesis/ (date of reference: 11.02.2022).

118. Science Horizons Leading-edge science for sustainable prosperity over the next 10-15 years // Royal Society of Chemistry. URL: rsc.org/globalassets/04-campaigning-outreach/campaigning/science-horizons/ science-horizons-report.pdf (date of reference: 11.02.2022).

119. Scientists make digital breakthrough in chemistry that could revolutionize the drug industry // CNBC. URL: https://www.cnbc.com/2020/10/24/how-a- digital-breakthrough-could-revolutionize- drug-industry.html (date of reference: 15.01.2022).

120. SciVal // SciVal. URL: scival.com/landing (date of reference: 11.02.2022).

121. Scopus // Scopus. URL: scopus.com/ (date of reference: 11.02.2022).

122. Smart Material Market Worth $98.2 Billion By 2025 | CAGR: 13.5% // Grand View Research. URL: grandviewresearch.com/ press-release/global-smart-materials- market (date of reference: 11.02.2022).

123. State and Trends of Carbon Pricing 2020 // World Bank. URL: openknowledge. worldbank.org/bitstream/han dle/10986/33809/9781464815867.pdf (date of reference: 11.02.2022).

124. Sustainable and circular business models for the chemical industry // Sitra. URL: media. sitra.fi/2020/05/28111719/sustainable-and-circular-business-models-for-the-chemical-industry.pdf (date of reference: 11.02.2022).

125. Sustainable Aviation Fuel Market by Fuel Type (Biofuel, Hydrogen Fuel, Power to Liquid Fuel, Gas to Liquid), Biofuel Manufacturing Technology (FT-SPK, HEFA-SPK, ATJ-SPK, HFS-SIP, CHJ), Biofuel Blending Capacity, Platform, Region - Global Forecast to 2030 // MarketsandMarkets. URL: marketsandmarkets.com/Market-Reports/sustainable-aviation-fuel-market-70301163.html (date of reference: 11.02.2022).

126. Technology // Twist Bioscience. URL: twistbioscience.com/technology (date of reference: 11.02.2022).

127. The evolution of digital R&D in chemicals // Accenture. URL: accenture.com/_acnmedia/ PDF-158/Accenture-Digital-Research-And-Development-Chemicals.pdf (date of reference: 11.02.2022).

128. The Future of Petrochemicals Towards more sustainable plastics and fertilisers // INTERNATIONAL ENERGY AGENCY. URL: iea. blob.core.windows.net/assets/bee4ef3a-8876-4566-98cf-7a130c013805/The_Future_of_Petrochemicals.pdf?_x_tr_sl=en&_x_tr_tl=ru&_x_tr_hl=ru&_x_tr_pto=sc (date of reference: 11.02.2022).

129. The future of work in chemicals // Deloitte. URL: www2.deloitte.com/content/dam/Deloitte/us/Documents/energy-resources/us-the-future-of-work-in-chemicals-pov.pdf (date of reference: 11.02.2022).

130. The Matter Lab // University of Toronto. URL: matter.toronto.edu/ (date of reference: 11.02.2022).

131. THE MOST VALUABLE MATCH // Excess Materials Exchange. URL: excessmaterialsexchange.com/en_us/ (date of reference: 11.02.2022).

132. The State of Industrial Digital Transformation // ptc. URL: ptc.com/ en/resources/iiot/white-paper/state- of-industrial-digital-transformation (date of reference: 11.02.2022).

133. These Countries Have Banned Animal Testing (2021) // Cruelty Free Soul. URL: crueltyfreesoul.com/animal-testing-banned-countries/ (date of reference: 11.02.2022).

134. Topic Prominence in Science // Elsevier. URL: elsevier.com/solutions/scival/features/topic-prominence-in-science (date of reference: 11.02.2022).

135. TRUCIRCLE™ portfolio and services // SABIC. URL: sabic.com/en/sustainability/circular-economy/trucircle-portfolio-and-services (date of reference: 11.02.2022).

136. U.S. Department of Energy Publishes New Energy Savings Forecast for Solid-State Lighting // Office of Energy Efficiency & Renewable Energy. URL: energy.gov/eere/ssl/articles/us-department-energy-publishes-new-energy-savings-forecast-solid-state-lighting (date of reference: 11.02.2022).

137. Universal Materials Incubator // UMI. URL: umi.co.jp/en/ (date of reference: 14.02.2022).

138. Welcome to the Open Reaction Database! // Open Reaction Database. URL: docs. open-reaction-database.org/en/latest/ (date of reference: 11.02.2022).

139. What We Do // Zymergen. URL: zymergen. com/what-we-do/ (date of reference: 11.02.2022).

140. Why refinery-petrochemical integration is the downstream trend to watch // Wood Mackenzie. URL: woodmac.com/news/opinion/why-refinery-petrochemical-integration-is-the-downstream-trend-to-watch/ (date of reference: 11.02.2022).

141. Why the future of oil is in chemicals, not fuels // C&EN. URL: cen.acs.org/business/petrochemicals/future-oil-chemicals-fuels/97/i8 (date of reference: 11.02.2022).

142. Zhoushan Green Petrochemical Base // NS Energy. URL: nsenergybusiness.com/projects/zhoushan-green-petrochemical-base/ (date of reference: 11.02.2022).

Appendix 1

Examples of global startups attracting leading investors

№	Company name	Public launch	Funding		Project focus
			Mln USD, USA	Investors	
Medicine					
1	Strike Pharma (strikepharma.com, Sweden)	2021	1,2	Almi Invest	Development of a new class **of toxins immunoconjugates** for a breakthrough in the treatment of cancer
2	Celeris Therapeutics (celeristx.com, Austria)	2021	1	Longevitytech.fund, R42 Group, APEX Ventures	Platform for predicting and designing molecular components, automating downstream chemical and biological problems. The platform Combines: **molecular design, automated synthesis and biological validation of results**
3	Rome Therapeutics (rometx.com, Cambridge, MA,USA)	2020	130	GV, Arch Venture Partners, Partners Innovation Fund, Section 32, etc.	Development of novel therapies cancer and autoimmune diseases using the ability to **repitome (repetitive genome sequences)**. The company has created platform for data analysis, which identifies diseases, builds prognosis, and predicts response to treatment
4	KOJIN THERAPEUTICS (kojintx.com, Cambridge, MA, USA)	2020	30	Polaris Partners, Newpath Partners и Cathay Health	Biopharmaceutical company developing **novel targeted therapeutic drugs based on cell states and ferroptosis biology**
5	EIKON THERAPEUTICS	2019	684	Column Group, Foresite Capital, Innovation Endeavors и Lux Capital	A biopharmaceutical company, using revolutionary technology **for imaging single molecules** at the intersection of chemistry, engineering and biology, to find new ways to treat dangerous diseases. The Eikon discovery platform is based on the revolutionary innovations of its founders (Nobel Prize, 2014)
6	ATAI Life Sciences AG (atai.life, Germany)	2018	384	Alpha Wave Global, Apeiron Investment Group, Pura Vida Investments, Thiel Capital, Subversive Capital, Fearless Ventures, Catalio Capital Management, Woodline Partners, Highline Capital Management, Neo Kuma Ventures	Development of innovative medicines for personalized psychological and psychiatric medicine, in particular The use of **intranasal filler technology based on solgel,** which can create new drugs with unique and optimized ways of delivery of various active ingredients
7	MOBILion SYSTEMS (mobilionsystems.com, Philadelphia, USA)	2015	115	D1 Capital Partners, aMoon, Agilent Technologies, IP Group, Hostplus, Cultivation Capital, etc (undisclosed investors)	Identification and analysis of complex Molecules by using **an analytical SLIM (using electric field technology**), superior to liquid chromatography and mass spectrometry.

№	Company name	Public launch	Funding		Project focus
			Mln USD, USA	Investors	
Materials					
1	Sudoc (sudoc.com, Charlottesville, Virginia; Boston; Pittsburgh; San Juan, Puerto Rico, USA)	2020	10	Family Foundation Hunter Lewis	Eco-friendly self-destructing commercial cleaning products with oxidation catalysts The focus: Effective and and safe products for the decomposition of toxic materials. The technology: **Super ultra-dilute oxidation catalysts**
2	Natural Fiber Welding (naturalfiberwelding. com, USA)	2015	30,8	Ralph Lauren, Allbirds, Smart Shirts, BMW i Ventures, Ethos Capital, For Good Ventures и Prairie Crest Capital	Creation of a closed-loop economy around soft goods. The key area: plant materials for production of textile products. Technology: **fiber welding and oil polymerization**. Clarus chemistry is based on the technology on which Haverhals founded NFW: fiber welding. Disassembling the product for recycling results in further shortening of the fibers. Creation of natural biodegradable polymers for production of new materials, especially textiles
Energetics					
1	Focused Energy (focused-energy.world, Germany)	2021	15	Marc Lore, Prime Movers Lab, Alex Rodriguez, Tony Florence	Development of **laser inertial controlled thermonuclear fusion technologies** with a focus on alternative energy
2	Hyme (hyme.energy, Denmark)	2021	12	Heartland A/S	**Network solution for thermal energy storage based on molten salts** for integration of sustainable energy into the energy system. Chemical control approach enables the use of inexpensive and stable hydroxide salts in compact high-temperature energy storage up to 700 °C
3	LionVolt (lionvolt.com, Netherlands)	2020	6	BOM Brabant Ventures, Sake Bosch, Innovation Industries	Development of new **3D solid-state Batteries,** characterized by improved safety, high performance, and use of stable materials that do not contain heavy heavy metal-free materials, in a circular economy. Lion Volt offers pioneering 3D solid state technology for next-generation batteries, that are 100% safe, weigh 50% less and their productivity is 200% higher compared to modern lithium-ion batteries
4	C-ZERO (czero.energy, California, USA)	2018	11,5	Breakthrough Energy Ventures, Eni Next, Mitsubishi Heavy Industries и AP Ventures	Development of a liquid catalyst that open a new era of turquoise hydrogen. Focus: Turquoise hydrogen. Technology: **a high-temperature liquid that catalyzes the pyrolysis of methane to hydrogen and elemental carbon.**

№	Company name	Public launch	Funding		Project focus
			Mln USD, USA	Investors	
5	Enerpoly (enerpoly.com, Sweden)	2018	2,8	Impact, Propel Capital, Vinnova, European Innovation Council, Swedish Energy Agency, Sting	The next-generation energy storage technology company is a pioneer in **zinc-ion battery chemistry**
6	Northvolt (northvolt.com, Stockholm, Sweden)	2016	4000	Goldman Sachs, Baillie Gifford, EIT InnoEnergy, Norrsken VC, Fjärde Ap-Fonden (Ap4), Första Ap-Fonden (Ap1), Scania, AMF, Daniel Ek, Andra Ap-Fonden (Ap2), Tredje Ap-Fonden (Ap3), Baron Capital, Volkswagen Group, Compagnia di San Paolo, Cristina Stenbeck, ATP, IMAS Foundation, Stena Metall, Bridford Investments, OMERS Capital Markets, PCS Holding ,etc	Manufacturer of lithium-ion batteries. **Green battery projects with 80% less carbon footprint** compared to batteries, made using carbon energy
7	Factorial Energy (factorialenergy.com, Woburn, MA, USA)	2013	65	Gatemore Capital Management и Wave Equity Partners	Bringing polymer-based solid electrolyte batteries to market. Focus: High-energy batteries for electric cars. Technology: **polymer-based solid electrolyte battery polymer-based electrolyte and a lithium-metal anode**
8	Neoen (neoen.com, Paris, France)	2008	77,1	Credit AgricoleLouis Dreyfus Natural Gas, Bpifrance Omnes Capital	One of the world's leading manufacturers of **green power plants and storage tanks**, a producer of energy exclusively from renewable sources
Ecology					
1	Carbo Culture (carboculture.com, Finland)	2017	7	True Ventures, Lifeline Ventures, Albert Wenger, Maija Itkonen, Paul Bragiel, David Helgason, Dan Bragiel, Cherry Ventures, Übermorgen Ventures, Moaffak Ahmed	Development of **bio-coal reactors** that use high pressure and high temperature for **conversion of plant waste into bio-coal,** a superstable carbon material
2	Cyclopure (cyclopure.com/lab), Chicago, USA)	2016	7,5	National Science Foundation, Irwin Jacobs, National Institute of on Health and the Environment	Technology for water purification using **β-cyclodextrin molecules, etc.**

№	Company name	Public launch	Funding		Project focus
			Mln USD, USA	Investors	
3	SCW Systems (scwsystems.com/ Maatschappij, Netherlands)	2016	16,9	Invest-NL	Creation of **supercritical (water) carbonation**. This is an innovative technology that **converts organic waste streams** such as sewage sludge, agricultural bio-mass, organic matter and industrial wastes into e**nvironmentally friendly raw materials for the chemical** industry and clean fuels for power industry. Conversion takes place at high pressure and temperature above the supercritical liquid. The outputs are **methane and green hydrogen**
4	Apix Analytics (apixanalytics.com, France)	2014	18,9	Bpifrance, Demeter Partners, BNP Paribas, Engie Rassembleurs d'Energies, Kreaxi, Banque Populaire Occitane, Supernova Invest, ALIAD (Air Liquide)	Production of miniature (20 times smaller than high-performance laboratory chromatographs) and modular **gas analyzers for industrial analysis and OEM applications**
5	Mosaic Materials (mosaicmaterials.com, USA)	2014	Нет данных	Baruch Future Ventures, Evok Innovations	**Metal-organic frameworks** carbon dioxide capture
6	Polystyvert (polystyvert.com, Canada)	2011	15	Cycle Capital Management, Anges Québec Capital, Anges Quebec, Energy Foundry	**Development of solution and technologies for polystyrene processing**. With these recycling or regeneration technologies, Polystyvert created a circular economy for polystyrene, which has a positive impact on the environment
7	QuantumScape (quantumscape.com, California, USA)	2010	1119	Bill Gates, Capricorn Investment Group, Qatar Investment Authority, TriplePoint Capital, SAIC Motor, Continental, Breakthrough Energy Ventures, Volkswagen Group, Fidelity	Lithium metal batteries. The technology: the solid-state lithium-metal battery is a battery which replaces the polymer separator used in conventional lithium-ion batteries with **a solid state separator.** **Replacement of the separator makes it possible to replace the carbon or silicon anode used in conventional li-ion batterieswith a lithium metal anode**. The lithium metal anode is more energy-intensive than conventional anodes, allowing the battery to store more energy in the same volume. Some solid-state structures use excess lithium, but the QuantumScape structure is "anode-free" in the sense that the battery is made without the anode in the discharged state, and the anode is formed in place during the first charge

№	Company name	Public launch	Funding		Project focus
			Mln USD, USA	Investors	
Other areas					
1	BOTA BIOSCIENCES (bota.bio, USA)	2019	118	BASF, Matrix Partners China, Meituan, Sequoia Capital China, Source Code Capital и др.	Technology: **enzyme engineering** and information technology. In fact, the Bota Freeway digital platform has a cyclic design, reflecting the union of digital technology and robotics in advanced autonomous laboratories. The data obtained in the design and creation of artificially created organisms are returned to the design phase and reentered into the cycle to further improve the process
2	Meatable (meatable.com, Delft, Netherlands)	2018	64,6	Good Seed Ventures, Albert Wenger, BlueYard Capital, Taavet Hinricus, Jeffrey Leyden, Richard Klausner, BlueYard Capital, DSM Venturing, Humboldt Foundation	Development of a new generation of clean **meat grown from animal cells using the latest advances in stem cell research**
3	BIOPHERO (biophero.com, Copenhagen, Denmark)	2016	20,5	DCVC Bio, FMC Ventures, Novo Holdings, Novo Seeds, Syngenta Group Ventures и Syddansk Innovation, as well as the amount of European Union grants from the Olefine and Phera	Growing insect pheromones in yeast cells for sustainable pest control. Technology: Production of insect sex pheromones in large fermenters. Starting with a modest 1-liter fermenter in 2018, BioPhero raised $3.5 million from a consortium that included agrochemical giant Syngenta. By 2020, the money helped the team to expand the fermenter to 180,000 liters. BioPhero is now preparing to commercially launch its first products with the support of a $17 million funding round announced in February 2021
4	Citrine (citrine.io, USA)	2013	36,3	UMI, Showa Denko, AGC, Michelin и LANXESS	Citrine Informatics is a materials informatics platform for data-driven material and chemical development. Developer of **the first artificial intelligence platform for research and development of materials and chemicals**

№	Company name	Public launch	Funding		Project focus
			Mln USD, USA	Investors	
Other areas					
5	Cascade SAS (lightcascade.com, France)	2012	7,9	European Innovation Council	Cascade develops **fluorescent formulations consisting of optically active substances that interact with light to create a "Cascade" effect.** These formulations have been integrated into the base material to provide the desired optical characteristics for end-use applications, including agricultural and photovoltaic applications. CASCADE's patented additives permit selective conversion of incident natural sunlight or any artificial light into wavelengths most efficiently perceived by light receptors in plants, solar cells, algae, the human eye, etc.
6	Ynsect (ynsect.com, France)	2011	271	Talis Capital, Bpifrance, Demeter Partners, Eurazeo, VisVires New Protein (VVNP), Quadia, Crédit Agricole, Caisse d'Epargne, Picardie Investissement	**Increase of protein productivity**. Cultivation of insects for the production of high quality natural premium ingredients for human, animal and plant nutrition and health

Sources:

1. C&EN's 2021 10 Start-Ups to Watch // ACS. URL: cen.acs.org/business/start-ups/CENs-2021-10-Start-Ups-to-Watch-cleantech/99/i42?utm_source=mostread&utm_medium=mostread&utm_campaign=CEN (date of reference: 10.02.2022).
2. It's a breakthrough: the ten most important technologies of 2021 // RBC.URL: trends.rbc.ru/trends/innovation/606ecf189a79470e64285ce2 (date of reference: 10.02.2022).
3. Presentation for investors, 12.08.2021 г. // QuantumScape. URL: ir.quantumscape.com/events-and-presentations/presentations/presentation-details/2021/Investor-Presentation/default.aspx (date of reference: 10.02.2022).
4. Universal Materials Incubator Ltd. (UMI) Announces Strategic Investment in Citrine Informatics // Citrine Informatics. URL: citrine.io/media-post/umi-announces-strategic-investment-in-citrine-informatics/ (date of reference: 10.02.2022).
5. Companies // European Startups. URL: app.europeanstartups.co/companies (date of reference: 11.02.2022).

Appendix 2

FAST-GROWING MARKETS FOR ADVANCED CHEMISTRY

Nanopesticides

Market growth is further stimulated by machine learning and artificial intelligence that can identify and predict the behavior of nanoparticles in soil and vegetation based on data sets, providing modeling capabilities in the R&D phase[70].

The global market for nanopesticides is expected to grow at an average rate of 15% per year, reaching more than $940 million in 2027 [71,72]. Nanoinsecticides are the largest segment, accounting for over 40% of total market revenue. COVID-19 had a strong negative impact on the market, but the tightening of regulatory laws in developed countries on the use of pesticides is stimulating market growth. Nanopesticides reduce the negative impact on the environment.

Nanotechnology in food industry

The food and agriculture-related sector also has a fast-growing market for chemical nano-technologies. The dynamics of the food nanotechnology market are largely driven by the growing introduction of new digital tools to improve agricultural productivity [73].

By 2025, the industry is projected to grow at an average annual rate of up to 25 %. One of the largest and fastest-growing segments is nanomaterials for food packaging, which increase the shelf life of products.

The key technologies on the market are polymer nanoparticles as high-barrier packaging materials and silver nanoparticles as potent antimicrobial agents, as well as nanomaterial-based nanosensors for food analysis[74].

Material informatics

The material direction has probably gained the greatest advantage in terms of R&D. Big data, high computational power, and advanced deep learning algorithms contribute to wide application of AI in the field of material informatics. Artificial Intelligence identifies patterns and forms prediction models. This is the difference between this field and computational chemistry, where the computer is just a calculator that uses human inputted formulas[75]. The market is made up of platform solutions such as Citrine Informatics, a materials informatics platform for data-driven material and chemical development[76].

The market was $91.7 million in 2021, with a projected growth rate of 27% by 2030. Innovations in artificial intelligence and major advances in data infrastructures have boosted the industry. The application of material informatics to the search for new solutions has proven successful. One striking example is the discovery of new superhard materials[77].

70 Shekhar S., Sharma S., Kumar A., et al (2021) The framework of nanopesticides: a paradigm in biodiversity. Materials Advances 2:6569-6588. DOI: /10.1039/d1ma00329a.

71 Credence Research. URL: credenceresearch.com/report/nanopesticide-market.

72 Shekhar S., Sharma S., Kumar A., et al (2021) The framework of nanopesticides: a paradigm in biodiversity. Materials Advances 2:6569-6588. DOI: /10.1039/d1ma00329a.

73 Technavio. URL: prnewswire.com/news-releases/food-nanotechnology-market-to-record-a-cagr-of-25-32-by-2025—technavio-301474651.html.

74 Duncan TV (2011) Applications of nanotechnology in food packaging and food safety: Barrier materials, antimicrobials and sensors. Journal of Colloid and Interface Science 363:1-24. DOI: /10.1016/j.jcis.2011.07.017.

75 Sha W., Guo Y., Yuan Q., et al (2020) Artificial Intelligence to Power the Future of Materials Science and Engineering. Advanced Intelligent Systems 2:1900143. DOI: /10.1002/aisy.201900143.

76 Citrine. URL: citrine.io.

77 Precedence Research. URL: globenewswire.com/en/news-release/2022/01/24/2372050/0/en/Material-Informatics-Market-Size-to-Surpass-US-782-2-Mn-by-2030.html.

Smart Materials

These are technologically sophisticated materials that can perceive and respond to a wide range of environmental stimuli. Their properties and behavior in the final product can be predicted thanks to digital solutions that help to carry out computer simulations[78].

The global market for smart materials will reach $98.2 billion by 2025, with a compound annual growth rate of 13.5% during the forecast period. The broader use of markets for motors, sensors, and structural materials is expected to strengthen the demand for smart materials in the next few years[79].

The market includes such technological solutions as shape-memory materials, piezoelectric, electrostrictive, magnetostrictive, and electrochromic materials. All of them are widely used in industry, along with shape memory ferromagnetic alloys, electroactive polymers, conductive polymers, and carbon nanotube actuators.

Organic electronics

This is another material-dependent market, so predictive capabilities of artificial intelligence helping to find the most efficient materials are essential to it.

The global market for organic electronics is expected to grow to $159 billion by 2027, with an average growth rate of 21% from 2020 to 2027. The development driver is the advantages of organic electronics over inorganic electronics (mechanical flexibility, light weight, low cost). Since organic devices are easier to recycle, their production is growing worldwide. Organic electronics operate with low power consumption, providing energy saving[80].

Key technologies: organic LEDs, organic field-effect transistors, organic conductors, photovoltaic materials.

Materials with a phase transition

Phase-transition materials are substances that absorb or release large amounts of "latent" heat when they undergo a change in their aggregate state. When machine learning algorithms and similar materials are used together, it is possible to control the temperature change of raw materials, which is a universal and necessary function for many industries and products[81].

The market volume should reach $ 1 billion by 2026, with an average annual growth rate of 16%. The development of the industry is negatively affected by the lack of industry awareness and the flammability of the materials. Nevertheless, a wide range of applications of materials with phase transition and their importance in many industrial areas provide for market growth[82].

78 Digital Engineering. URL: digitalengineering247.com/article/making-smart-materials-smarter-multiphysics-simulation.

79 Grandview Research. URL: grandviewresearch.com/press-release/global-smart-materials-market.

80 Allied Market Research. URL: alliedmarketresearch.com/printed-organic-and-flexible-electronics-market.

81 Tietze T., Szulc P., Smykowski D., et al (2021) Application of Phase Change Material and Artificial Neural Networks for Smoothing of Heat Flux Fluctuations. Energies 14:3531. DOI: /10.3390/en14123531.

82 Markets and Markets. URL: marketsandmarkets.com/Market-Reports/advanced-phase-change-material-pcm-market-1087.html.

Synthetic Biology

Biotechnology is increasingly dependent on the use of big data about relationships and patterns in chemistry.

The synthetic biology market, estimated at $6.4 billion in 2020, is projected to grow to $28.8 billion by 2026, growing at an average of 28.1% over the analyzed period. The oligonucleotides and synthetic DNA segment is expected to grow at an average annual growth rate of 29.5%, reaching $16.1 billion. This dynamic is due to the growing consumption of synthetic RNA, synthetic DNA and synthetic genes, which are used in a multitude of applications. In the face of the COVID-19 pandemic, scientists see synthetic biology as a way to accelerate vaccine development. Other factors contributing to the market expansion include an increase in synthetic biology research organizations, the growing demand for hybrid animals, the increase in the number of oil spills in the ocean, improved funding for drug R&D, and increased demand for sustainable energy resources, particularly biofuels [83].

Key technologies: genetic and post-translational modification, technological solutions in DNA synthesis, genome engineering, in vitro transcription applications, continuous and cell-free evolution formats.

83 Global News Wire. URL: globenewswire.com/news-release/2022/01/21/2370810/28124/en/Global-Synthetic-Biology-Market-Report-2021-Market-to-Reach-28-8-Billion-by-2026-Oligonucleotides-Synthetic-DNA-is-Projected-to-Account-for-16-1-Billion.html.

84 Global News Wire. URL: globenewswire.com/en/news-release/2021/07/12/2261393/0/en/Precision-Medicine-Market-Size-Worth-USD-126-14-Billion-by-2025-at-12-48-CAGR-Report-by-Market-Research-Future-MRFR.html.

85 NIH. URL: cancer.gov/publications/dictionaries/cancer-terms/def/personalized-medicine.

Personalized medicine

A new field of health care has been developing rapidly in recent years. The topic of personalized medicine is the focus of researchers and industry working on the overall sequencing of the human genome. Advances in technology have paved the way for new scientific and business models. The market is growing rapidly worldwide and is expected to reach its peak in the next few years.

It is predicted that by 2025 the market will reach a volume of 126 billion dollars at an average annual rate of 12.5%. The growth of the precision medicine market will be supported by the cooperation of the pharmaceutical and biotechnology sectors with the healthcare industries working with big data during the forecasted period[84].

Recent advances in personalized medicine solutions (ultra-high-throughput sequencing and next-generation sequencing) have enabled physicians to better understand the health status of their patients and develop specific treatments for each patient individually. Personalized medicine includes the use of targeted therapies to treat certain types of cancer cells, such as HER2-positive breast cancer cells, or oncomarker testing for cancer diagnosis. The field is also called precision medicine[85].

Solar energy

The solar energy market is directly dependent on scientific achievements in the field of materials. It also depends on the predictive capabilities of artificial intelligence to find the most efficient compounds for power generation.

Solar energy has been booming in recent years thanks to the demand for renewable energy and sustainable energy initiatives. In January 2022 the EU proposed a new 0 % VAT rate for solar panels. Tax incentives and research and development have also boosted solar power production in the U.S., another region where the market is booming. Some states have required suppliers to purchase a certain amount of energy from renewable reserves, with photovoltaic solar modules remaining the most popular[86].

The market's key technologies include photovoltaic solutions, such as various types of solar panels.

Batteries for electric cars

The battery market could get a boost from AI, as its predictive capabilities create the most successful material chemistry solutions for efficient conservation of electricity at the lowest cost[87].

The global market for batteries for electric vehicles was $22 billion in 2020. It is projected to grow to $155 billion in 2028 at an average annual growth rate of 28.1% over the period of 2021-2028. Currently, the main energy source for electric cars is lithium-ion batteries. According to a 2018 U.S. International Trade Commission (USITC) assessment report, lithium-ion batteries account for more than 70% of the battery market. In addition, the cost of batteries per kilowatt hour has fallen to less than $200 in 2019, down from $1,000 in 2010. This is expected to boost the market for batteries for electric vehicles[88].

The market is mainly represented by the following technologies: nickel-metal hydride, lithium-ion, and lead-acid batteries.

Recycling of lithium-ion batteries

The battery recycling market relies heavily on chemical technologies. First, high-quality methods of their recycling are very effective. Second, new useful substances and materials can be produced on the basis of recycled materials.

By 2030, the world market for lithium-ion battery recycling will reach $24 billion with an average annual growth rate of 21.4%. The need for battery-powered electric vehicles is increasing and leading to market growth over the forecast period. There has been a paradigm shift toward low-carbon vehicle fleets in developed and developing countries, driving the industry forward. The emergence of different types of electric vehicles over the years has led to a large number of batteries coming to the end of their useful life. The clean energy trend will also serve as a reliable source of growth for the market over the forecast period [89].

86 Global News Wire. URL: prnewswire.com/news-releases/at-25-7-cagr-solar-panels-market-size-expected-to-reach-usd-902-55-bn-globally-by-2028—says-brandessence-market-research-301460328.html.

87 Wired. URL: wired.com/story/ai-is-throwing-battery-development-into-overdrive/.

88 Global News Wire. URL: globenewswire.com/news-release/2021/10/27/2321353/0/en/At-28-1-CAGR-EV-Battery-Market-Size-is-Projected-to-Grow-from-USD-27-30-Billion-in-2021-to-USD-154-90-Billion-in-2028.html.

89 Global News Wire. URL: globenewswire.com/news-release/2021/12/06/2346181/0/en/Lithium-ion-Battery-Recycling-Market-to-rise-at-CAGR-of-21-43-through-2030-Report-by-Market-Research-Future-MRFR.html.

Green jet fuel

At the research stage, the biofuel market in general can benefit from the use of neural networks. Their use provides reliability, accuracy, ability for fast learning in the most complex models in predicting biofuel quality parameters[90]. The same is true for certain market segments (e.g. jet biofuels): AI has the potential to change the research approach as one of the digital analysis tools [91].

The market for sustainable aviation fuels is expected to grow from $219 million in 2021 to $15 billion by 2030, at an average annual growth rate of 60.8% over the forecast period. The expansion of commercial aircraft fleets by airlines due to the increase in air traffic has contributed greatly to the development of the industry. This, in turn, stimulates demand for environmentally friendly aviation fuel in line with strategies to reduce greenhouse gas emissions[92].

In terms of social and economic benefits, the most promising sustainable aviation fuels are synthetic, environmentally friendly jet, bioreactive and hydrogen fuels.

Carbon capture and utilization

Technological advances are expanding offshore oil and gas exploration and production activities, facilitating the introduction of enhanced oil recovery by gas injection, including the use of carbon dioxide for crude oil production. All these factors combined are the drivers of the sector growth.

The global carbon capture, utilization and storage market was estimated at $1.9 billion in 2020 and is projected to reach $7 billion by 2030, growing at an average of 13.8 percent from 2021 to 2030. Carbon capture, utilization and storage is the process of capturing carbon dioxide from fuel combustion or industrial processes, transporting the CO2 by sea or pipeline, and using it as a resource to create valuable products and services or permanently storing it deep underground in geological formations. Global demand here is primarily driven by a growing focus on CO2 reduction, support for government initiatives, and increasing demand for CO2-EOR methods. To reduce the carbon footprint, governments in many developed and developing countries (USA, Netherlands, UK, China, India) are setting up large numbers of CO2 capture and storage plants. This factor is expected to drive market growth over the forecast period.

90 Barradas A. O., Amorim I. M. Applications of Artificial Neural Networks in Biofuels. In: El-Shahat A, editor. Advanced Applications for Artificial Neural Networks. London: IntechOpen. DOI: 10.5772/intechopen.70691.

91 Ong M. Y., Nomanbhay S., Kusumo F., et al (2021) Modeling and Optimization of Microwave-Based Bio-Jet Fuel from Coconut Oil: Investigation of Response Surface Methodology (RSM) and Artificial Neural Network Methodology (ANN). Energies 14:295. DOI: /10.3390/en14020295.

92 Markets and Markets. URL: marketsandmarkets.com/Market-Reports/sustainable-aviation-fuel-market-70301163.html.

93 Allied Market Research. URL: alliedmarketresearch.com/carbon-capture-and-utilization-market-A12116.

Biodegradable materials

Neural networks and other algorithms use data sets with compound descriptions, and are able to classify biodegradability with a fairly high level of accuracy[94].

The market for biodegradable materials is estimated at $14 billion in 2020, and is expected to reach roughly $87 billion by 2026, at annual average growth rate of 26.5%. The stable cost of agricultural raw materials compared to petrochemical products is likely to increase the use and popularity of bio-based materials in the world. These products are also environmentally friendly: they are recyclable and do not contribute to greenhouse gas emissions. In addition, bio-based materials help minimize the economy's dependence on oil, and their biodegradable properties reduce the toxic impact on the environment[95]. Regulatory standards such as the European REACH are pushing manufacturers towards the use of such materials and their evaluation. Increase in the demand for these materials combined with digital tools, will allow the market to develop dynamically in the future.

Technologies for bio-based materials from renewable raw materials based on organic polymers from corn, starch, and sugar cane which decompose in the environment within a year also look quite promising.

94 Putra R. I. D., Maulana A. L., Saputro A. G. (2019) Study on building machine learning model to predict biodegradable-ready materials. AIP Conference Proceedings. DOI: /10.1063/1.5095351.

95 Global News Wire. URL: globenewswire.com/news-release/2021/12/17/2354362/0/en/Global-Bio-Based-Materials-Market-Size-Is-Expected-To-Reach-About-USD-87-Billion-by-2026-at-a-CAGR-of-26-5-Facts-Factors.html.

The report was preceded by a foresight session "Frontiers in the New Sciences", organized by the Center for Strategic Research "North-West" Foundation together with the Foundation for the Support of Innovation and Youth Initiatives of St. Petersburg with the support of the Government of St. Petersburg and the Ministry of Science and Higher Education of Russia.

Date: November 9-10, 2021

Format: Conference and joint work in groups.

Topics: new chemistry, synthetic biology, artificial intelligence for industry, "green transition" in industry and cities.

Participants: 168 participants representing Russian universities, scientific organizations and business companies from 19 regions of the Russian Federation.

The results for each research area:

— identified trends in the development of research topics in focus until 2030 and 2050;

— identified the most relevant topics for high-risk research (BlueSkyResearch);

— designed training programs for key researchers of the PI school.

ISBN 978-5-9909736-5-7

CENTER FOR STRATEGIC RESEARCH NORTH WEST

INNOVATION AND YOUTH CREATIVITY FOUNDATION OF ST PETERSBURG