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CHAPTER V. ARTIFICIAL INTELLIGENCE IN CHEMISTRY: CURRENT STATE AND PROSPECTS

DOI

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Abstracts. The monograph is devoted to a comprehensive analysis of the implementation of artificial intelligence (AI) in various fields of chemistry. The work considers modern directions of AI application for the discovery of new drugs, development of innovative materials, prediction of chemical reactions, automation of laboratory experiments, spectroscopy and analytical chemistry. The benefits of using deep learning, machine learning algorithms, and generative models, as well as the challenges associated with data quality, ethics, and model interpretability, are analyzed in detail. Particular attention is paid to the evolution of AI in chemistry, the current state of research, and predictions for integration with other technologies, including robotics and quantum computing. The monograph aims to facilitate interdisciplinary dialog between chemists, computer scientists, and industry representatives for the effective implementation of AI in chemical research.

Keywords: artificial intelligence, chemistry, machine learning, deep learning, drug development, materials science, reaction prediction, spectroscopy, automation, analytical chemistry, innovative technologies.

Introduction. The rapid development of science and technology puts more and more difficult tasks before chemical research. The need to accelerate the opening of new medicines, the development of innovative materials with unique properties, optimization of chemical processes and the analysis of huge amounts of data requires new approaches and tools. One of these promising areas is the use of artificial intelligence (AI). Artificial intelligence is defined as the ability of machines to simulate cognitive functions of a person, such as learning, solving problems and decision - making. The main sub -sectors of the AI include machine learning (MN) and deep training (GN). Unlike traditional computer programs that apply to clearly defined rules, AI systems are designed in such a way as to understand the relationships between data and find new solutions for complex problems. Machine training, in turn, includes various paradigms, including teaching with the teacher (based on labeled data), learning without a teacher (identifying patterns in unmarked data) and training with reinforcement (training based on rewards and punishments) [4, 12].

The relevance of the use of AI in chemistry is emphasized by the fact that the International Union of Theoretical and Applied Chemistry (IUPAC) has recognized as one of the ten most promising technologies in chemistry in 2023 4. This report is intended to provide a comprehensive review of the current state and prospects for the development of artificial intelligence in various fields of chemistry. The report will consider the use of AI to open and develop new medicines, in material science, to forecast chemical reactions, in spectroscopy and other analytical methods, as well as to analyze the advantages and disadvantages of using AI in chemical research and future trends in this field [7, 16].

In addition to the above areas, an important aspect of the use of AI in chemistry is the automation of laboratory experiments using robotic systems guided by machine learning algorithms. Such "smart laboratories" are able to plan experiments independently, analyze the results in real time and adapt further actions to achieve optimal results. This not only reduces the time and cost of research, but also reduces the likelihood of human mistake [2, 18].

Also popular is the use of artificial intelligence to interpret large volumes of spectroscopic, chromatographic and mass spectrometric data. Due to the ability to identify hidden patterns in complex data kits, AI algorithms help to identify substances more accurately and faster, to predict their activity or toxicity, which is especially valuable in pharmaceutical and environmental chemistry. Another promising area is the development of new catalysts with given properties. With the use of AI, it is possible to model the surface of the catalyst at the atomic level and to predict its activity in different conditions. This opens up new opportunities for green chemistry and sustainable development, where process efficiency is critical [4, 7].

However, despite all the advantages, the introduction of AI in chemistry is accompanied by certain challenges. These include the need for large and high -quality data training arrays, limited interpretability of some algorithms, as well as ethical issues related to autonomy decision -making. To overcome these difficulties, an interdisciplinary approach that combines knowledge in chemistry, computer science, statistics and ethics is important [6, 15].

As a result, the development of artificial intelligence opens a new era in chemical research. Its integration into scientific processes can accelerate the discovery of new substances, improve understanding of complex reactions and make chemical science more effective, safe and focused on the future [9, 11].

The use of artificial intelligence in chemistry has gone a significant path of evolution, from early conceptual developments to modern rapid implementation in various research and industrial processes. Particularly noticeable is the increase in interest and activity in this field after 2015, which is reflected in a significant increase in the number of publications and patents related to the use of AI methodologies in chemistry. Thanks to the AI, researchers were able to process and analyze data at such a pace that would be impossible when using traditional manual methods, which would take decades manually. To date, artificial intelligence is widely used in many key areas of chemical research. Among them is an important place to predict the various properties of molecules, such as bioactivity, toxicity, solubility and stability. AI is also actively used to develop new molecules with predetermined properties, which is critical for the creation of innovative medicines and materials. In addition, AI algorithms are used to predict the results of chemical reactions, optimize the conditions of their conduct, as well as to analyze complex spectral data, which significantly increases the efficiency of experimental work [1, 14].

CAS Content Collection plays an important role in understanding and contextualization of the modern landscape. CAS is a recognized leader in the field of scientific information decisions, making the customization, binding and analysis of valuable data published in scientific literature around the world, in order to accelerate scientific breakthroughs. The CAS Scientists and Experts Team uses CAS Content

Collection, the world's largest chemical library for classification and quantitative evaluation of all chemical publications related to AI, from 2000 to 2020. [2, 15].

The rapid increase in the use of AI in chemistry after 2015 indicates qualitative changes in approaches to chemical research. This turning point is probably related to the progress in the development of more powerful deep learning algorithms and a significant increase in computational capacity. The analysis of the dynamics of publications demonstrates exponential growth after this period, which correlates with the general tendency of development of deep learning in other scientific fields. It is at this time that deep learning models have reached a level of maturity sufficient for effective use to complex chemical data. In addition, chemistry disciplines, in which the level of implementation of AI remains relatively low, can represent significant opportunities for future research and innovation. If certain areas of chemistry are lagging behind in the use of AI, it may indicate the undisclosed potential to increase the efficiency, accuracy and speed of research processes in these areas. Detection and elimination of obstacles that interfere with the introduction of AI in such disciplines can lead to significant scientific breakthroughs and discoveries [11, 17].

The traditional process of developing new medicines is extremely long, expensive and is characterized by a high level of failure. Usually, from identifying a potential target to the release of the drug to the market is over ten years, and the cost of developing one successful medicinal product can reach billions of dollars. In this case, much of the candidates for the medicine fail in the stages of preclinical or clinical trials. Artificial intelligence plays an increasingly important role in accelerating and improving the efficiency of each stage of this complex process. At the stage of targeting and validation, the AI algorithms are able to analyze huge volumes of biological data, such as genomic and proteom data, to detect molecular targets (eg, proteins or genes) related to diseases. An excellent example is the use of the DeepMind Alphafold tool that has revolutionized the three -dimensional protein structure, which is critical for understanding their function and developing medicines that interact with these proteins [14, 17].

In the field of design and optimization of AI molecules, it helps to generate new molecular structures with the desired properties. To represent molecules, a simplified system of introduction of molecular rows (SMILES) is used, which allows the AI algorithms to process chemical structures as text 9. Generative models, such as variational auto codes (VAE) and generative-magnifying networks (GAN) are used to create new molecules. AI is also effectively used to predict the properties of molecules, including their solubility, toxicity and bioactivity. For this purpose models of quantitative ratio of structure-activity (QSAR) are developed, which establish the relationship between the chemical structure of the compound and its biological activity [3].

Results of the study. At the stage of virtual screening and identification of medical massacles, the AI helps to predict the interaction of potential medicinal products with target proteins 7. There are different approaches to predicting interactions, including methods based on the analysis of features of molecules and their similarity, as well as deep learning methods, such as Deeepdta, Padda, WEAPTA, WEDDA. AI also finds the use in clinical trials, where it is used to optimize research protocols, selection of patients, forecast treatment results and identify potential side effects. For example, a Trialgpt algorithm has been developed to help select potential volunteers to participate in clinical trials. Another important area is the re -profiling of medicines, that is, the search for new therapeutic applications for existing medicines. For this purpose, machine learning methods are used that analyze large amounts of data on medicines, diseases and their relationships, for example, the "Guilt by Association" approach [1, 8].

The Lab in Lab in A Loop concept involves the integration of the generative AI into all stages of drug development. Data obtained in the laboratory and during clinical trials are used to teach AI models, which then generate new hypotheses and forecasts for potential medicinal targets and molecules that are again checked experimentally, creating a continuous cycle of improvement [2].

There are already many examples of successful use of AI in the discovery of medicines. Among them is the detection of a new antibiotic capable of combating bacteria resistant to medicines; identification of potential methods of treatment of rare genetic disorders; development of exscientia drug from obsessive-compulsive disorder; use of Benevalentai to detect Baricitinib as a possible treatment for Covid-19; and the use of Alphafold to identify new genes associated with lateral amyotrophic sclerosis (BAS) [4].

It is important to note that AI not only significantly accelerates the process of developing medication, but also increases the likelihood of success of clinical trials. Studies show that drugs found by AI have a higher percentage of success in the first phase of clinical trials compared to drugs developed by traditional methods. This indicates that AI helps to more effectively select promising candidates in the early stages [4, 7].

Despite significant successes, a number of problems related to the quality and availability of data, ethical considerations on their use and transparency and interpreting models of AI, need to be fully realized in the development of medicinal products in the development of medicines. The quality of data is critically important for teaching effective models, and ethical aspects and transparency of decision -making models need special attention to ensure confidence and responsibility [4, 7].

Traditional methods for developing new materials are often slow and largely dependent on experiments conducted by trial and error. Finding materials with certain characteristics, such as durability, electrical conductivity or heat resistance, can take considerable time and require a lot of resources. Artificial intelligence plays an increasingly important role in accelerating the discovery and development of new materials with predetermined properties. One of the key areas is to predict the properties of materials, including their mechanical, electronic, magnetic and thermal characteristics. Various machine learning algorithms, including graphic neural networks (GNN) and physically sound neural networks (Pinn) are used for this purpose [2, 6].

An approach known as material science based on data informatics involves the use of AI algorithms to analyze large arrays of data on existing materials to identify patterns and to predict the behavior of new, not yet synthesized compounds. AI also contributes to the development of reverse design, when the purpose is to design materials with predetermined properties. An example of this approach is the Microsoft Mattergen tool developed, which uses generative models to create new materials with the desired characteristics. Generative models of AI, such as DeepMind Gnome and diffusion models, are not only able to predict properties, but also to offer completely new materials with given characteristics. Gnome, for example, has already discovered hundreds of thousands of new stable materials, including potential superconductors [4, 7].

There are already a number of examples of materials designed or open by artificial intelligence. Among them is nanomaterial, which is light as foam, but strong as steel; new materials for improved energy -intensive batteries; materials for effective carbon capture; and high energy density and heat resistance polymers for use in condensers [14, 17].

An important advantage of using AI is the ability not only to predict the properties of existing materials, but also to carry out the so -called "reverse design". This means that researchers can start with the desired characteristics of the material and use AI algorithms to determine the optimal chemical structure and composition that would provide these properties. The traditional approach to the development of materials has often been the synthesis and study of the properties of existing or random compounds. The reverse design with the help of AI opens the path to purposeful creation of materials for specific needs and use [10, 15].

However, despite the considerable potential of AI in materials science, one of the main obstacles to its wider application remains the problem of lack of quality and sufficient data for training models. Effective learning of machine learning algorithms requires large and various data sets on materials properties, their structure, composition and conditions of synthesis. Collection and preparation of such data is a complex and often expensive process. The development and use of generative models, as well as data of data, can be a partial solution to this problem, allowing you to create synthetic data to expand the training sets [14, 17].

Accurate forecasting of chemical reactions and their products is extremely important for many sectors of chemistry, including organic synthesis, drug development and material science. Traditional forecasting methods are often dependent on the knowledge and intuition of experienced chemists, which can be time -pointed and not always accurate. Artificial intelligence, especially machine training, offers powerful tools for predicting chemical reactions, conditions of their conduct and possible by -products. Smiles system is often used to represent molecules and chemical reactions. Popular models of "sequence-sequence" (SEQ2SEQ) and architecture based on transformers, which have demonstrated high efficiency in the tasks of forecasting chemical reactions. AI is also used to predict thermochemical parameters of reactions, which is important for understanding their energy [6, 20].

The Chemreactome Platform, developed by Cambridge University researchers together with Pfizer, is an example of a successful combination of automated experiments and artificial intelligence to predict chemical reactions 68. There are also specialized AIs, such as IBM RXN for CHEMISTRY. offer synthetic paths. A special place is the use of AI in retrosynthesis, that is, in the automated planning of synthetic pathways to obtain target molecules. There are different types of retrosynthesis models, including template, semi -shaped and cumulative methods. Research on integration of machine learning with chemical works for automation of experimental processes is also underway [4, 7].

AI is also used to predict optimal conditions of reactions, such as temperature, pressure, type of catalyst and solvent. There are a number of successful examples of using AI to predict chemical reactions. For example, a model of machine learning has been developed to predict catalytic oxidation products on the gold surface with an accuracy of up to 93%. The IBM RXN platform is successfully used to predict the results of organic reactions. Chemreactome platform demonstrates significant progress in understanding chemical reactivity and reactions predicting. It is important to note that AI not only helps to predict the results of already known reactions, but also contributes to the discovery of new reactionary pathways and deepening understanding of the fundamental principles of organic chemistry [15, 17].

Not only the choice of the appropriate algorithm of artificial intelligence, but also the quality and representativeness of the data on which the model is studied, is crucial for the effective forecasting of chemical reactions. The accuracy of AI forecasts depends directly on how well the model was trained in various and high quality chemical reactions. Insufficiency or bias of educational data can lead to inaccurate or incomplete forecasts, which emphasizes the importance of careful selection and preparation of data for teaching models of machine learning in chemistry [8, 22].

Traditional methods of spectroscopy and analytical chemistry are often time -

consuming and require deep expert knowledge for the proper interpretation of the data obtained. The process of analyzing spectra and identification of compounds can be long -lasting and prone to subjective errors [14, 17].

Artificial intelligence offers significant opportunities to automate the analysis of spectral data, improve the accuracy of compound identification, and gain new, deeper insights in chemical research. In the field of nuclear magnetic resonance (NMR), AI is used to predict chemical shifts, model spectra, structurally identify unknown compounds, and analyze complex mixtures. In mass spectrometry (MS), AI is used to identify and quantify compounds, in proteomics and metabolomics, and to analyze data from large repositories. In infrared (IR) and Raman spectroscopy, machine learning helps to identify functional groups, perform qualitative and quantitative analysis, and is used for medical diagnostics. In chromatography (gas, liquid, liquid chromatography-mass spectrometry), AI is used to optimize separation conditions, identify peaks, and quantify components of mixtures. In X-ray diffraction (XRD), AI algorithms help in phase identification and crystal structure determination of materials [4, 7].

There are also intelligent material analysis systems, such as ZEISS ZEN core, that use artificial intelligence to automatically recognize material properties. An interesting application of AI is to predict the chemical composition of substances based on the analysis of their photographs, which can be used in various fields, including forensics and environmental monitoring [9, 17].

The use of AI in spectroscopy and analytical chemistry not only automates routine procedures, but also identifies complex, non-obvious patterns in the data, leading to deeper insights that were previously unavailable to researchers 8. The ability of AI algorithms to process large volumes of heterogeneous data and recognize subtle relationships between spectral characteristics and chemical structure of compounds opens up new opportunities for in-depth understanding of complex chemical systems and processes [14, 21].

However, for the successful application of AI in spectroscopy and other analytical methods in chemistry, it is critical to have large, high-quality, and properly annotated datasets to train machine learning models. The effectiveness of AI models directly depends on the quality of the data they are trained on. Collecting and preparing such data can be a complex and resource-intensive task, but it is a key factor in achieving high accuracy and reliability of the analysis results [4, 7].

The use of artificial intelligence in chemical research offers significant advantages. AI can significantly accelerate the pace of scientific discovery and development by quickly analyzing large amounts of data and identifying potential new compounds and materials. It also leads to increased efficiency and productivity of research processes, optimization of reaction conditions, and automation of routine tasks. Due to the high accuracy of data analysis, AI helps to identify subtle patterns and connections that may be missed by humans, which contributes to the discovery of more effective compounds and materials. The use of AI can also significantly reduce research and development costs by reducing the need for manual labor and increasing the accuracy of predictions. In addition, AI plays an important role in promoting green chemistry and sustainable practices by helping to predict the environmental impact of new chemicals and materials. Overall, AI is expanding the possibilities for developing new medicines and materials with desirable properties, opening up new horizons in chemical science and industry [9, 20].

However, the use of AI in chemical research is also associated with certain disadvantages and challenges. One of the main drawbacks is the dependence on the quality and quantity of training data. AI models require large amounts of high-quality data to perform effectively; insufficient or poor quality data can lead to inaccurate results. The “black box” problem, where it is difficult to understand how an AI model makes decisions, is also a significant challenge, especially in regulated industries such as pharmaceuticals. Implementing and maintaining AI systems requires highly skilled professionals with knowledge of both chemistry and computer science, which can be a problem due to their lack of availability. Training and deploying complex AI models often requires significant computing resources. The use of AI in chemistry also raises important ethical issues related to data privacy, intellectual property rights, and the potential misuse of AI-generated knowledge or compounds. There is also a risk of model bias if the training data contains systematic errors or is not representative [9, 11]

AI models trained on specific datasets may have limited ability to generalize to new, previously unknown data, which is important in chemistry, where new compounds and reactions are constantly emerging. Integrating AI with existing laboratory processes can be challenging and require significant changes. The potential risks associated with human error when using complex AI systems should also not be overlooked. Finally, results obtained with AI often require experimental validation, as AI is a powerful predictive tool but does not replace physical experiments. Despite its significant advantages, the widespread adoption of AI in chemistry is hampered by a number of technical, organizational, and ethical challenges. To overcome these barriers, joint efforts of scientists, developers, industry, and regulators are needed [1, 5].

Successful AI implementation requires not only significant investments in information technology and infrastructure, but also the development of relevant skills among chemists and the creation of effective interdisciplinary teams combining deep expertise in both chemistry and computer science. To use AI effectively, chemists need to understand its capabilities and limitations, and AI specialists need to have a thorough knowledge of the chemical industry [8, 14].

The future of artificial intelligence in chemistry looks extremely promising and promising. Further progress is expected in the development of more sophisticated machine and deep learning algorithms, including improved generative models that can create new chemical structures with desired properties and reinforcement learning methods that can optimize complex chemical processes. One of the key trends is the increasing integration of AI with other advanced technologies, such as robotics and automated laboratory systems, which will lead to the creation of fully autonomous research platforms. The development of quantum computing may also open up new opportunities for modeling complex chemical systems and reactions with unprecedented accuracy [6, 15]. User-friendly AI-based platforms and tools are expected to emerge and become more widely available, addressing the needs of a wide range of chemists, even those without deep computer science knowledge. The increase in the amount and quality of chemical data suitable for training AI models is also an important trend that will contribute to the accuracy and reliability of predictions [8, 11]. In the future, AI will be increasingly used to solve fundamental and applied problems in chemistry, such as predicting the mechanisms of chemical reactions at the atomic level, developing new, more efficient and selective catalysts, and creating materials with extreme properties that were previously considered unattainable [4,12].

Table 1.

SWOT ANALYSIS

• **(Strengths)** ➢ Accelerating research and discovery ➢ High accuracy in predicting molecular properties ➢ Ability to analyze large amounts of data ➢ Automation of routine experimental processes ➢ Possibility to create new materials with unique properties	• **(Weaknesses)** ➢ Dependence on the quality and volume of training data ➢ Limited interpretability of some algorithms ➢ High cost of implementing and maintaining AI systems ➢ The need for specialists with interdisciplinary knowledge ➢ Risk of model bias
(Opportunities) ➢ Development of new drugs and materials ➢ Optimization of chemical processes ➢ Deepening interdisciplinary cooperation ➢ Development of "green chemistry" ➢ Creation of fully automated research platforms	**(Threats)** ➢ Ethical issues in the use of AI ➢ Potential risks to data security and privacy ➢ Resistance to changes in traditional research approaches ➢ Possible job losses ➢ Regulatory restrictions and implementation challenges

Interdisciplinary cooperation between chemists, computer scientists, and representatives of other scientific disciplines is expected to increase, which is a prerequisite for the successful implementation and development of AI in chemistry. Another important aspect is the development of ethical standards and regulatory frameworks for the use of AI in chemical research, which will help ensure the responsible and safe application of this powerful technology [8, 16].

The future of chemistry is inextricably linked to the further development and widespread adoption of artificial intelligence, which opens up qualitatively new opportunities in both fundamental research and practical applications in industry. It is predicted that AI will become an integral part of chemical research, transforming approaches to the development of drugs, materials, catalysts, and analytical methods [5, 19].

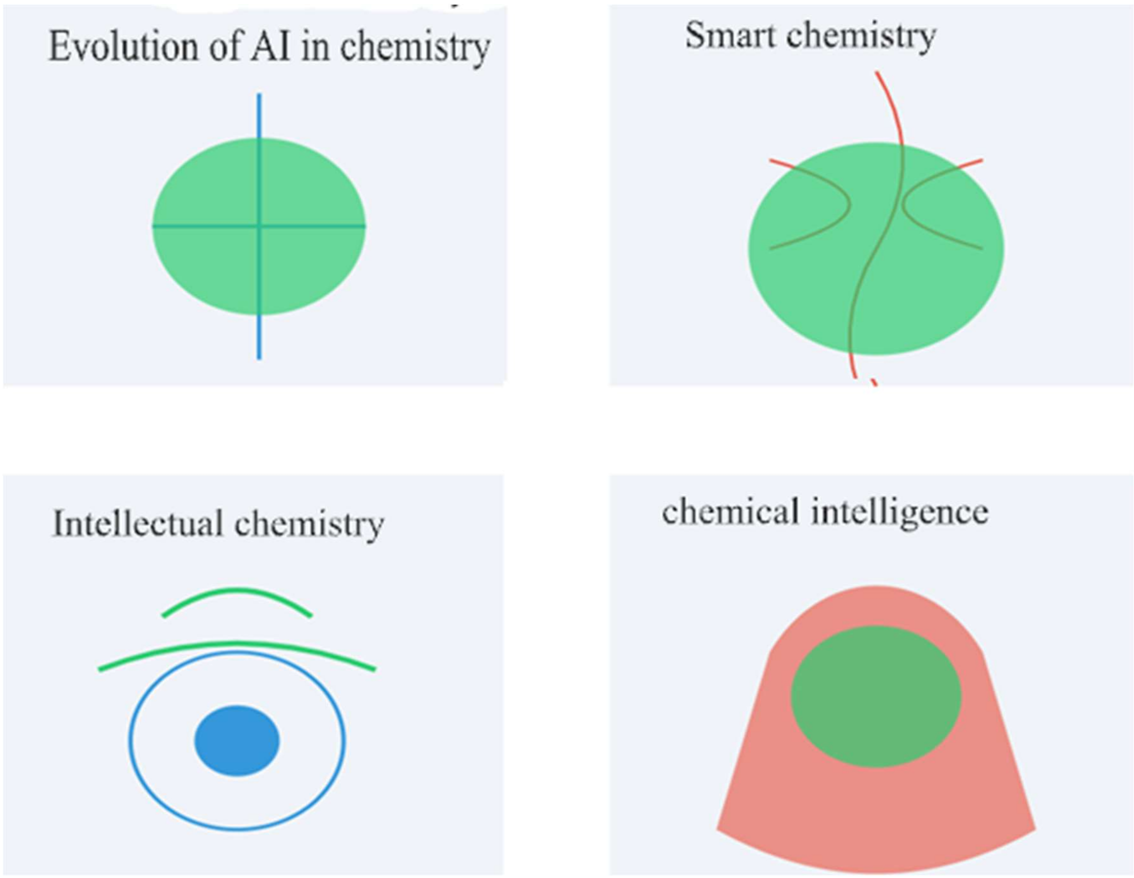

Fig. 1. Conceptual approaches to the integration of artificial intelligence into chemical science: evolution, intellectualization, and smart technologies.

To realize the full potential of artificial intelligence in chemistry, it is crucial to focus on creating reliable, transparent, and ethical systems that effectively integrate the deep knowledge of chemists with the powerful computational capabilities of AI. Future successes in this area will largely depend on the ability to develop AI models that are not only highly accurate in their predictions but also understandable to chemists, as well as ensuring that the data used in training and applying these models is properly secured and confidential [18, 22]. Artificial intelligence is already demonstrating impressive results in various fields of chemistry. In pharmaceuticals and biotechnology, one of the most famous examples is the AlphaFold algorithm developed by DeepMind, which made a breakthrough in accurately predicting the three-dimensional structure of proteins, which is critical for identifying drug targets and developing new drugs. BenevolentAI has successfully used AI to repurpose existing drugs, including the discovery of a potential treatment for COVID-19. Insilico Medicine is another leader in this field, using AI to rapidly develop new drugs and identify biomarkers. It is also worth noting Pfizer's collaboration with IBM Watson to utilize AI capabilities in cancer research. New antibiotics capable of fighting drug-resistant bacteria were discovered with the help of AI [15, 21].

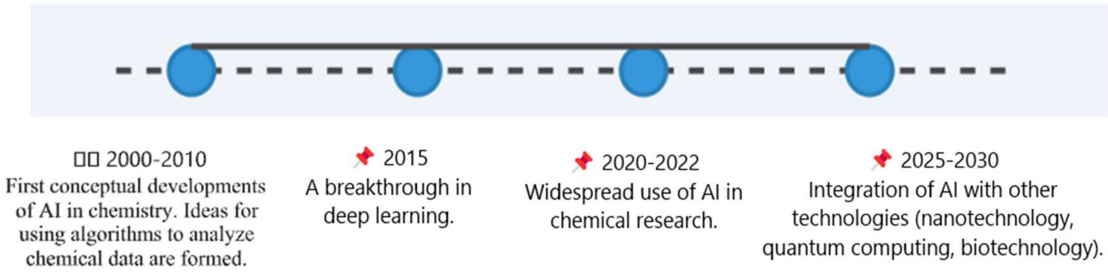

Fig. 2. Evolution of AI in chemistry

In materials science, significant progress has been achieved through the use of generative AI models. For example, the GNoME tool developed by DeepMind has discovered hundreds of thousands of new stable materials, including potential superconductors, which could have revolutionary consequences for various industries, from quantum computers to energy. Microsoft has developed a powerful tool called MatterGen, which allows you to generate new materials with specified properties, opening up endless possibilities for creating innovative materials. AI is also used to develop new polymers with improved characteristics for various applications, as well as research in the field of nanomaterials design using machine learning methods [1, 12]. In the chemical industry, AI is used to optimize production processes and increase their efficiency. The IBM RXN platform is successfully used to predict the outcome of chemical reactions and optimize synthetic routes, which reduces research time and costs. Companies such as PPG and Dow Chemical use AI to optimize the production of coatings and predict the properties of new materials. DuPont is introducing AI-controlled robots to perform hazardous tasks and automate production processes. Borealis uses AI to improve the energy efficiency of chemical production [3, 17].

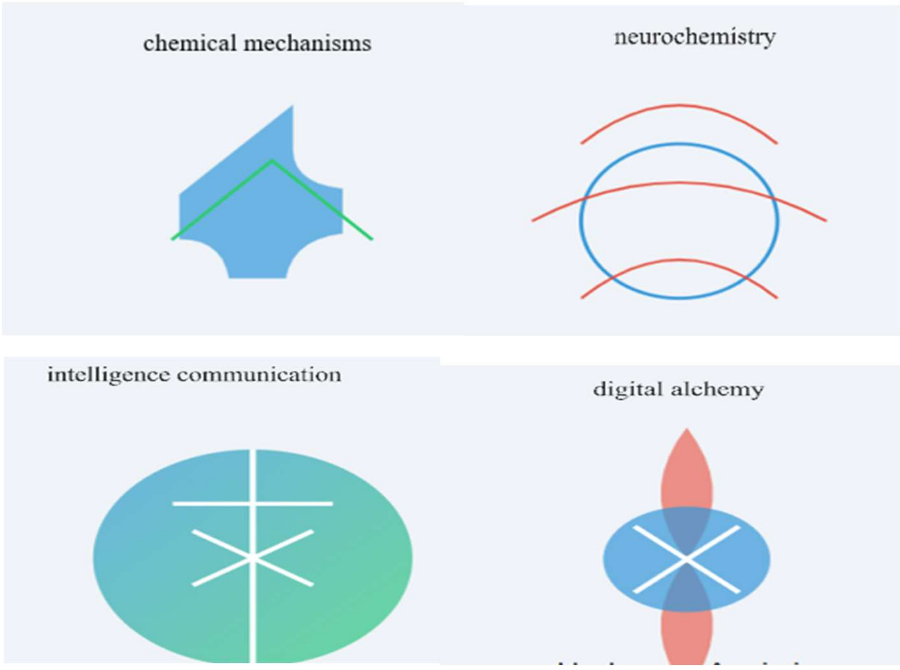

Fig. 3. The interaction of artificial intelligence and chemistry

Analytical chemistry also has examples of successful AI applications. Researchers from Florida State University have developed a machine learning-based tool that accurately determines the chemical composition of salt solutions from their photographs, opening up new opportunities for inexpensive and fast chemical analysis [6, 20].

These numerous examples of successful applications of artificial intelligence in various fields of chemistry clearly demonstrate that AI is already a powerful tool that brings real results, ranging from basic scientific research to practical applications in industry. These examples clearly illustrate how AI helps solve complex scientific and industrial problems, reduce development time, cut costs, and open up new opportunities that previously seemed unattainable [4, 7].

An important prerequisite for the successful application of artificial intelligence in chemistry is close cooperation between the developers of machine learning algorithms and experts in the relevant fields of chemical science. In order for AI to be a truly effective tool, it is necessary to ensure that models are trained on high-quality and relevant data, and that their results are carefully interpreted and validated by expert chemists.

Conclusion. Artificial intelligence is rapidly transforming the landscape of chemical research and industry, offering unprecedented opportunities to accelerate scientific discovery, develop innovative materials, and optimize chemical processes. AI applications are already showing significant success in key areas such as drug discovery, materials science, chemical reaction prediction, and analytical chemistry. The further development of machine and deep learning algorithms, their integration with other advanced technologies, and the growth in the volume and quality of available chemical data open up new prospects for solving complex scientific and technological problems.

Despite existing challenges related to data quality, model transparency, and ethical considerations, the potential for AI to revolutionize chemistry is enormous. To fully realize this potential, further research and development in this area is needed, as well as active interdisciplinary collaboration between chemists, computer scientists, and other professionals. Given the rapid progress in the field of artificial intelligence, it is safe to predict that in the future AI will play a key role in solving global problems related to chemistry, such as developing new effective treatments for diseases, creating environmentally friendly and sustainable materials, and optimizing chemical processes for sustainable development.

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