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On the Technologies of Artificial Intelligence and Machine Learning for 2*D* Materials

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Abstract—Nowadays, an important area of research in the field of two-dimensional (2*D*) materials and their surface characteristics is acceleration of the process of searching for synthesis parameters for new structures with unique properties. The achieved level of development of artificial intelligence and especially machine learning makes it possible to use these techniques to solve a wide range of problems, including in the field of 2*D*-materials science. This article describes the current state of technologies of artificial intelligence and its subset, machine learning. The presented literature review describes the capabilities of machine-learning technologies for solving problems in the field of 2*D*-nanomaterials both at the stages of computer design and chemical synthesis and diagnostics of the obtained 2*D*-nanostructures and their surfaces. Much attention is given to the application of machine-learning technologies to find new 2*D* materials with specified characteristics that can be successfully used in a number of promising areas of application.

Keywords: artificial intelligence, machine learning, two-dimensional materials, graphene

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INTRODUCTION

Two-dimensional nanostructures occupy a special place among nanomaterials. An important stage in the development of this area was the discovery of graphene and the subsequent study of its unique properties [1]. Due to their unique characteristics, graphene-like materials are now in demand in various fields, including biomedical technologies [2]. Unfolding on a wide front, research has opened the way for a number of innovative applications [3]. Recently, scientific research in this area has not been limited only to graphene-like nanostructures [4]. 2*D* materials have extremely interesting properties for use in electrocatalytic processes [5]. Two-dimensional nanocatalysts turned out to be no less promising for photocatalytic processes of CO_2 reduction [6].

An important feature of two-dimensional nanostructures with a developed surface is the possibility of their use as highly sensitive sensors [7]. The unique characteristics of some classes of two-dimensional nanostructures make it possible to use them in new types of electrochemical batteries and fuel cells [8]. Recent research in the field of defect engineering has allowed an increase in the efficiency of 2*D* photocatalysts for organic synthesis processes [9]. Recently, active research has begun on new classes of substances—van der Waals heterostructures, which are based on two-dimensional layers [10]. New classes of two-dimensional materials such as borophenes [11] and MXenes [12] may turn out to be very promising for practical innovative application. It should be noted that, due to the special characteristics of two-dimensional nanostructures, various special approaches are being developed for their study, including for nanodiagnostics using synchrotron-radiation sources [13]. The demands for development of the high-tech sector of the economy dictate the need to accelerate the search for new two-dimensional materials, and new end-to-end technology based on artificial intelligence opens up significant prospects in this area.

The objective of this paper is to review current research in the field of artificial intelligence and machine-learning technologies for two-dimensional materials.

INTRODUCTION TO ARTIFICIAL-INTELLIGENCE TECHNOLOGY AND METHODS OF MACHINE LEARNING

In over half a century of development, artificial intelligence has acquired a solid theoretical base, establishing itself as an independent scientific direction, mainly related to the field of computer science. Nevertheless, the problems raised by artificial intelligence are manifested in related scientific fields, for example, in the theory of control systems, neurosci-

ences, applied mathematics, linguistics, philosophy and psychology.

Approaches to the formation and construction of scientific research in artificial intelligence, as well as in other scientific fields, can be divided into abstract-symbolic and computational-pragmatic directions, as shown in Fig. 1. The abstract-symbolic direction in artificial intelligence goes back to the set-theoretical and logical foundations of the most abstract and at the same time the most practical of all fundamental sciences, i.e., mathematics.

On the basis of predicate logics of the first order, theoretical logic systems are successfully created, used in artificial intelligence for automatic theorem proving, for example, a formal logic system of automatic inference based on the deductive theory of residues modulo [14]. Applied software implementations of systems for automatic theorem proving by means of first-order logic [15] and libraries of test problems for automatic theorem proving using clause normal forms [16] are also being developed quite intensively. There are also modern implementations in the logic language SWI-Prolog, designed for the automatic generation of expert text processing systems based on deductive inference on clause graphs [17].

The other side of symbolic intelligence and the representation of knowledge in artificial-intelligence systems is associated with an obvious fact: an exclusive part of real information that is input to artificial-intelligence systems is ill-conditioned and systematized, having a possibility and probabilistic nature. One of the methods for describing this feature of symbolic intelligence is fuzzy logic. Techniques and approaches that are used in fuzzy logic have now gone far beyond the consideration of logic as such. The half-century development of fuzzy logic in work [18] is given by its founder L. Zadeh and in work [19], by D. Dubois and A. Prade, well-known scientists in this field. The spread of ideas and methods of fuzzy logic in the field of artificial intelligence turned out to be so wide that at present it can be considered one of the "symbols" of not only symbolic, but also computational artificial intelligence. Fuzzy logic, constructed on the basis of the mathematical apparatus of fuzzy sets, has been many times subjected to improvements and extensions that are of particular importance for artificial-intelligence systems, for example, for a complex-valued representation of data [20] in the direction of plausible inference on intuitionistic fuzzy sets [21], fuzzy analytical [22] and fuzzy cognitive [23] approaches to decision making.

The main attention in modern approaches to the representation of knowledge in artificial-intelligence systems is paid not so much to the very principles of organizing and formalizing knowledge bases as a set of agreements of an ontological nature, that is, ensuring structuredness, coherence, and then the process of interpretability, transfer of knowledge into a machine format. For this, numerous families of description logics [24] are widely used, including description ontologies [25] and languages for representing ontologies such as OWL (Web Ontology Language).

The processes and methods of comparing the artificial knowledge of reality seem to be much more complex, and in such a way that, on the one hand, reproduced artificial knowledge does not break away from reality, is not based on conjectures and has properties that are confirmed in the external world. On the other hand, it is necessary that plausible reasoning in artificial-intelligence systems be pragmatically suitable and effective for their formal execution in computing systems that in some cases, for example, in autonomous mobile platforms, have limited computing resources. For this, different approaches to plausible reasoning of the theory of artificial intelligence use different ways of describing and formally determining the measure of information uncertainty, confidence and conviction in knowledge, together with the degree of plausibility of the reasoning process itself. Difficult-to-formalize concepts of uncertainty and disconfidence as the initial prerequisites for the research process gave rise to a significant number of mathematical directions and approaches, the apparatus of which was subsequently used in the theory of artificial intelligence. These include classical and Bayesian probabilistic approaches, evidence theory, theory of possibilities, interval non-classical probabilities, probabilistic logic, situational and event calculus, the theory of reconsiderable reasoning, argumentation theory, Kripke models, multi-agent and granular computation, as well as broad classes of plausible inference systems based on induction and abduction. Under conditions of the entry of large amounts of information into artificial-intelligence systems, the modern development of methods of argumentation theory, such as the automatic extraction and structuring of arguments [26] and artificial computational argumentation [27], becomes important.

The directions of abstract-symbolic intelligence, discussed above, refer to the so-called "top-down" approaches in the theory of artificial intelligence. No less well-known are the "bottom-up" approaches, which originate from the tasks of studying and modeling the neurobiological principles of the functioning of natural organisms and the human brain. Particularly well-known and extremely widespread today is the apparatus of artificial neural networks, which is constantly supplemented not only with new technical capabilities, but also constantly undergoing revision and approaching the imitation of human cognitive and thinking abilities.

At present, it is more important that the very mathematical apparatus of artificial neural networks, without pretending to be extremely accurate in reproducing neurobiological processes occurring in natural organisms, supplemented by the colossal computing

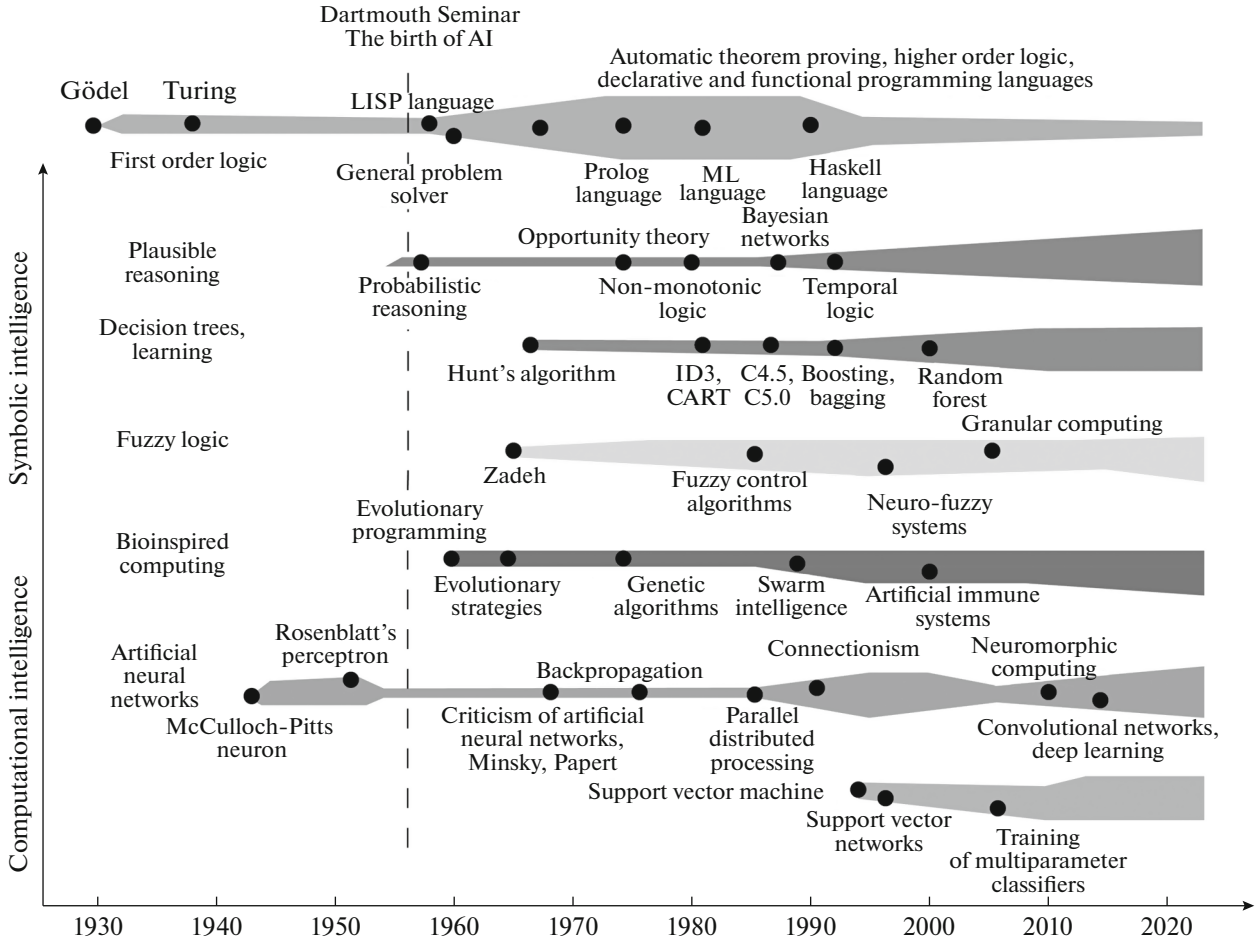

Fig. 1. Modern trends in artificial intelligence.

capabilities of modern computers and infocommunication networks, can be used everywhere in a wide range of applied areas, where there are problems of object classification and pattern recognition.

The great popularity of artificial neural networks is facilitated by the principles of their functioning, fairly simple (if considered at the initial level) and understandable to the vast majority, a huge number of scientific and popular articles, books and manuals on the creation, training and use of artificial neural networks, as well as their many implementations in in the form of software modules and libraries that even a non-specialist in the field of programming can use. Indeed, the principle of functioning of an elementary artificial neuron was initially very simple: a weighted sum of input numerical values transmitted from receptors or artificial synaptic connections of the previous layer activates a simple jump-like threshold function, which either transfers or does not allow further propagation of the output value from this element to the next one. Naturally, one artificial neuron could not adequately solve the problem of classifying a set of objects, in addition, the requirement for the presence of many inputs from various sensory devices, i.e., artificial receptors, gave rise to the emergence of various options for connecting artificial neurons into network structures called topologies of artificial neural networks. Over time, various types of threshold functions have become more complex, which are usually called the activation functions of artificial neurons. Now an artificial neural network is a massively parallel distributed information processing system, the supercomputer implementations of which can number tens of millions of artificial neurons with a much larger number of artificial synaptic connections between them. Obviously, before using such a network, or one with a significantly smaller size, it is necessary to choose a goal and present the desired end result to make efforts aimed at minimizing incorrect classification options, incorrect sampling, inappropriate choice of alternatives formed by the output of an artificial neural network. In a simplified sense, training an artificial neural network is a procedure for changing the weights and biases of a network, performed in accordance with some learning algorithm, and designed to "teach" the network to give a specific answer to a specific set of

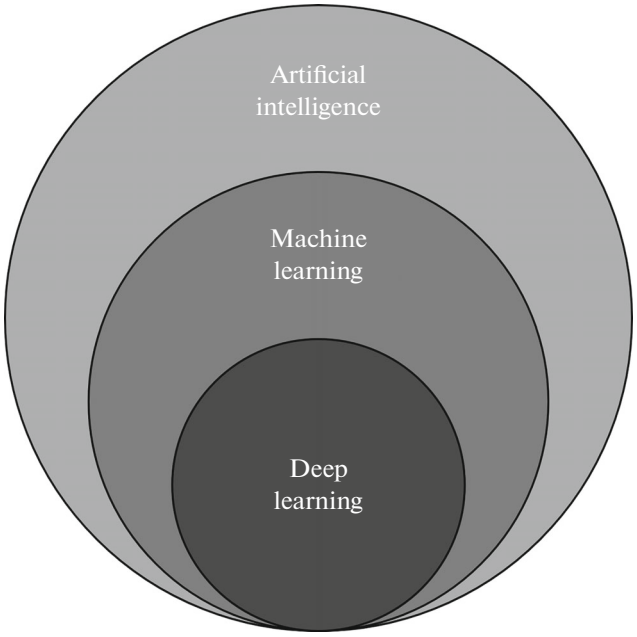

Fig. 2. Position of machine learning in artificial intelligence.

input data. Learning algorithms are very important, both in terms of accuracy of the output classification, together with the adequacy of their inputs, and in terms of computational complexity, which characterizes the time spent on the process of preliminary network training.

The choice of the general architecture and algorithms for training artificial neural networks remains a rather nontrivial task to this day and requires at least initial knowledge from the researcher in many areas related to artificial intelligence, especially mathematical skills. It is not always possible to successfully solve the main problems of classification, clustering, pattern recognition based on relatively simple architectures and learning algorithms for artificial neural networks. In such cases, they resort to the use of complex multilevel architectures of artificial neural networks, due to which it becomes possible to represent the input data for the task at various levels of abstraction using various nonlinear computational nodes, i.e., neurons. This distinction is emphasized in the name of a group of machine-learning methods called "deep learning" and often by the presence of a super-precise structure of artificial neural networks. This area of machine learning uses a multi-level representation of the function to be trained and often has many parameters, and the learning process itself is performed on big data to improve the accuracy of object classification or to predict processes. A natural consequence of this complication is a significant increase in both technical resources and the time spent on training such a multilevel and heterogeneous artificial-neural-network architecture at each of the levels. With the advent of corresponding computer hardware and effective computing tools, deep-learning technologies for artificial neural networks are now at the stage of growth and significant interest in many applied areas of using artificial-intelligence systems.

In addition, in the modern world, machine-learning methods, and especially deep learning, are actively used to solve a wide range of problems, both applied and scientific. Machine learning is one of the areas of artificial intelligence (Fig. 2), which received a powerful impetus to development due to the increased computing power of modern computer technology and the availability of a large amount of data.

The problem that machine-learning methods solve is finding an unknown relationship in the data, which is called a training sample. Learning is the process of finding an algorithm that would approximate the unknown dependence in an optimal way. There are three main types of machine-learning methods:

(1) Supervised learning. For this type of methods, the training sample is represented by object-response pairs. The main problems of supervised learning methods are:

(a) classification—the case when the set of answers is finite;

(b) regression—the case when the set of answers is infinite (real numbers).

(2) Unsupervised learning. In this case, the training sample is only a set of objects. Typical problems of unsupervised learning include:

(a) clustering—dividing the sample into several non-intersecting sets;

(b) dimensionality reduction—representation of a training sample in a space of a lower dimension;

(c) data visualization—displaying data in the form of graphs on a plane and others.

(3) Reinforcement learning. A machine-learning method called an agent learns through interaction with its environment. During training, the agent learns to act in such a way as to maximize the potential gain.

Supervised learning algorithms include:

(1) Bayesian classifier [28] is based on the application of Bayes theorem. After finding the posterior probabilities of the classes for the object under consideration, described by a set of features, the algorithm selects the most probable class as an answer. Used primarily for classification problems.

(2) Support vector machine [29, 30] constructs an optimal dividing hyperplane in the parameter space of the training sample. It is a good method for solving classification problems, but also used for regression problems.

(3) Decision tree [31] is a tree structure intended for decision making. Decision trees consist of decision rules according to which branching occurs, and first of all, features with the minimum entropy are selected.

The method can be used for both classification and regression.

(4) The *k*-nearest neighbors method [32] is a simple metric classification algorithm. The object is assigned a class, the objects of which are the most among the *k* nearest neighbors. The method can also be used for regression problems, in this case, the average value of *k* nearest neighbors is assigned to the object.

An example of unsupervised learning algorithms are:

(1) Algorithm of *k* means [33] is an iterative clustering algorithm that assigns an object to the cluster, the center of which is closer. Cluster centers are recalculated at the end of each iteration.

(2) Principal component analysis (PCA) [34, 35] is one of the main methods for solving the problem of dimensionality reduction, which constructs new components losing the least amount of information. Principal components can be found by the singular value decomposition (SVD) of feature objects.

MACHINE-LEARNING TECHNOLOGIES FOR SEARCHING FOR NEW MATERIALS AND STRUCTURES

Traditional trial and error methods tend to impede large-scale searches for new functional materials. Multiscale computer-modeling approaches, enhanced by machine-learning methods, take the process of finding new functional materials to a fundamentally new level.

For example, Schleder et al. used machine-learning technologies to define thermodynamically stable two-dimensional materials [36]. For this, the materials were classified according to the energies of formation. Based on data on the composition and symmetry (without using information on atomic positions), the materials were assigned to the class with low, medium, or high stability. The proposed approach made it possible to identify the most promising new two-dimensional materials for a more thorough analysis. More than a thousand new structures were generated to test the applicability of the model. For some of them, the classification was confirmed by calculations in the density functional theory (DFT) approximation. As a result, a new material was proposed that has a potentially high efficiency for the photoelectrocatalytic decomposition of water: Sn_2SeTe.

In [37], a method was proposed that combines high-performance *ab initio* calculations and machine-learning approaches to predict the structures of two-dimensional octahedral oxyhalides with improved optoelectronic properties. For this, a model was developed based on an extensive dataset that included 300 structures of two-dimensional octahedral oxyhalides, generated based on calculations in the DFT approximation. The model allowed acceleration of the validation of 5000 potential optoelectronic materials based on octahedral oxyhalides. The distortion factors of folded octahedra played a key role in predicting the optoelectronic properties in this model. Based on the developed model, it was shown that $Bi_2Se_2Br_2$, Bi_2Se_2BrI, and $Bi_2Se_2I_2$ have optimal optoelectronic properties: a moderate band gap, high mobility of charge carriers, and superhigh absorption coefficients.

The authors of [38] used a combination of machine learning and the high-performance screening of two-dimensional materials for photovoltaics [8]. As a result, twenty-six most promising candidates were selected from 187093 inorganic crystal structures. In addition to predicting materials with the highest energy-conversion efficiency, the model made it possible to establish a fundamental pattern of structure and properties: the packing factor affects the likelihood of having suitable physical properties. The results showed that Sb_2Se_2Te, Sb_2Te and Bi_2Se_3 have a high energy conversion efficiency and are candidates for use in photovoltaics.

In [39], Frey et al. used the Positive and Unlabeled learning method to determine the likelihood of synthesizing theoretically proposed two-dimensional materials based on transition metal carbides, carbonitrides, and nitrides. On the basis of the model, 18 materials with the highest probability of the possibility of synthesis were identified, while the highest probability was shown by a two-dimensional material based on zirconium: Zr_2GaC.

In [40], Momeni et al. in their review considered various combinations of theoretical calculations of two-dimensional materials and machine-learning methods. In particular, the features of predicting the thermodynamics and kinetics of the synthesis of two-dimensional materials were shown. The authors suggest that there will be two main approaches for the design and synthesis of new two-dimensional materials. One approach assumes that before the synthesis of materials, computer simulation will be carried out, taking into account the physicochemical conditions of synthesis. The second approach will involve a closed loop in which the synthesis conditions will be adjusted in real time.

Fujikake et al. in [41] used interatomic potentials to model guest lithium atoms in graphene, graphite, and amorphous carbon nanostructures. To train the neural network, the data from the DFT calculations were used. Instead of considering the complete Li–C system, the energy and force differences resulting from the intercalation of lithium atoms were considered. It was shown that consideration of the pair potential made it possible to detect the interaction between lithium atoms, which improved the model of the Gaussian potential. Thus, the possibility of using pair potentials obtained on the basis of machine-learning algorithms was shown.

Table 1. Functional 2*D* materials predicted by artificial-intelligence technologies

Material	Application	Source
Sn_2SeTe	Water splitting photocatalyst	[36]
$Bi_2Se_2Br_2$, Bi_2Se_2BrI and $Bi_2Se_2I_2$	Photovoltaics	[37]
Sb_2Se_2Te, Sb_2Te and Bi_2Se_3	Photovoltaics	[38]
Zr_2GaC	–	[39]

The atomic structure of boron-doped graphene was investigated in [42]. To analyze the data set, the authors used a machine-learning method such as Monte Carlo tree search with Bayesian unfolding to find the most stable structure of B graphene with a boron concentration of up to 31.25%. It was found that in free-standing, pure graphene, doped boron atoms replace carbon atoms at various sublattice sites, with the B–B configuration dominating in cases of a high boron concentration. Doping with boron can increase the work function of graphene by 0.7 eV at a boron content above 3.1%.

Table 1 shows functional two-dimensional materials predicted on the basis of artificial-intelligence technologies.

ARTIFICIAL-INTELLIGENCE TECHNOLOGIES FOR PREDICTING THE PHYSICAL PROPERTIES AND STRUCTURAL CHARACTERISTICS OF 2D MATERIALS

In recent years, artificial-intelligence tools have been proposed to improve the efficiency of diagnostic methods for 2*D* materials. In addition, the use of artificial-intelligence algorithms allows prediction of the structural characteristics, electronic and thermal properties of various two-dimensional structures.

To investigate 2*D* materials, machine-learning algorithms integrated with other approaches can be used to quantify the thickness of the graphene layer and the amount of impurities in it. For example, Leong et al. presented a fast and non-destructive approach to using artificial intelligence to assess the quality (i.e., packing order and number of layers) of centimeter-sized graphene samples by analyzing Raman spectroscopy data [43]. To use the artificial-intelligence tool to analyze Raman data, end users only need to download the Raman spectra collected from the graphene samples under study as input, and analysis of the Raman data will be performed automatically. When using this technique, three parameters ω_G, ω_{2D}, and Γ_{2D} (ωG and ω_{2D} are the positions of the *G* and 2*D* bands, respectively, Γ_{2D} is the half-width at half-height of the 2*D* peak) were extracted from each Raman spectrum, then they were chosen as functions clustering in the *k*-means algorithm. For example, using this method, two clusters were identified, which were a single layer and a two-layer graphene. In addition, it was shown that, although only three parameters are considered, the proposed analysis makes it possible to recognize graphene with a thickness of one to five layers and approximately estimate their twist angles. It is reported that this algorithm is fully automated, does not require human intervention, is highly reliable (accuracy 99.95%) and can be extended to other 2D materials for which Raman analysis is a convenient method for studying the number of layers in layered compounds such as GeS, SnS, MoS_2 and others. In addition, the developed method of quality control using artificial intelligence is not limited to analysis of the Raman spectrum and can be applied to the analysis results using other methods for determining the characteristics of 2*D* materials, such as scanning electron microscopy, scanning probe microscopy, etc.

Other characteristics of graphene have also been investigated using artificial intelligence algorithms. For example, Garg et al. [44] proposed a new computational approach to assess the mechanical properties of graphene samples. In this method, factors influencing the shear modulus of graphene structures are analyzed using molecular dynamics (MD) modeling. The resulting data is then processed using gene expression programming. Moreover, this approach makes it possible to formulate an explicit dependence of the shear modulus of a graphene nanostructure on the aspect ratio of graphene sheets, the temperature, the number of atomic planes, and the number of defects. It was found that the shear modulus predicted using the proposed model is in good agreement with the experimental results obtained from publications (the R^2 value is about 0.94). In addition, in order to find out the specific influence of each of the input parameters of the system on the shear modulus of graphene structures, the sensitivity of the method to the input values was estimated. The results showed that it is the number of defects that has the greatest influence on the shear modulus for each graphene sheet, and then, in decreasing order of influence, are the temperature, the number of layers, and the aspect ratio.

The paper [45] demonstrated the use of machine learning to predict the differences between the electronic properties of graphene nanostructures at two levels of approximation: the Density Functional method and the Self-consistent Charge Density

Functional Tight Binding method. In doing so, model optimization and feature selection were performed for 70% of the dataset, while the remaining 30% were used to test the predictive ability of the models. As a result, the prediction accuracy of the proposed machine-learning model was determined, which was 94 and 88% for the Fermi level energy and for the band gap, respectively. In another study by the aforementioned research group [46], machine learning was used to predict the band-gap energy of graphene nanoflakes using the Topological Autocorrelation Vectors method. The data sample consisted of the band-gap energies of 662 optimized graphene nanoparticles. Machine-learning modeling has shown that the most suitable relationships appear at topological distances in the range from 1 to 42 with a prediction accuracy of more than 80%. The proposed model can statistically significantly distinguish graphene nanoflakes with different energy gaps based on their molecular topology.

Dopant atoms play a key role in shaping the electronic properties of many materials. However, the number of possible combinations of types and concentrations of doping atoms leads to a significant number of possible atomic configurations. Dong et al. used deep machine-learning approaches to predict the band gap of graphene doped with boron and nitrogen atoms [47]. To train the neural network, data sets obtained on the basis of *ab initio* calculations were used. The resulting model successfully predicts a band gap with an accuracy of better than 90% with a root-mean-square deviation of about 0.1 eV.

In addition, the electronic properties of not only graphene nanostructures, but also two-dimensional transition-metal carbides and nitrides (Mxenes) were investigated using machine-learning models. For example, Rajan and colleagues have built statistical learning models to accurately predict the band gap of this vast class of materials [48]. The models were developed using nuclear ridge regression, support vector regression, Gaussian process, and bagging using the properties of Mxenes such as boiling and melting points, group numbers, atomic radii, phases, bond lengths, etc. as input functions. It was noted that among them, the Gaussian process model predicts the band gap with the smallest root-mean-square error of 0.14 eV within a few seconds. At the same time, the authors of the paper developed a metal-semiconductor classification model with an accuracy of 94%.

Patra et al. in [49] used supervised machine learning, MD simulation, and high-resolution transmission electron microscopy to fully understand the phase transformation in 2*D* transition metal dichalcogenides. Genetic algorithms were combined with MD to study the extended structure of point defects, their dynamic evolution, and their role in inducing a phase transition between the semiconductor (2H) and metallic (1T) phases in a MoS_2 single layer. The genetic algorithm is used to efficiently search for the most energetically favorable distribution of atomic defects, which, as was found, is the organization of the predominant type of defects (sulfur point vacancies) into extended lines in the MoS_2 layer. Using high-resolution transmission electron microscopy, the results were confirmed and a phase transformation from the 2H- to the 1T phase, which is localized near these linear defects when exposed to high doses of an electron beam, was assumed. The MD simulation, in turn, explains the molecular mechanism of this defect-induced phase transformation. It consists in the fact that sulfur atoms locally slide to defects and lead to the formation of an intermediate α phase, which triggers the formation of the 1T phase. It is noted that the final amount of the 1T phase can be retained by increasing the concentration of defects and temperature.

Yang et al. used machine learning to determine the interfacial thermal resistance in thermally conductive materials based on graphene and hexagonal boron nitrite based on data on the system temperature, adhesion forces, and in-plane strain expansion [50]. The training dataset was obtained using calculations in the MD approximation. The best results were shown by methods based on a two-layer neural network.

Han et al. in [51] used an algorithm based on a neural network architecture (encoder-decoder) to identify and determine the thickness of 2*D* samples by real-time pixel-by-pixel recognition of optical microscopy images of various 2*D* materials using semantic segmentation. It has been shown that the trained network can extract graphical features such as contrast, color, edges, shapes, scale sizes and distributions, from which an approach is developed to predict the most important physical properties of 2*D* materials. In addition, the algorithm was found to find correlations between optical microscopy images and the physical properties of 2*D* materials. For example, it was predicted that 1T'ould be similar to 1T–$HfSe_2$ in the trained group, which corresponds to the similar crystal structure of these materials. Thus, the proposed approach can be used to predict the properties of new, not yet investigated 2*D* materials.

Machine learning has been successfully applied to the optical identification of 2*D* nanostructures such as graphene, MoS_2, and heterostructures of these two materials [52]. In the course of this study, an approach was developed based on the trained and automatic analysis of the red, green, and blue information of optical photographs of 2*D* nanostructures using the support vector machine. It turned out that when identifying 2*D* heterostructures, the regions of the substrate, graphene, MoS_2, heterojunction, as well as the resist residues from the transfer process, can be automatically recognized with an accuracy of 90.16%. The experimental results show that the developed approach allows one to accurately characterize graphene, molybdenum disulfide, and their hetero-

Table 2. Properties and characteristics of two-dimensional materials predicted by artificial-intelligence technologies

Material	Properties and characteristics	Artificial-intelligence tools	Source
Graphene	Number of layers	*k*-means algorithm	[43, 53]
Graphene	Shear modulus	Gene expression programming method	[44]
Graphene	Fermi energy and band gap	Multiple linear regression, decision tree, random forest, support vector machine	[45]
Mxenes	Band gap	Nuclear ridge regression, support vector machines, Gaussian process regression and bagging	[48]
MoS_2	Distribution of point defects	Genetic algorithm	[49]
Graphene, MoS_2	Thickness of samples, presence of impurities in them	Support vector machine	[52]
Van der Waals heterostructures	Interlayer distance and band gap	Feed-forward neural network, support vector machine, relevant vector machine, random forest	[55]

structures in terms of sample thickness, the presence of impurities in them, and even the packing order.

For the analysis of optical images of 2*D* materials, it was proposed in [53] to develop an approach for the fast identification of 2*D* materials, the essence of which is a combination of a reflection model based on Fresnel law and machine learning. In this study, such three effective indices as optical contrast (OC), total color difference, and red-green-blue index analysis were used to determine the optimal Si/SiO_2 substrates and the number of layers of 2*D* materials deposited onto the substrate using optical microscopy. In doing so, firstly, the OC and the total color difference were used to determine the suitable substrates that maximize the difference not only between the 2*D* material and the substrate, but also between the 2*D* material of different layers. In this case, the algorithms of *k*-means and *k*-nearest neighbors are used to obtain a database of the thickness of 2*D* materials (graphene and MoS_2 on a Si/SiO_2 substrate) and to test their optical images using the "red–green–blue" index.

Wang et al. in [54] independently developed such machine-learning approaches as Materials Genome Integration System Phase and Property Analysis (MIPHA) and rMIPHA (based on the R programming language) for predicting the 2*D* properties of 2*D* materials. When using them, the two-dimensional and three-dimensional microstructural analysis of steels, direct analysis of property predictions and reverse analysis of the dependence of properties on microstructure were carried out. At the same time, quantitatively determined data on the microstructure and properties constitute the "genomes of materials" used for subsequent forward and reverse analyses, on the basis of which stress-strain curves were then predicted.

As noted earlier, recently, new classes of substances — van der Waals heterostructures – have been actively studied. In principle, the number of different structures that can be synthesized is not limited. Therefore, even the theoretical modeling of possible structures in the DFT approximation is very time consuming. The combination of computer modeling and machine-learning methods is a more efficient alternative to both DFT calculations and chemical synthesis. Parameters such as the interlayer spacing and band gap for hybrid van der Waals heterostructures were predicted based on machine-learning methods [55].

Table 2 shows the properties and characteristics of two-dimensional materials predicted on the basis of artificial-intelligence technologies.

CONCLUSIONS

A review of current published data on the use of artificial-intelligence technologies and especially machine learning shows that this new end-to-end technology is already being actively used to solve a wide range of problems, including in the field of two-dimensional materials science at all stages of research (computer design, chemical synthesis and subsequent diagnostics of the characteristics of the obtained nanomaterials). This makes it possible to give a significant new impetus to a new stage in the development of studies of surfaces and two-dimensional nanostructures both in the search for parameters for the synthesis of new 2*D* materials and in predicting their physicochemical characteristics, promising in terms of practical application.

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