Engineering and Technology Journal
Journal homepage: https://etj.uotechnology.edu.iq

# Applications of artificial intelligence in nanotechnology

**Shahad M. Eabd Alrida[a], Ola D. Obed[a], Elaf M. Taha[a], Thamer A. Abdullah[a]*, Mustafa M. Hathal[b], Viola Somogyi[b]**

[a]Applied Sciences Dept., University of Technology-Iraq, Alsina'a street, 10066 Baghdad, Iraq.
[b]Asustainability Solutions Research Lab, Faculty of Engineering, University of Pannonia-Veszprém, Hungary.
*Corresponding author Email: 100249@uotechnology.edu.iq

## HIGHLIGHTS

- Simulating nanoscale systems is challenging due to the lack of real optical images.
- AI can enhance simulation quality and simplify analysis.
- Machine-aided design is essential for synthetic molecular design at the nanoscale.
- Renewable energy is vital for global sustainability and energy security.
- AI shows promise in developing efficient materials for power conversion and supply.

## ARTICLE INFO

**Handling editor:** Qusay F. Alsalhy

**Keywords:**

Nanomaterials; Machine Learning; Nanocomposites; Artificial Neural Networks; Molecular Design; Artificial intelligence; Nanotechnology; AI.

## ABSTRACT

Artificial intelligence (AI) is emerging as a prominent technological advancement. It is the act of replicating human intelligence for many purposes. In contrast to conventional methodologies, artificial intelligence (AI) is undergoing tremendous advancements. The present state of artificial intelligence (AI) technology enables them to effectively address numerous intricate difficulties with proficiency comparable to a human's. The significance of advancements in AI is particularly evident in machine learning, where the techniques and algorithms are effectively applied to address many problems, including those in nanotechnology. In contemporary nanotechnology, it is crucial to expedite the search for the most favorable synthesis parameters while developing novel nanomaterials. The convergence of machine learning and nanotechnology necessitates a comprehensive examination of existing data on the application of artificial intelligence (AI) in addressing challenges in the nanomaterials science field. This review should encompass various stages, including computer design, chemical synthesis, and diagnostics of the resultant nanomaterials. Significant emphasis is placed on employing machine-learning technologies to investigate the thermal and dynamic characteristics of nanofluids, the sorption processes of nanocomposites, the catalytic activity of nanoparticles, and the toxicity of nanoparticles. Additionally, these technologies are utilized to address nanosensor issues and process experimental data acquired during the diagnostics of different nanomaterial properties.

## 1. Introduction

Multidisciplinary research integration is still underway. AI has used biological inspiration to construct neural networks and evolutionary algorithms, while nanotechnology mixes physics, chemistry, and engineering. Integrating present-day artificial intelligence with nanosciences can advance both areas of study, ushering in a new era of information and communication technology with far-reaching societal effects—possibly even bringing biology and technology together as shown in Figure 1. Nanoscience research, both theoretical and applied, has used AI to decipher experimental procedures and create novel nanomaterials and gadgets. A few research have examined how nanoscience will boost computing power for present and future AI systems. This study tackles these concerns in the context of rapid progress in several fields, how advances in computational intelligence could improve nanotechnology, and how it could be utilized to build new paradigms for artificial intelligence, thereby increasing their application and combining them with biotechnology. There are several applications of AI paradigms in nano research. When applied to the working size of nanotechnology, physics has limitations distinct from macroscopic physics. Therefore, nanotechnology must deal with the proper interpretation of outcomes from any system or instrument at this scale [1], which makes the situation worse because multiple elements often strongly influence the signal. Numerical simulations are commonly utilized to accurately interpret experimental results because analytical approximations are challenging to construct; this is where AI techniques like machine learning paradigms can help provide scientific results and develop nano applications.



http://doi.org/10.30684/etj.2024.148957.1736
Received 21 April 2024; Received in revised form 07 August 2024; Accepted 09 August 2024; Available online 12 September 2024
2412-0758/University of Technology-Iraq, Baghdad, Iraq

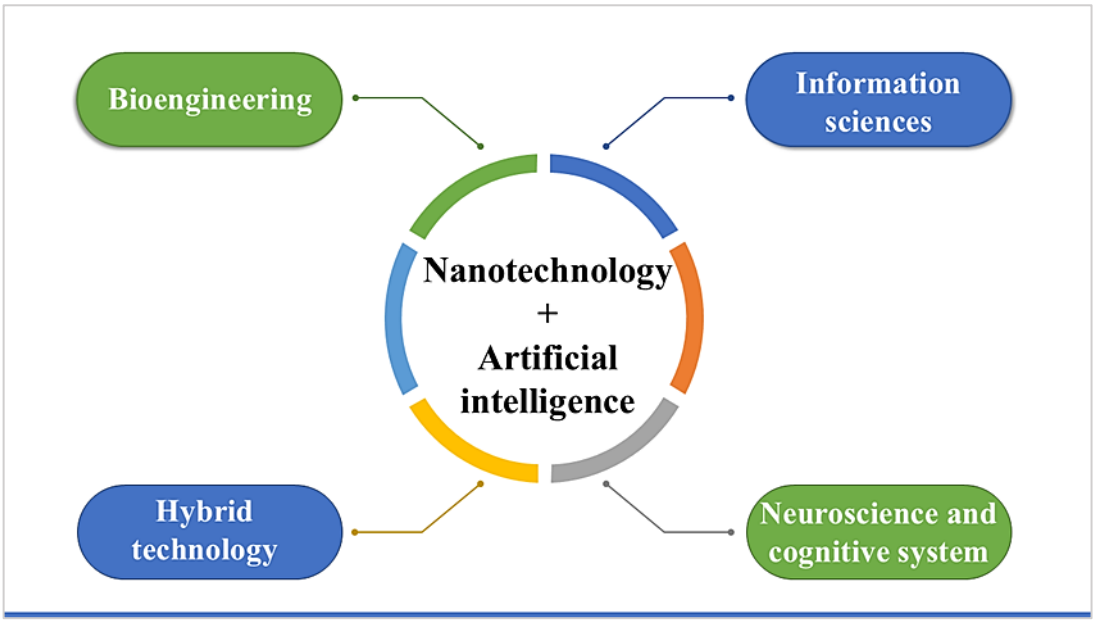


**Figure 1:** Nanotechnology and artificial intelligence

Nanotechnology and artificial intelligence are anticipated to have an impact on various fields, including bioengineering, cutting-edge information sciences based on innovative computer architectures and data depictions, hybrid technologies that combine biological entities with nanotechnological machines, as well as studies into cognitive systems and neuroscience as shown in Figure 1 [1,3,5]. With machine learning techniques, complicated or unknown functions or data can be described and generalized, and numerous interacting parameters can be treated quickly [2,3]. Artificial neural networks (ANNs) are used to learn input-output functions using supervised or unsupervised algorithms to calculate their connection weights. Different bio-inspired AI paradigms use genetic or evolutionary algorithms for optimization and search problems. For categorization, grouping, association, prediction, data mining, and control, support vector machines, decision trees, Bayesian networks, and various similar techniques can be utilized to solve complex problems in nanotechnology research. Machine Learning (ML) has identified compounds and materials with excellent conductivity, aqueous solubility, bioavailability, and toxicity. This makes it feasible to search millions of molecules, discard dangerous candidates, and pick compounds with desired features for pharmacological, medicinal, and environmental chemistry [4]. This is safe, cost-effective, and sustainable. ML already outperforms classic computation. Shindo and Matsumoto [5] Considering the molecule's atomic coordinates, a neural network ML algorithm predicted atomization energy, maximal absorption intensity, excitation energy at maximal absorption, HOMO, LUMO, initial excitation energy, ionization potential, electron affinity, and polarizability. It learned organic chemicals by the bunch. Results were efficient, accurate, and better than DFT quantum-chemical models for all characteristics. Computational toxicology uses complex models to identify hazardous interaction variables. To provide relevant findings, the model must consider all substance interactions. New toxicity assessment methods were developed as AI and ML evolved Figure 2 and Tables 1, 2. The biokinetics, destiny, and dynamics of the substance's biological response after it reaches the target organ are all interrelated in nanomaterial computational modeling. An ideal mathematical model for simulating nanotherapeutics and engineered nanomaterials (ENMs) in experimental systems is based on biology. ML simulations of nanomaterial biokinetics and interaction in different environments have been successful [6]. Mathematical models that are based on the structure of nanomaterials, methods such as Markov Chain Monte Carlo, & Bayesian procedures are the methodologies that are most commonly utilized in the process of assessing the toxicity that is induced by nanomaterials. Much research is being done on quantitative structure-activity relationships (QSAR) at the nanoscale, also called nano-QSAR [7]. QSAR uses physicochemical features and theoretical descriptors of molecules to predict biological function. QSARs are the most studied and accurate as contemporary DFT-based physicochemical property models. Nanomaterial physicochemical parameters are essential for QSAR modeling. One QSAR method relies solely on a theoretical model. The QSAR of a substance can be derived from chemical reactivity based on molecular orbital energies. Statistical QSAR modeling uses pattern recognition to correlate descriptors with predicted effects [8]. The hybrid QSAR model uses mechanical reasoning and statistical fit to discover predictive descriptors using theoretical considerations [9]. Statistical models calibrate molecular descriptor parameters well. Surface charge, corona, aggregation, solubility, and other physicochemical parameters can predict nanomaterial biological activity. Open-source ML tools can predict a range of nanomaterial qualities using quantitative structure-property relationship (QSPR) methodology that is cross-platform and easy to integrate into nano-informatics workflows [10].

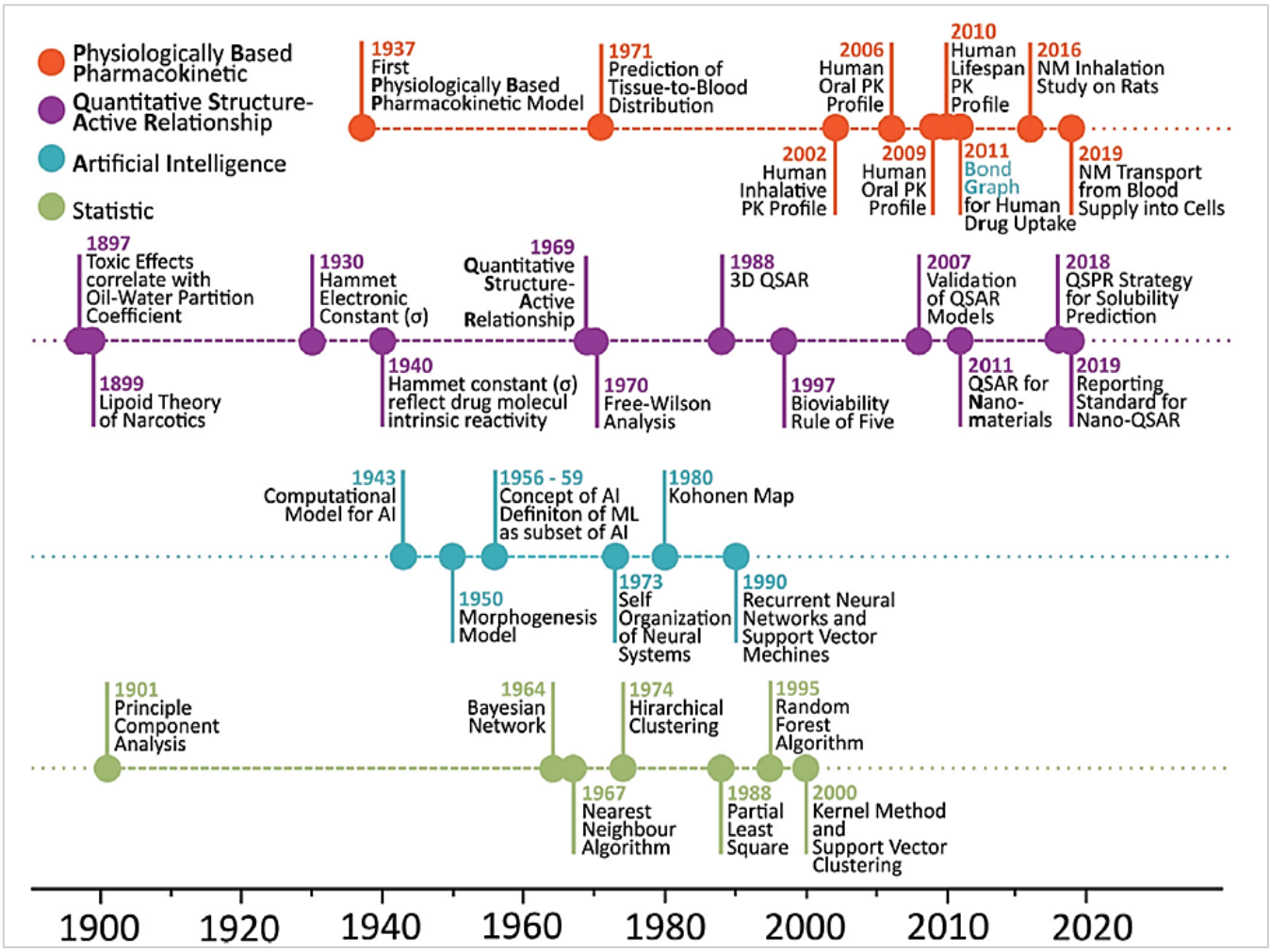


**Figure 2:** Timeline of relevant developments of AI [**12**]

Using them independently or feeding them into more advanced physiologically based pharmacokinetic (PBPK) models is possible. Biological activities and potential interaction partners that could trigger a harmful reaction can be predicted by simulations utilizing QSAR data. Throughout the past few years, numerous computer systems have been created to improve simulations and generate findings that can be relied upon. With QSAR, the hypothesis of border molecular orbitals is an extra parameter that can be used for prediction. A decrease in stability and an increase in conductivity are the results of increasing the difference between the energy levels of the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO). This results in an improvement in the rate at which reactions occur [11]. Figure 2 depicts a timeline of the key developments that have occurred to construct a combining machine learning (ML) based QSAR-PBPK modeling [12,13] for nanomaterial (NM) adsorption, distribution, and metabolism entering the human body through the prediction of the properties of the nanomaterial being studied. During the 20th century, numerous statistical methods for discriminating [14], clustering or grouping [15], prediction [16], and regression [17] of various sets of data were created and extensively utilized in machine learning (ML). In the field of artificial intelligence (AI) and, more specifically, in the field of machine learning (ML), neural networks [18] along with support vector machines [19] were all initially presented to forecast, evaluate, and optimize these data sets. Models for the forecasting of quantitative structure-activity correlations (QSAR) [20] and physiologically basis pharmacokinetic (PBPK) [21] of medications and other chemicals have been introduced simultaneously to predict the behavior of these substances. For PBPK models, the most important input parameters are the partition coefficient [22], biological activity [23], and the other parameters. QSAR, which depends on the Hammet constant [24], can be used to make predictions regarding bioavailability [25]. At the start of the 21$^{st}$ century, QSAR models were expanded by incorporating technique confirmation, NMs, and the forecasting of the solubility of substances for the first time. The most essential developing stages of the PBPK models are human inhalation [26] oral [27], and lifetime [28] PK profiles. Recently developed models describe the absorption, adsorption, and dispersion of NM in rates (after inhalation) [29], as well as the transit of NM from the blood supply into cells [30].

**Table 1:** (AI) Primary machine learning methods and their pros/cons in nanotoxicology and nanomedicines

| Models | Application | Advantages | Disadvantages | Ref. |
|---|---|---|---|---|
| Regression | Forecasts and predictions | Its transparency in delivering important physicochemical descriptor information | Restricted to linear relationships, susceptible to outliers. | [31] |
| Decision tree | All Categories nanomaterials | Auto-selection of input variables, eliminating irrelevant descriptors, and finding valuable data in noisy or large datasets. | It is unable to process non-numerical data. Training takes longer than other types of models. | [32] |
| Support vector machines (SVM) | Nonlinear connections, collinear descriptors, small/large datasets, overfitted models. | Handles classification and regression issues, nonlinear connections, collinear descriptors, restricted datasets, and model overfitting with high precision and conjecture. | Model performance depends on design elements like kernel functions, and SVM result interpretation is difficult. | [33] |
| Artificial neural network (ANN) | Massive datasets and nonlinear data relationships | Allows handling nonlinear structure-activity relationships and massive descriptor collections, including superfluous variables. | Challenges in choosing optimal complexity and overfitting. Broad generalization sensitivity to parameter and network topology changes | [34] |
| Partial least square (PLS) | Reduced variables to make them better suited for additional analysis | It works effectively with frequent noise sources and associated descriptors. | Challenges in evaluating independent latent variable loading and unknown distributional features of estimates. | [35] |
| Principal component analysis (PCA) | Remove the correlation among input variables (physicochemical descriptors) without deleting irrelevant datasets. | Reduces dataset features, Minimise overfitting, Reduces high-dimensional data to two dimensions for easy visualization. | The interpretability of independent variables decreases. The total number of Principal Components may overlook some information relative to the original list of features if not carefully selected. | [36] |

**Table 2:** Artificial intelligence (AI) Modelling and algorithms for nanotoxicology & nanomedicine

| Models | Nanomaterial | Algorithm | In vitro/in vivo/in silico | Ref. |
|---|---|---|---|---|
| PBPK | $CeO_2$ nanoparticles as small as 5 and 30 nanometers | Using linear regression and the Gear method vs. the Berkeley Madonna | In vivo rat model | [37] |
| | Carbon nanotube | The proportion of particles deposited in human alveoli using particle dosimetry | In silico | [38] |
| MPPD | Aerosols and particles (nano-to microparticles) containing copper | Sprague-Dawley rats, male rhesus monkeys, lambs, pigs, and mice (Balb/c and B6C3F1) with an algorithm that deciphers variability. | In silico | [39] |
| | aerosol/airborne nanoparticles | Evaluation of computational fluid dynamics (CFD) and mass transfer over a single path | In vivo | [40] |
| Nano-QSAR/QSPR | Modification of iron oxide nanoparticles | Using linear regression | In silico | [40] |
| | classifies NPs | Artificial neural networks (ANN) | In silico | [41] |
| | Metal oxide NPs | Logistic linear regression with expectation minimization algorithm | In silico | [42] |
| ADMET | classifies NPs | Neighbor-to-neighbor (k-NN) | In silico vnn web server | [43] |
| | All classifies of NPs with a single QSPR model | Machine learning, decision tree, artificial neural network, regression | In silico | [44] |
| | All classifies of NPs | Integrated algorithm | In silico | [45] |
| i-TASSER | Compact nanoflowers encased in peptide gold | Iterative threading and refinement | In vitro and silico | [46] |
| | Distinct SnO2 Nanoparticles | Iterative threading and refinement | In vitro and silico | [47] |
| Quantitative feature–activity relationships (QFAR) | ZnO, CuO, $Co_3O_4$, and $TiO_2$ nanoparticles | CORAL | In silico | [48] |

## 2. Artificial intelligence applied to scanning probe microscopy

Scanning probe microscopy is a popular nanoworld imaging method. This broad idea includes any technique that captures images from probe-sample interactions. Many methods have been created depending on the interaction, even though topographers [49]. The scanning tunneling microscope, created in 1981, is widely acknowledged as the pioneering technology in scanning electron microscopy (SPM), encompassing numerous fundamental components. Despite recent advances in

resolution [50] and atomic manipulation capabilities [51], deciphering microscopy signals remains a formidable obstacle [52]. The primary problem is that most interactions between tips and samples are complex and parameter-dependent. Artificial intelligence methods work well for these problems. Multi-modal SPM imaging, which uses numerous channels to offer complementary picture information, has come a long way in recent years. Several examples include SPM with dual excitation frequencies, multiple harmonic imaging [53], 3D modes [54], banded excitation SPM [55], and quick digital lock-ins [56]. This massive amount of data exponentially increases the challenge of deciphering certain material qualities. Nikiforov et al. [57]. Functional recognition imaging, also known as FR-SPM, was created to overcome this issue. Utilizing neural networks trained on expert examples, this technique can immediately recognize local behaviors based on the spectroscopic responses that have been seen.

Through cleaning and beautifying the data sent to the neural network, artificial neural networks (ANNs) are utilized in conjunction with principal component analysis (PCA) to minimize the number of distinct variables. Without this treatment, well-designed ANNs could still gather appropriate data from duplicate datasets. Using PCA, ANN completes the work more quickly and accurately. Micrococcus lysodeikticus and Pseudomonas fluorescens were detected by FR-SPM on a mica substrate coated with poly-L-lysine (PLL). A multilayer perceptron that has been trained using back-propagation is utilized in this investigation [58]. They used three hidden layer neurons, six inputs, and three outputs. Transfer functions for the sigmoid hidden layer and the purlin output layer were present at each node.

## 3. Simulations of artificial intelligence at the nanoscale

Simulating the system under study is a significant challenge for nanoscale scientists. Real optical pictures are not possible at the nanoscale. This size of images requires interpretation, and numerical simulations are sometimes best. Many programs and applications accurately imitate atomic-effect systems today [59]. When appropriately used, these approaches can give a precise image characterization. However, they are still complex and require numerous parameters to depict the system accurately. Artificial intelligence can increase simulation quality and make them easier to get and analyze. ANNs have shown many benefits in nanoscale numerical simulations. The program can be manually modified to balance numerical precision and physical meaning [60]. The usual least-squares minimization (LSM) method is used in these models to reduce the electrostatic potential inaccuracy at the surface of the tip. Changing the tip point weights is one of the reduction routines that is sometimes used [61].

## 4. The merging of artificial intelligence with nanocomputing

Artificial intelligence and nanoscience can tackle nanoscale microscopy, nanomaterial science, and simulation challenges. Numerous applications may result from combining AI with nanocomputing, encompassing current and future technologies [62]. Since the early attempts at building nanocomputers [63]. Various stages of nanocomputing device modeling, design, and prototype construction have used artificial intelligence paradigms [62, 64]. Using machine learning techniques, nano hardware can replace semiconductor-based hardware, ushering in a new era of smaller, more affordable, and powerful computer technology for processing and controlling sensory data. Recent developments in nanotechnology have shifted the emphasis to the fabrication and analysis of discrete parts, such as nanowires for connections or molecules for switches [64]. Quantum computing and memory provided by nanotechnology [65] have the most significant potential to address complicated NP-complete optimization problems. Big data applications that demand computational intelligence are especially prone to these issues. This definition of natural computing encompasses at least three ways [66]: (1) individuals who find solutions in nature and use that knowledge to create new methods of tackling problems, (2) systems that rely on the computational synthesis of natural events and (3) systems that use nanoscale computation enabled by natural materials. Within this final notion are methods currently the subject of extensive research, such as DNA computing [67] and quantum computing [68].

## 5. Machine learning for chemistry

Chemistry has a unique opportunity to enhance molecular technologies beyond synthetic efforts. Machine learning algorithms use error minimization in various ways to detect patterns in enormous amounts of data. Google search results, Apple Voice assistant, and Facebook personalized site feeds use ML reduction techniques. Academic research in almost every scientific discipline uses machine learning.

Figure 3 shows that artificial intelligence (AI) refers to any software with human-like intelligence. Machine learning AI can adjust its parameters with more data. ML programs can self-construct adjustments, making them less dependent on humans. Machine learning algorithms discover how a data set affects a property. The neural network (s)' complexity determines the relationship's quality. The neural network's hidden algorithm and inputs provide predictions. Deep learning is a neural network with several hidden layers as shown in Figure 4. The complexity of hidden layers determines the mathematical sophistication of the input and output layers. These hidden layers allow the neural network to process inputs sequentially. Making facial identification more accessible, the first hidden layer detects lines in a photo, while the second layer identifies the eyes, mouth, and nose. The final layer uses those attributes to establish the person's identity and output an answer.

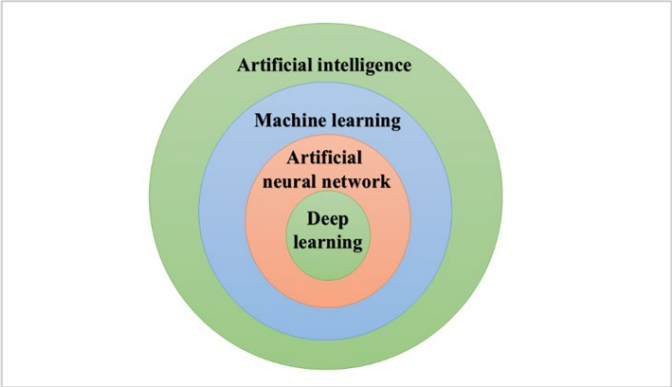


**Figure 3:** Diagram of AI terms

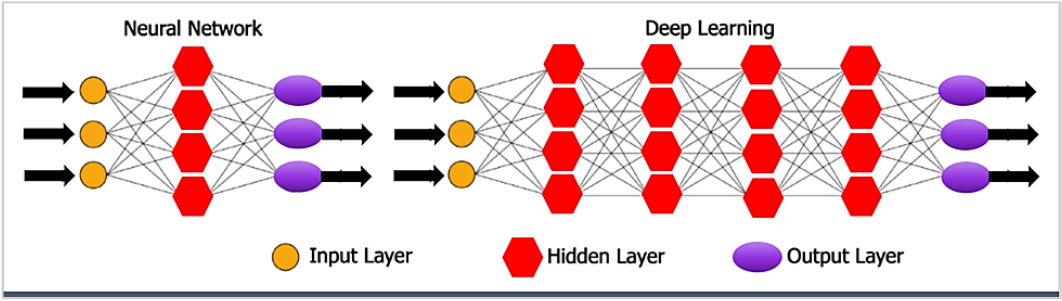


**Figure 4:** Neural networks and Deep learning

Two types of neural networks, superficial and deep, are shown in Figure 4. The hidden layer [red] receives the inputs [orange]. The input is fed into the hidden layer, producing the blue output. The result of deep learning is achieved by applying many hidden layers (alphabold) [69]. There will be practical applications of machine learning to various chemical challenges shortly, as the area is still in its early stages of development. The following applications of ML are being explored: reaction mechanism determination, molecular dynamic simulations, optimal condition prediction, chemical optimization, protein folding structure prediction, analytical tools, quantum sensing, and approximations of density functional theory (DFT) functionals, Cova and Pais, Wang , Senior, Evans, and Jumper, [70-72]. Four ML applications are interesting: quantum molecular simulations, molecular property prediction, screening, developing new compound synthesis techniques, and genetic programming-based molecular design. The entire procedure produces stable molecular patterns with desirable features.

## 6. AI for molecular property prediction

Chemical characteristics are determined by nuclear and electronic structure. The estimated PES can provide structural information since stable structures are linked to local or global minima along the potential energy surface. Using chemical structure, AI can anticipate hypothetical molecule properties without experimentation. Compounds' beneficial qualities could be screened without synthesis. ML program screens millions of chemicals and delivers the most promising medicine and material discovery options. Synthesis conditions can be predicted to maximize product yields and reaction rates, Ahneman [73]. It is possible to handle reaction prediction and retrosynthesis at the same time. One way to prepare an organic molecule for synthesis is through retrosynthesis, which involves cutting it into smaller pieces. Incorporating over a million organic reaction datasets, Segler and Waller, [74] turned in reaction predictions with 97% accuracy and retrosynthesis predictions with 95% accuracy. The work was initially applied to organic molecules with lesser molecular weights and is not yet applicable to the bigger scale. Granda, [75, 76] brought an ML algorithm into play through an organic synthesis robot. With its 18 available chemicals, the robot could carry out 969 distinct reactions. Protein structure prediction is being enhanced with machine learning and deep learning techniques. With this program, we can foretell which proteins will bind to which targets and which will catalyze which reactions, Torrisi, Pollastri, and Le, [77].

Vectorized representations of molecules, capturing exact information about their atomic structures, are used in molecular fingerprinting. Different problems call for varying levels of granularity in fingerprinting. A coarser fingerprint might be defined in cases where the precision of the prediction is not paramount, such as when estimating the electrical or mechanical strength of materials. It may be related to the material's composition or other general characteristics of the atoms that make it up (e.g., band gap).

However, if predictions involving total energies and atomic forces are to be accurate, the solid-state space groups that fingerprint must be more precise with atomic-level structural information [78]. One possible input for a neural network is a reaction fingerprint, often created by joining together a small number of fingerprints of molecules that are reactants and reagents [79]. Extended connection fingerprints are a common type of fingerprint [80]. As shown in Figure 5, the featurization method involves breaking a molecule down into smaller pieces, or substructures, that have a binary fingerprint of a defined

length. These pieces are then put into an array where each element is either 1 or 0. Typical applications of fingerprinting include grouping, virtual screening, and similarity searches.

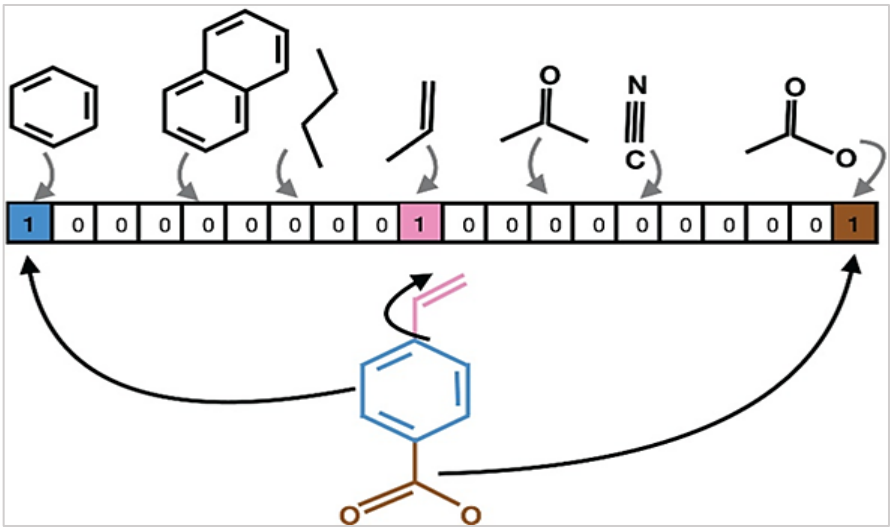


**Figure 5:** A molecular fingerprint's representation encoded whether specific substructures in a compound were present (1) or not (0). Twenty binary digits comprise the vector representing this molecule [80]

## 7. AI for molecular design

Complex molecular-scale designs in biology demonstrate remarkable skills. Genetically engineered molecular systems and macro-scale inventions are more sophisticated than synthetic molecular designs. Unfortunately, the quantum process is counterintuitive; humans cannot create molecular structures with hundreds of atoms. Due to the disparity in physical spaces, applying macroscale design approaches to nanoscales is inefficient and restricting. Machine-aided design is needed to overcome human creativity's limits in synthetic molecular design. Yi [81] offer a tool architecture with seven parts: simulator, constraints, requirements, GP, visualizer, evaluator, and control interface. A quantum-chemical simulator is needed to analyze physically viable molecules and structures. These simulators have computational limits using traditional approaches, but ML could solve this. The AI GP algorithm will iteratively search for designs that meet the parameters and maximize the evaluator score. The software would also have a visualizer to track AI progress and a control interface to access modular components, Figure 6.

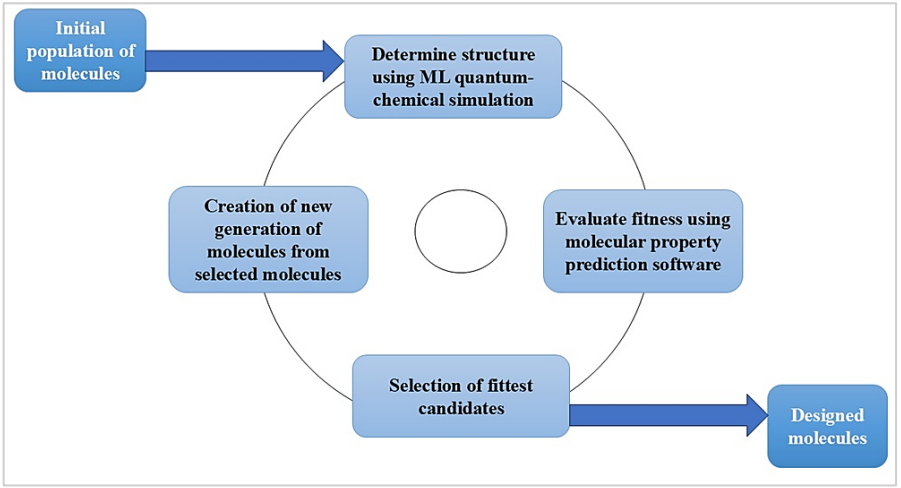


**Figure 6:** Diagram of steps for one generation done by AI for molecular design

More parts can be added to the AI. Because of their high computing cost, quantum-mechanical simulations should only be undertaken if a more cost-effective method of estimating the design's quality is employed beforehand. Researchers currently use inefficient processes that can take years or even decades to alter molecular modifications to find the proper structure to attach to such a receptor. Numerous treatments, including those for Alzheimer's, are presently the focus of such research [82]. AI molecular design software might efficiently and cheaply do this and subsequent testing and synthesis development tasks. Candidates may outperform human-made chemicals since GP can test and develop intelligent molecules. Due to fewer chemicals failing, experimental testing and health screenings would considerably reduce synthesis and screening time. Protein-based enzymes can affect the response rate trillion-fold. AI is important to predict the cancer. AI tools predicted the responses

of individual cells to both single drugs and drug combinations which would help in cancer field [83]. Due to our poor molecular design skills, such technology is unattainable. Software that uses molecular dynamic modeling could create new enzymes for new processes. A designed fitness function related to the pace at which reactants generate products and specifications to only amino acid fragments for the planned molecule is needed. The synthesized enzyme might be dismantled into its amino acid chain. This script could be used to create an RNA string. Our cells' ribosomes could manufacture the enzyme utilizing the specified RNA.

## 8. Application of AI in nanomaterials

As AI develops the future paradigms in material science, it becomes increasingly crucial for the exploration, examination, and design of nanomaterials. Because of AI, data-driven science has replaced the expensive and time-consuming empiric trial-and-error method in material science. Artificial intelligence is essential for the automated discovery and fabrication of functional nanomaterials exhibiting desirable properties. AI can speed up the development of new paradigms, predict material properties, synthesize and characterize materials, and explore the vast chemical design space for specific purposes. AI enables the intelligent and efficient investigation of suitable synthesis parameters to create materials with better properties. Predicting properties, designing inversely, synthesizing, characterizing, and extracting information are all examples of ML applications in this area of the detection and advancement of nanomaterials.

### 8.1 Property prediction

ML is often used to forecast properties in material development. The quantitative structure-activity relationship (QSAR) among materials' structural information and target attributes can be established and predicted using ML models based on previous experimental or computational data. ML has solved these QSAR modeling problems well and promisingly. The ML models anticipate target qualities in regions without experimental data, making navigating the vast design space easy. Machine learning (ML) boosts the efficiency of first-principle computations by combining it with an examination framework for property prediction. Using ML as a replacement model has simplified large-scale material screening procedures while reducing computing time and expense for DFT. Previous reviews [84, 85] provide great explanations of the beneficial link between first-principle calculations and ML, and this method has been applied in various publications. The following sections will discuss additional details. ML can make first-principle calculations more precise or tackle complex issues that traditional computing approaches cannot handle. A neural network-based functional DM21 from Deep Mind [86] solves DFT's long-standing fractional electron difficulties better than conventional functionals. ML offers alternatives to improve material calculation for property prediction.

Many areas of molecular research have succeeded with ML algorithms, providing more accurate and quicker results than conventional approaches (such as QM calculations, DFT, MM-based methods, etc.). A molecule structure has a predictable link with its properties [87]. Learning the underlying QSPRs of an issue, even from simple chemical representations, is made possible by ML models' flexibility (e.g., universal approximation theorem for ANNs) [88, 89].

Multiple criteria allow for the categorization of ML methods. One way to categorize ML systems is according to whether or not they require human oversight. Figure 7 shows the three main categories of ML techniques based on this: supervised, unsupervised, and reinforcement learning. This section provides a concise overview of some well-known ML approaches that have been applied to address issues in molecular science [90].

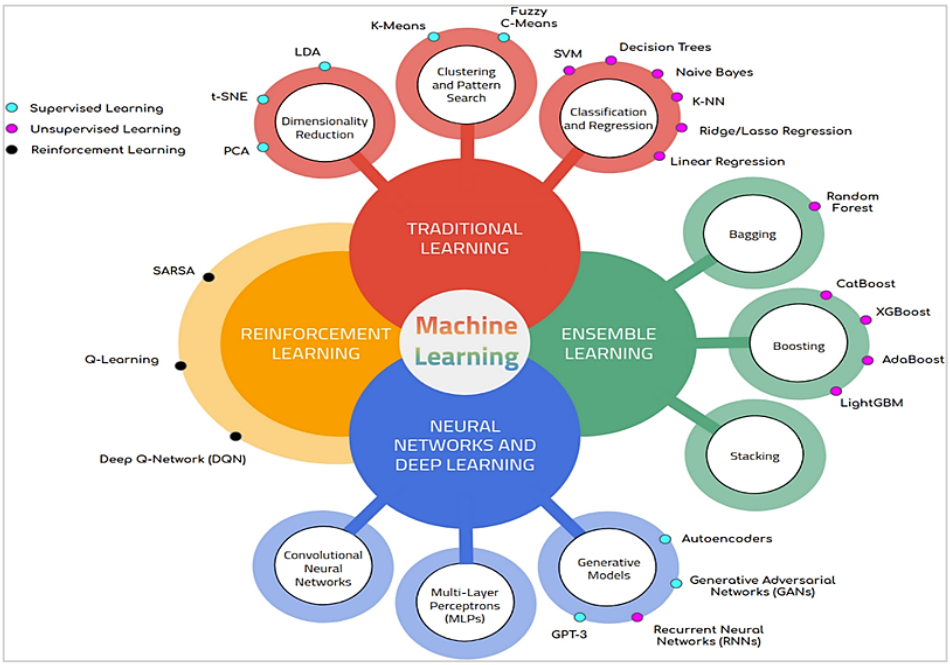


**Figure 7:** Examples of machine learning approaches and algorithms [90]

### 8.2 Material inverse design

Machine learning models are utilized for large-scale applications such as high-throughput material screening. This is because these models can analyze massive amounts of candidate materials effectively and find materials that possess the required properties while maintaining low costs. Unfortunately, the forward design method is quite sensitive to the pool of candidate materials; if the pool is too small, the effective search for necessary attributes may be severely hindered. It appears that inverse design could be a promising approach to this issue. Inverse design involves inverting the input and output of ML models to predict information about the structure of materials with desired attributes directly. Utilizing generative adversarial networks and variational autoencoders are two techniques used in inverse design. Kim et al. [91] accomplished the design of zeolites by using a generative adversarial network (GAN), which consists of a generator and a discriminator. When a discriminator attempts to tell accurate data from fake in an adversarial learning process, the generator fools him, resulting in realistic zeolite materials. The next step is to employ GAN to make zeolites with a methane adsorption heat of 4 kJ/mol. Generative models can be used in inverse design processes to output the materials of preference and their chemical and structural properties for more efficient material design. By leveraging AI, the inverse design framework can efficiently scour the vast design space, surpassing the time-consuming and error-prone traditional trial-and-error approach that relies on the researcher's expertise.

### 8.3 Material synthesis

Conditions and pathways during synthesis determine the material's performance. ML can find the best synthesis pathways and settings to produce nanomaterials with the desired properties. Automated machinery, such as Ro-bots, can incorporate the suggested synthesis protocol for high-throughput experiments, making it easier to scour the enormous material design space for conventional inorganic crystals, organic compounds, and bio-mixed materials [92]. Mekki-Berrada et al. [93] Utilized repeated active learning on a high-throughput microfluidic chip to discover the ideal conditions for synthesizing silver nanoparticles with the specified absorbance spectra. A deep neural network (DNN) was used to forecast the relationship between the chemical composition and optical performance after improving nanomaterials production using Gaussian process-based Bayesian optimization. Using machine learning according to the expected enhancement decision, Rao et al. [94] Designed conditions for synthesizing single-wall carbon nanotubes (SWCNTs) with a limited diameter distribution. Which proved the potential advantages of optimizing diameter using machine learning. A more complete summary of machine learning-aided nanoparticle production is available in earlier reviews [95].

### 8.4 Material characterization

Fast progress in material characterization approaches has led to an explosion in material data from devices like SEM, TEM, and XANES. Due to data growth, manual data analysis procedures are typically excessively laborious. ML gives a more efficient and automated way to analyze data that even experts find difficult. Kim et al. [95] used machine vision and ML to quantify SEM pictures. These ML algorithms automatically extract morphology and nanoparticle sizes from SEM pictures. Based on these algorithms, a user-friendly, adaptable program that may be used for additional SEM/TEM imaging analysis tasks was built. Liu et al. [96] constructed structural descriptors by training convolutional neural networks with theoretical spectra, which then "inverted" experimental XANES data. While evaluating average cluster sizes on copper oxide clusters, transforming reaction conditions, and distinguishing structural motifs, a convolutional neural network (CNN) model functioned admirably. Timoshenko et al. [97] created a machine-learning method to reconstruct the three-dimensional geometry of metal catalysts using experimental XANES spectroscopy. They determined the median quantity of coordinates for the initial of several shells of coordination and utilized neural networks to describe the nanoparticles' size and three-dimensional structure. The rapid advancement of high-resolution spatial imaging techniques like scanning probes, optical microscopy, electron and ion systems, and multi-scale and multi-modal imaging approaches has made investigating and characterizing material structural features all the more important [98]. Such approaches have the potential to unify experimental characterization data sets of varying sizes onto a single, essential data application platform. A new KAIST initiative called material and molecular modeling, imaging, information systems, and integration (M3I3) employs ML approaches and scientific knowledge to expedite materials' discovery, design, and development. For nanoscale systems, our AI-based characterization approaches can high-throughput and time-dependently extract structural characteristics from material images [99].

## 9. Artificial intelligence aided nanotechnology for renewable energy

Due to their continuous extraction and exploitation, the accelerated exhaustion of finite resources (such as fossil fuels) threatens worldwide energy sustainability and worsens environmental concerns [100]. Therefore, greener renewable energy options must be explored. Every recent global agenda has prioritized sustainable energy development due to rising global energy consumption due to population growth and a booming economy [101]. The objectives of newly passed energy legislation are creating energy sources with zero or low carbon emissions and guaranteeing future energy security. In 2015, renewable energy accounted for 23% of power generation; by 2060, that number is projected to rise to 41-60%. With this additional contribution from renewables, we should be able to cover almost all the predicted increases in power consumption in 2060 [102]. There will be a dramatic shift in the future of energy due to the widespread availability of renewable resources and the positive social, economic, and environmental impacts of these technologies [103]. To achieve the aim of keeping the average surface temperature above 2 °C and to satisfy the growing global energy demand, it is essential to utilize renewable energy resources [104]. Improving energy infrastructure to use renewable energy sources better to meet demand is equally

critical. Enhanced energy materials with nanostructures are used for this purpose. Researchers are interested in designing and manufacturing high-performance energy storage devices for large-scale deployment that integrate pseudocapacitive and nanofibrous nanomaterials. These materials have outstanding electrochemical and rate capabilities and a high specific surface area [105]. Artificial intelligence (AI) in fields like inverse design, information extraction, and materials property prediction has shown promising results in developing more dependable and efficient materials for power conversion and supply. This could pave the way for commercial, large-scale green energy systems that rely on these materials [106-112].

## 10. AI Models

The XAI community is likely still in the early stages of development regarding the supervised (regression and classification) and unsupervised (clustering) tasks that form the basis of most AI applications. The authors of the selected articles used well-established AI/ML models to accomplish their goals. Neural networks (NN), ensemble models (EM), Bayesian models (BM), fuzzy models (FM), tree-based models (TM), linear models (LM), nearest neighbor models (NNM), support vector machines (SVM), neuro-fuzzy models (NFM), and case-based reasoning (CBR) were the key categories into which the methods were grouped. Table 3 displays the grouped works of these models according to their kinds. Furthermore, the table contains the overall count of studies, a rundown of all the AI/ML model versions, and citations for the articles that showcase the models. Many academics are showing a lot of interest in neural networks and ensemble techniques. It's safe to infer that these models were selected with explainability in mind because of how well they function across different domains. Table 4. Assessment of machine learning models for energy system comparison.

**Table 3:** Various models are employed to address the main objective of classification or regression

| Model Types | Models | Ref. |
|---|---|---|
| Bayesian Models (BM) | Gaussian Naive Bayes Classifier/Regressor (GNBC/GNBR), Bayesian Rule List (BRL), and Bayesian Network (BN): | [95-97, 106-107, 113] |
| Neuro-Fuzzy Models (NFMs) | The following systems: ANFIS, iChIMP, LeNet with a Fuzzy Classifier, Mamdani, Sugeno-Type, and ALMMo-0*—Autonomous Learning Multiple-Model Adaptive Networks and Fuzzy Inference Systems | [103-107, 114-115] |
| Linear Models (LMs) | Logistic Regression (LgR), Linear Regression (LnR), and Linear Discriminant Analysis (LDA) | [116,117] |
| Support Vector Machines (SVMs) | SVM Kernels with Linear and Radial Basis Function (RBF) | [118,119] |
| Tree-Based Models (TB) | One-class tree (OCTree), Multi-Operator Temporal Decision Tree (MTDT), Conditional Inference Tree (CTree), Decision Tree (DT), Fuzzy Hoeffding Decision Tree (FHDT), Fast and Frugal Trees (FFTs), and more. | [79-80, 120,121] |
| Neural Networks (NNs) | VGG19; YOLO; ApparentFlow-net; Temporal Convolutional Netwrok (TCN); Convolutional Neural Network (CNN); RestNet; ROINet; Deep Neural Network (DNN); Region-Based CNN (RCNN); Recurrent Neural Network (RNN); Deep Reinforcement Learning (DRL); Multilayer Perceptrons (MLP); MatConvNet; Nilpotent Neural Network (NNN); Explainable Deep Neural Network (xDNN); Explainable Neural Network (ExNN); Locally Guided Neural Networks (LGNN); Global–Local Capsule Networks (GLCapsNet); Knowledge-Shot Learning (KSL); GoogleLeNet; Gramian Angular Summation Field CNN (GASF-CNN); Hopfield Neural Networks (HNN); LVRV-net; Knowledge-Aware Path Recurrent Network; LeNet-5; Long/Short-Term Memory (LSTM); | [89-111,112, 122,123] |
| Nearest Neighbours Models (NNMs) | Distance-weighted k-nearest Neighbours (WkNN) and k-nearest Neighbours (kNN) | [124,125] |

**Table 4:** Evaluation of machine learning models for energy system comparison [126]

| Model of ML | User-Friendliness | Complexity | Speed | Accuracy |
|---|---|---|---|---|
| ANN | Low | Reasonably high | Reasonable | High |
| MLP | Reasonable | Reasonable | High | Reasonably high |
| ELM | Reasonably high | Reasonable | Reasonably high | Reasonable |
| SVM | Low | Reasonably high | Low | High |
| DT | Low | Reasonable | Reasonable | Reasonable |
| DL | Reasonable | High | Reasonable | High |
| Ensemble | Low | High | High | Reasonable |
| WNN | Low | Reasonable | Low | High |
| ANFIS | Reasonable | Reasonable | High | Reasonable |
| Hybrids | High | Reasonable | High | High |

## 11. Conclusion

A sophisticated artificial intelligence system designed for molecular design has the potential to systematically explore molecules exhibiting intricate motion patterns, hence facilitating the development of novel molecular design approaches with unforeseeable practical implications. The artificial intelligence (AI) system autonomously identifies potential nanomachine candidates that can use molecular motion to facilitate the desired task or can be manually prompted to generate mobile molecules. The shift from human-theoretical chemistry to AI-developed methodologies will likely be one of the most substantial transformations in science thus far. The inference is that human-made molecular designs would require aid beyond human capabilities to compete with nanochemistry, which is present in life and has evolved through evolutionary processes. Hence, an alternate approach is needed to address these restrictions and facilitate the design of molecules through a process distinct from human creativity. The proliferation of computer science, artificial intelligence (AI), and machine learning (ML) technologies has controlled the emergence of diverse tools. Utilizing this approach in the field of chemistry will enable us to replicate the evolutionary mechanism to generate novel synthetic designs. Implementing this instrument would provide significant breakthroughs in synthetic molecule design, leading to notable progress in chemical research. The popularity of AI systems in several domains can be attributed to their capacity to achieve accuracy, precision, and continuous error-free operation. Artificial intelligence (AI) has proven effective in various domains, particularly monitoring. AI technologies, particularly machine learning, enable the examination of concealed connections between the structure and properties of materials at the nanoscale. These computational tools are characterized by their speed, high efficiency, and resource-saving nature. They are utilized to research the parameters of nanoparticles and anticipate the potential characteristics of nanomaterials before their creation. Machine learning has novel prospects for addressing nanofluids' thermal and dynamic characteristics, chemical adsorption, diagnostics of NP imaging outcomes, and nanosensors. Artificial neural networks have proven to be effective in classifying extensive datasets about the spectra and pictures of nanoparticles (NPs). The assessment of nanomaterial toxicity, forecasting the in vivo behavior of nanoparticles, and identifying the most effective chemical compositions of nanoparticle surfaces for their entry into the body are conducted with greater speed and accuracy. The $Al_2O_3$–$H_2O$ nanofluid accurately predicts important parameters, including the heat transfer coefficient, thermal conductivity, and dynamic-viscosity ratio.

### Author contributions

Conceptualization, Sh. Eabd Alrida and O. Obed; data curation, E. Taha.; formal analysis, Th. Abdullah.; investigation, M. Hathal; methodology, V. Somogyi; project administration, M. Hathal, resources, Sh. Eabd Alrida; supervision, Th. Abdullah; writing—original draft preparation, O. Obed; writing—review and editing, Sh. Eabd Alrida. All authors have read and agreed to the published version of the manuscript.

### Funding

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

### Data availability statement

The data that support the findings of this study are available on request from the corresponding author.

### Conflicts of interest

The authors declare that there is no conflict of interest.

## References

**[1]** L. Dung, L. Paramonov, C. Davidson, J. Ramsden, H. Wright, N. Holliman, J. Hagon, M. Heggie, C. Makatsoris, The Matter Compiler-towards atomically precise engineering and manufacture, Nanotech. Perce., 7 (2011) 199-217. https://doi.org/10.56801/nano-ntp.v7i3.68

**[2]** Mitchell, T. M. Machine learning; MA: McGraw-Hill, Boston, 1997.

**[3]** Bishop,C.M., Nasrabadi, N.M. Pattern Recognition and Machine Learning; Springer, New York, NY, USA, 2006.

**[4]** T. F. Cova, and A. A. Pais, Deep learning for deep chemistry: optimizing the prediction of chemical patterns. Front. Chem., 7 (2019) 809. https://doi.org/10.3389/fchem.2019.00809

**[5]** H. Shindo, Y. Matsumoto, Gated Graph Recursive Neural Networks for Molecular Property Prediction, https://doi.org/10.48550/arXiv.1909.00259

**[6]** Reisfeld, B. Mayeno, A.N. What is Computational Toxicology?; Humana Press: Springer Protocols, NJ, USA, 2012.

**[7]** G. Chen, M.G. Vijver, Y. Xiao, W. J. G.M., Peijnenburg, A Review of Recent Advances towards the Development of (Quantitative) Structure-Activity Relationships for Metallic Nanomaterials. Materials, 10 (2017) 1013. https://doi.org/10.3390/ma10091013

**[8]** B. Saini, S. Srivastava, Nanotoxicity prediction using computational modelling - review and future directions, IOP Conf. Ser. Mater. Sci. Eng., 348 (2018) 012005. https://doi.org/10.1088/1757-899X/348/1/012005

**[9]** C. Zhao, E. Boriani, A. Chana, A. Roncaglioni, E. Benfenati, A new hybrid system of QSAR models for predicting bioconcentration factors (BCF), Chemosphere, 73 (2008) 1701. https://doi.org/10.1016/j.chemosphere.2008.09.033

**[10]** Leszczynski, J., Kaczmarek-Kedziera, A., Puzyn, T., Papadopoulos, M. G., Reis, H., Shukla, M. K. Handbook of Computational Chemistry; Springer Cham: Springer International Publishing, Switzerland, 2017.

**[11]** H. Kubinyi, From Narcosis to Hyperspace: The History of QSAR, Quant. Struct.-Act. Relat, 21 (2002) 348.

**[12]** A. Singh, M. Ansari, D. Rosenkranz, R. Maharjan, F. Kriegel, K. Gandhi, A. Kanase, R. Singh, P. Laux, A. Luch, Artificial Intelligence and Machine Learning in Computational Nanotoxicology: Unlocking and Empowering Nanomedicine, Adv. Healthc. Mater., 9 (2020) 170. https://doi.org/10.1002/adhm.201901862

**[13]** K. Pearson, LIII. On lines and planes of closest fit to systems of points in space, London Edinburgh Dublin Philos. Mag. J. Sci., 2 (1901) 559-572. https://doi.org/10.1080/14786440109462720

**[14]** A. Ben-Hur, D. Horn, H.T. Siegelmann, Support Vector Clustering, J. Mach. Learn. Res., 2 (2001) 125-137.

**[15]** T. K. Ho, Proceedings of 3rd International Conference on Document Analysis and Recognition, Montreal, Canada, August 1995. https://doi.org/10.1109/ICDAR.1995.598929

**[16]** S. Vanhuffel, J. Vandewalle, The partial total least squares algorithm J. Comput. Appl. Math., 21 (1988) 333-341. https://doi.org/10.1016/0377-0427(88)90317-2

**[17]** T. Kohonen, Self-organized formation of topologically correct feature maps, Biol. Cybern., 43 (1982) 59–69. https://doi.org/10.1007/BF00337288

**[18]** M. Sato, A real time learning algorithm for recurrent analog neural networks, Biol. Cybern., 62 (1990) 237–241. https://doi.org/10.1007/BF00198098

**[19]** B.E. Boser, COLT '92: Proc. of the Fifth Annu.Workshop on Computational Learning Theory, Association for Computing Machinery: New York, 1992.

**[20]** C. Hansch, Quantitative approach to biochemical structure-activity relationships, Acc. Chem. Res.., 2 (1969) 232–239. https://doi.org/10.1021/ar50020a002

**[21]** T. Teorell, Kinetics of distribution of substances administered to the body, II: The extravascular modes of administration, Arch. Int. Pharmacodyn. Ther., 57 (1937) 226-240. https://api.semanticscholar.org/CorpusID:53883583

**[22]** Overtone, F. Applied Physiology: Including the Effects of Alcohol and Narcotics; American Book Company: New York, 1897.

**[23]** J.W. Wilson, S.M. Free, A mathematical contribution to structure-activity studies, J. Med. Chem., 7 (1964) 395–399. https://doi.org/10.1021/jm00334a001

**[24]** C.A. Lipinski, F. Lombardo, B.W. Dominy, P.J. Feeney, Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings, Adv. Drug Delivery Rev., 23 (1997) 3-25. https://doi.org/10.1016/S0169-409X(96)00423-1

**[25]** Hammett, L. P., Physical Organic Chemistry; McGraw-Hill: New York, 1940.

**[26]** M. Hosseini-Yeganeh, A.J. McLachlan, Antimicrob. Agents Chemother., 46 (2002) 2219-2228. https://doi.org/10.1128/AAC.46.7.2219-2228.2002

**[27]** S. Persiani, M. D'Amato, A. Jakate, P. Roy, J. Wangsa, R. Kapil, L.C. Rovati, Pharmacokinetic Profile of Dexloxiglumide, Clin. Pharmacokinet., 45 (2006) 1177-1188. https://doi.org/10.2165/00003088-200645120-00003

**[28]** R. Beaudouin, S. Micallef, C. Brochot, A stochastic whole-body physiologically based pharmacokinetic model to assess the impact of inter-individual variability on tissue dosimetry over the human lifespan, Regul. Toxicol. Pharmacol., 57 (2010) 103. https://doi.org/doi:10.1016/j.yrtph.2010.01.005

**[29]** D.S. Li, M. Morishita, J.G. Wagner, M. Fatouraie, M. Wooldridge, W.E. Eagle, J. Barres, U. Carlander, C. Emond, O. Jolliet, In vivo biodistribution and physiologically based pharmacokinetic modeling of inhaled fresh and aged cerium oxide nanoparticles in rats, Part. Fibre Toxicol., 13 (2016) 45. https://doi.org/10.1186/s12989-016-0156-2

**[30]** E. Price, A.J. Gesquiere, An in vitro assay and artificial intelligence approach to determine rate constants of nanomaterial-cell interactions, Sci. Rep., 9 (2019) 13943. https://doi.org/10.1038/s41598-019-50208-x

**[31]** T. Puzyn, B. Rasulev, A. Gajewicz, X. Hu, T.P. Dasari, A. Michalkova, H.-M. Hwang, A. Toropov, D. Leszczynska, J. Leszczynski, Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles, Nat. Nanotechnol., 6 (2011) 175. https://doi.org/10.1038/nnano.2011.10

**[32]** Y. Bengio, O. Delalleau, C. Simard, Decision trees do not generalize to new variations, Comput. Intell., 26 (2010) 449-467. https://doi.org/10.1111/j.1467-8640.2010.00366.x

**[33]** H. Mei, Y. Zhou, G. Liang, Z. Li, Support vector machine applied in QSAR modelling, Chin. Sci. Bull., 50 (2005) 2291-2296. https://doi.org/10.1007/BF03183737

**[34]** B. Saini, S. Srivastava, Nanotoxicity prediction using computational modelling - review and future directions, IOP Conf. Ser.: Mater. Sci. Eng., 348 (2018) 012005. https://doi.org/10.1088/1757-899X/348/1/012005

**[35]** A.V. Singh, MHD Ansari, D. Rosenkranz, R. S. Maharjan, F. L. Kriegel, K. Gandhi, A. Kanas, R. Singh, P. Laux, A. Luch, Artificial intelligence and machine learning in computational nanotoxicology: unlocking and empowering nanomedicine, Adv. Heal. Mater., 17 (2020) 1901862. https://doi.org/10.1002/adhm.201901862

**[36]** Tran, L., Banares, M.A., Rallo, R., Modelling the Toxicity of Nanoparticles; Springer: Berlin, 2017.

**[37]** U. Carlander, D. Li, O. Jolliet, C. Emond, G. Johanson, Toward a general physiologically-based pharmacokinetic model for intravenously injected nanoparticles, Int. J. Nanomed., 11 (2016) 625-640. https://doi.org/10.2147/IJN.S94370

**[38]** Erdely, M. Dahm, B.T. Chen, P.C. Zeidler-Erdely, J.E. Fernback, M.E. Birch, D.E. Evans, M.L. Kashon, J.A. Deddens, T. Hulderman, Carbon nanotube dosimetry: from workplace exposure assessment to inhalation toxicology, Part. Fibre Toxicol., 10 (2013) 53. https://doi.org/10.1186/1743-8977-10-53

**[39]** F.J. Miller, B. Asgharian, J.D. Schroeter, O. Price, Influence of alveolar mixing and multiple breaths of aerosol intake on particle deposition in the human lungs, J. Aerosol Sci., 99 (2016) 14. https://doi.org/10.1016/j.jaerosci.2022.106050

**[40]** S. Anjilvel, B. Asgharian, ultiple-path model of particledeposition in the rat lung, Fundam. Appl. Toxicol., 28 (1995) 41.

**[41]** D.A. Winkler, E. Mombelli, A. Pietroiusti, L. Tran, A. Worth, B. Fadeel, M.J. McCall, Applying quantitative structure-activity relationship approaches to nanotoxicology: current status and future potential, Toxicology, 313 (2013) 15. https://doi.org/10.1016/j.tox.2012.11.005

**[42]** L.M. Gilbertson, F. Melnikov, L.C. Wehmas, P.T. Anastas, R.L. Tanguay, J.B. Zimmerman, Toward safer multi-walled carbon nanotube design: Establishing a statistical model that relates surface charge and embryonic zebrafish mortality, Nanotoxicology, 10 (2016) 10-19. https://doi.org/10.3109/17435390.2014.996193

**[43]** P. Schyman, R. Liu, V. Desai, A. Wallqvist, vNN Web Server for ADMET Predictions, Front. Pharmacol., 8 (2017) 1-14. https://doi.org/10.3389/fphar.2017.00889

**[44]** H. Gonzalez-Diaz, ADMET-Multi-Output Cheminformatics Models for Drug Delivery, Interactomics, and Nanotoxicology, Curr. Drug Deli., (2016). https://pubmed.ncbi.nlm.nih.gov/27417300/

**[45]** A.V. Singh, T. Jahnke, S. Wang, Y. Xiao, Y. Alapan, S. Kharratian, M.C. Onbasli, K. Kozielski, H. David, G. Richter, J. Bill, P. Laux, A. Luch, M. Sitti, Anisotropic Gold Nanostructures: Optimization via in Silico Modeling for Hyperthermia, ACS Appl. Nano Mater., 1 (2018) 6205-6216. https://doi.org/10.1021/acsanm.8b01406

**[46]** A.V. Singh, T. Jahnke, Y. Xiao, S. Wang, Y. Yu, H. David, G. Richter, P. Laux, A. Luch, A. Srivastava, P.S. Saxena, J. Bill, M. Sitti, Peptide-Induced Biomineralization of Tin Oxide (SnO2) Nanoparticles for Antibacterial Applications, J. Nanosci. Nanotechnol., 19 (2019) 5674-5686. https://doi.org/10.1166/jnn.2019.16645

**[47]** A.P. Toropova, A.A. Toropov, D. Leszczynska, J. Leszczynski, CORAL and Nano-QFAR: Quantitative feature – Activity relationships (QFAR) for bioavailability of nanoparticles (ZnO, CuO, $CO_3O_4$, and $TiO_2$), Ecotoxicol. Environ. Saf., 139 (2017) 404-407. https://doi.org/10.1016/j.ecoenv.2017.01.054

**[48]** R. Young, J. Ward, F. Scire, The Topografiner: An Instrument for Measuring Surface Microtopography, Rev. Sci. Instrum., 43 (1972) 999–1011. https://doi.org/10.1063/1.1685846

**[49]** G. Binnig, H. Rohrer, C. Gerber, E. Weibel, Surface Studies by Scanning Tunneling Microscopy, Phys. Rev. Lett., 49 (1982) 57–61. https://doi.org/10.1103/PhysRevLett.49.57

**[50]** C.I. Enriquez-Flores, J.J. Gervacio-Arciniega, E. Cruz-Valeriano, P. De Urquijo-Ventura, B.J. Gutierrez-Salazar, F.J. Espinoza-Beltran, Fast frequency sweeping in resonance-tracking SPM for high-resolution AFAM and PFM imaging, Nanotechnology, 23 (2012) 495705. https://doi.org/10.1088/0957-4484/23/49/495705

**[51]** Y.Q. Xie, F. Liu, L. Huang, Lateral manipulation of small clusters on the Cu and Ag(1 1 1) surfaces with the single-atom and trimer-apex tips: Reliability study, Appl. Surf. Sci., 256 (2010) 4084–8. https://doi.org/10.1016/j.apsusc.2010.01.088

**[52]** R. Miotto, F.D. Kiss, A.C. Ferraz, Changes in a nanoparticle's spectroscopic signal mediated by the local environment, Nanotechnology, 23 (2012) 485202. https://doi.org/10.1088/0957-4484/23/48/485202

**[53]** A. Raman, J. Melcher, R. Tung, Cantilever dynamics in atomic force microscopy, Nano Today, 3 (2008) 20–27. https://doi.org/10.1016/S1748-0132(08)70012-4

**[54]** B.J. Rodriguez, C. Callahan, S.V. Kalinin, R. Proksch, Dual-frequency resonance-tracking atomic force microscopy, Nanotechnology, 18 (2007) 475504. https://doi.org/10.1088/0957-4484/18/47/475504

**[55]** Gómez, A. Gil, M. Álvarez, P. J. De Pablo, F. Herrero, I. Horcas, R. Sánchez, J. Colchero, J. Gómez and A. M. Baró, Scanning force microscopy three-dimensional modes applied to the study of the dielectric response of adsorbed DNA molecules, Nanotechnology, 13 (2002) 314–7. https://doi.org/10.1088/0957-4484/13/3/315

**[56]** S. Jesse, S.V. Kalinin, R. Proksch, A.P. Baddorf, B.J. Rodriguez, The band excitation method in scanning probe microscopy for rapid mapping of energy dissipation on the nanoscale, Nanotechnology, 18 (2007) 32. https://doi.org/10.1088/0957-4484/18/43/435503

**[57]** A.B. Kos, D.C. Hurley, Nanomechanical mapping with resonance tracking scanned probe microscope, Meas. Sci. Technol., 19 (2008) 015504. https://doi.org/10.1088/0957-0233/19/1/015504

**[58]** M.P. Nikiforov, V.V. Reukov, G.L. Thompson, A.A. Vertegel, S. Guo, S.V. Kalinin, S. Jesse, Functional recognition imaging using artificial neural networks: applications to rapid cellular identification via broadband electromechanical response, Nanotechnology, 20 (2009) 405708. https://doi.org/10.1088/0957-4484/20/40/405708

**[59]** D.E. Rumelhart, G.E. Hinton, R.J. Williams, Learning representations by back-propagating errors, Nature, 323 (1986) 533–536.https://doi.org/10.1038/323533a0

**[60]** O. Kwon, H. Kim, J. W. Kang, Energy exchange between vibration modes of a graphene nanoflake oscillator: Molecular dynamics study, Curr. Appl. Phys., 13 (2013) 789-794. https://doi.org/10.1016/j.cap.2013.11.027

**[61]** E. Castellano-Hernández, F. Rodríguez, E. Serrano, P. Varona, G. Sacha, The use of artificial neural networks in electrostatic force microscopy, Nanoscale, Res. Lett., 7 (2012) 250. https://doi.org/10.1186/1556-276X-7-250

**[62]** G. Sacha, Method to calculate electric fields at very small tip-sample distances in atomic force microscopy, Appl. Phys. Lett., 97 (2010) 033115. https://doi.org/10.1063/1.3467676

**[63]** J. Arlat, Z. Kalbarczyk, T. Nanya, Nanocomputing: Small Devices, Large Dependability Challenges, IEEE Secur. Priv. Mag., 10 (2012) 69-72. https://doi.org/10.1109/MSP.2012.17

**[64]** G. Tseng, J. Ellenbogen, Toward nanocomputers, Science, 294 (2001) 1293-1294. https://doi.org/10.1126/science.1066920

**[65]** M. Uusitalo, J. Peltonen, T. Ryhänen, Machine Learning: How It Can Help Nanocomputing, J. Comput. Theor. Nanosci., 8 (2011) 1347–1363. https://doi.org/10.1166/jctn.2011.1821

**[66]** P. Maurer, G. Kucsko, C. Latta, L. Jiang, N. Yao, S. Bennett, F. Pastawski, D. Hunger, N. Chisholm, M. Markham, D. Twitchen, J. Cirac, M. Lukin, Room-Temperature Quantum Bit Memory Exceeding One Second, Science, 336 (2012) 1283–1286. https://doi.org/10.1126/science.1220513

**[67]** L. DeCastro, Fundamentals of natural computing: an overview, Phys. Life Rev., 4 (2007) 1–36. https://doi.org/10.1016/j.plrev.2006.10.002

**[68]** M. Razzazi, M. Roayaei, Using sticker model of DNA computing to solve domatic partition, kernel and induced path problems, Inform. Sci., 181 (2011) 3581-3600. https://doi.org/10.1016/j.ins.2011.04.026

**[69]** X. Zha, C. Yuan, Y. Zhang, Generalized criterion for a maximally multi-qubit entangled state, Laser Phys. Lett., 10 (2013) 045201. https://doi.org/10.1088/1612-2011/10/4/045201

**[70]** J. Schmidhuber, Deep learning in neural networks: An overview, Neur. Net. 61 (2015) 85-117. https://doi.org/10.1016/j.neunet.2014.09.003

**[71]** T. Cova, A. Pais, Deep Learning for Deep Chemistry: Optimizing the Prediction of Chemical Patterns, Front. Chem., 7 (2019) 809. https://doi.org/10.3389/fchem.2019.00809

**[72]** J. Wang, S. Olsson, C. Wehmeyer, A. Pérez, N. Charron, G. Fabritiis, F. Noé, C. Clementi, Machine Learning of Coarse-Grained Molecular Dynamics Force Fields, ACS Cent. Sci., 5 (2019) 755–767. https://doi.org/10.1021/acscentsci.8b00913

**[73]** A. Senior, R. Evans, J. Jumper, J. Kirkpatrick, L. Sifre, T. Green, C. Qin, A. Žídek, A. Nelson, A. Bridgland, H. Penedones, S. Petersen, K. Simonyan, S. Crossan, P. Kohli, D. Jones, D. Silver, K. Hassabis, Improved protein structure prediction using potentials from deep learning, Nature, 577 (2020) 706–710. https://doi.org/10.1038/s41586-019-1923-7

**[74]** D. Ahneman, J. Estrada, S. Lin, S. Dreher, A. Doyle, Predicting reaction performance in C–N cross-coupling using machine learning, Science, 360 (2018) 186–190. https://doi.org/10.1126/science.aar5169

**[75]** M. Segler, M. Waller, Neural-Symbolic Machine Learning for Retrosynthesis and Reaction Prediction, Chem. Eur. J., 23 (2017) 5966–5971. https://doi.org/10.1002/chem.201605499

**[76]** J. Donina, V. Dragone, De. Cronin, controlling an organic synthesis robot with machine learning to search for new reactivity, Nature, 559 (2018) 377–381. https://doi.org/10.1038/s41586-018-0307-8

**[77]** M. Torrisi, G. Pollastri, Q. Le, Deep learning methods in protein structure prediction, Comput. Struct. Biotechnol. J., 18 (2020) 1301–1310. https://doi.org/10.1016/j.csbj.2019.12.011

**[78]** N. Alwash, H. Kareem, Detection of COVID-19 Based on Chest Medical Imaging and Artificial Intelligence Techniques, Eng. Technol. J., 39 (2021) 1588–1600. https://doi.org/10.30684/etj.v39i10.2200

**[79]** S. Raghunathan, U. Priyakumar, Molecular representations for machine learning applications in chemistry, Int. J. Quantum, Chem., 122 (2022) e26870. https://doi.org/10.1002/qua.26870

**[80]** D. Cao, Y. Liang, Q. Xu, Molecular Descriptors Guide, Description of the Molecular Descriptors Appearing in the ChemoPy Software Package, China Computational Biology Drug Design, 2012.

**[81]** H. Yi, Visualized Co-Simulation of Adaptive Human Behavior and Dynamic Building Performance: An Agent-Based Model (ABM) and Artificial Intelligence (AI) Approach for Smart Architectural Design, Sustainability, 12(16) (2019) 6672. https://doi.org/10.3390/su12166672

**[82]** V. Gautam, A. Gaurav, N. Masand, V. Sanghiran Lee, V.M. Patil, Artificial intelligence and machine-learning approaches in structure and ligand-based discovery of drugs affecting central nervous system, Mol Divers, 27 (2023) 959–985. https://doi.org/10.1007/s11030-022-10489-3

**[83]** E. Pintelas, M. Liaskos, I. Livieris, S. Kotsiantis, P. Pintelas, Explainable Machine Learning Framework for Image Classification Problems: Case Study on Glioma Cancer Prediction, J. Imaging., 6 (2020) 37. https://doi.org/10.3390/jimaging6060037

**[84]** B. Mehrazma, A. Rauk, Exploring Amyloid-β Dimer Structure Using Molecular Dynamics Simulations, J. Phys. Chem. A, 123 (2019) 4658- 4670. https://doi.org/10.1021/acs.jpca.8b11251

**[85]** J. Li, K. Lim, H. Yang, Z. Ren, S. Raghavan, P. Chen, T. Buonassisi, X. Wang, AI Applications Through the Whole Life Cycle of Material Discovery, Matter, 3 (2020) 393- 432. https://doi.org/10.1016/j.matt.2020.06.011

**[86]** Y. Jia, X. Hou, Z. Wang, X. Hu, Machine Learning Boosts the Design and Discovery of Nanomaterials, ACS Sustainable Chem. Eng., 9 (2021) 6130 - 6147. https://doi.org/10.1021/acssuschemeng.1c00483

**[87]** D. Rogers, M. Hahn, Extended-connectivity fingerprints, J. Chem. Inf. Model., 50 (2010) 742-754. https://doi.org/10.1021/ci100050t

**[88]** A. Karthikeyan, U. Priyakumar, Artificial intelligence: machine learning for chemical sciences, J. Chem. Sci., 134 (2022). https://doi.org/10.1007/s12039-021-01995-2

**[89]** M. Butkiewicz, E. Lowe, R. Mueller, J. Mendenhall, P. Teixeira, C. Weaver, J. Meiler, Benchmarking Ligand-Based Virtual High-Throughput Screening with the PubChem Database, Molecules, 18 (2012) 735-756. https://doi.org/10.3390/molecules18010735

**[90]** A. Karthikeyan, U. Priyakumar, Artificial intelligence: machine learning for chemical sciences, J. Chem. Sci., 134 (2022) https://doi.org/10.1007/s12039-021-01995-2

**[91]** B. Kim, S. Lee, J. Kim, Inverse Design of Porous Materials Using Artificial Neural Networks, Sci. Adv., 6 (2020) eaax9324. https://doi.org/10.1126/sciadv.aax9324

**[92]** P. Mastracco, A. González-Rosell, J. Evans, P. Bogdanov, S. Copp, Chemistry-Informed Machine Learning Enables Discovery of DNA-Stabilized Silver Nanoclusters with Near-Infrared Fluorescence, ACS Nano, 16 (2022) 16322–16331. https://doi.org/10.1021/acsnano.2c05390

**[93]** F. Mekki-Berrada, Z. Ren, T. Huang, W. Wong, F. Zheng, J. Xie, I. Tian, S. Jayavelu, Z. Mahfoud, D. Bash, K. Hippalgaonkar, S. Khan, T. Buonassisi, Q. Li, X. Wang, Two-step machine learning enables optimized nanoparticle synthesis, Npj, Co mput. Mater., 7 (2021) 1–10. https://doi.org/10.1038/s41524-021-00520-w

**[94]** R. Rao, J. Carpena-Núñez, P. Nikolaev, M. Susner, K. Reyes, B. Maruyama, Advanced Machine Learning Decision Policies For Diameter Control Of Carbon Nanotubes, npj . Comput. Mater., 7 (2021) 157. https://doi.org/10.1038/s41524-021-00629-y

**[95]** H. Kim, J. Han, T. Han, Machine Vision-Driven Automatic Recognition of Particle Size And Morphology In SEM Images, Nanoscale, 12 (2020) 19461–19469. https://doi.org/10.1039/d0nr04140h

**[96]** Y. Liu, N. Marcella, J. Timoshenko, A. Halder, B. Yang, L. Kolipaka, M. Pellin, S. Seifert, S. Vajda, P. Liu, A. Frenkel, Mapping XANES Spectra On Structural Descriptors Of Copper Oxide Clusters Using Supervised Machine Learning, J. Chem. Phys., 151 (2019) 164201. https://doi.org/10.1063/1.5126597

**[97]** J. Timoshenko, D. Lu, Y. Lin, A. Frenkel, Supervised Machine-Learning-Based Determination Of Three-Dimensional Structure Of Metallic Nanoparticles, J. Phys. Chem. Lett., 8 (2017) 5091–5098. https://doi.org/10.1021/acs.jpclett.7b02364

**[98]** A. Belianinov, A. Ievlev, M. Lorenz, N. Borodinov, B. Doughty, S. Kalinin, F. Fernández, O. Ovchinnikova, Correlated Materials Characterization via Multi-modal Chemical and Functional Imaging, ACS Nano, 12 (2018) 11798–11818. https://doi.org/10.1021/acsnano.8b07292

**[99]** S. Hong, C. Liow, J. Yuk, H. Byon, Y. Yang, E. Cho, J. Yeom, G. Park, H. Kang, S. Kim, et al., Reducing Time to Discovery: Materials and Molecular Modeling, Imaging, Informatics, and Integration, ACS Nano, 15 (2021) 3971–3995. https://doi.org/10.1021/acsnano.1c00211

**[100]** J. Szargut, A. Ziebik, W. Stanek, Depletion of The Non-Renewable Natural Exergy Resources As A Measure Of The Ecological Cost, Energy Conv. Manag. , 43 (2002) 1149–1163. https://doi.org/10.1016/S0196-8904(02)00005-5

**[101]** T. Kober, H. Schiffer, M. Densing, E. Panos, Global Energy Perspectives To 2060 − WEC's World Energy Scenarios 2019, Energy Strategy Reviews, 31 (2020) 100523. https://doi.org/10.1016/j.esr.2020.100523

**[102]** D. Gielen, F. Boshell, D. Saygin, M. Bazilian, N. Wagner, R. Gorini, The Role of Renewable Energy In The Global Energy Transformation, Energy Strategy Reviews, 24 (2019) 38–50. https://doi.org/10.1016/j.esr.2019.01.006

**[103]** N. Glanemann, S. Willner, A. Levermann, Paris Climate Agreement Passes The Cost-Benefit Test, Nat. Commun., 11 (2020) 110. https://doi.org/10.1038/s41467-019-13961-1

**[104]** Y. Zhao, J. Yan, J. Yu, B. Ding, Advances in Nanofibrous Materials for Stable Lithium-Metal Anodes, ACS Nano, 16 (2022) 17891–17910. https://doi.org/10.1021/acsnano.2c09037

**[105]** A. Chen, X. Zhang, L. Chen, S. Yao, Z. Zhou, A Machine Learning Model On Simple Features For CO2 Reduction Electrocatalysts, J. Phys. Chem. C, 124 (2020) 22471–22478. https://doi.org/10.1021/acs.jpcc.0c05964

**[106]** A. Dubaish, A. Jaber, State-of-the-Art Review into Signal Processing and Artificial Intelligence-based Approaches Applied in Gearbox Defect Diagnosis, Eng. Technol. J., 42 (2024) 157-172. http://doi.org/10.30684/etj.2023.142462.1535

**[107]** H. Rashid, K. Sultan, H. Anead, Thermal Performance of an Evacuated-Tube Solar Collector Using Nanofluids and an Electrical Curtain Controlled by an Artificial Intelligence Technique, Eng. Technol. J., 40 (2022) 8-19. http://doi.org/10.30684/etj.v40i1.2021

**[108]** D. Rogers, M. Hahn, Extended-connectivity fingerprints, J. Chem. Inf. Model., 50 (2010) 742-754. https://doi.org/10.1021/ci100050t

**[109]** A. Karthikeyan, U. Priyakumar, Artificial intelligence: machine learning for chemical sciences, J. Chem. Sci., 134 (2022). https://doi.org/10.1007/s12039-021-01995-2

**[110]** M. Butkiewicz, E. Lowe, R. Mueller, J. Mendenhall, P. Teixeira, C. Weaver, J. Meiler, Benchmarking Ligand-Based Virtual High-Throughput Screening with the PubChem Database, Molecules, 18 (2012) 735-756. https://doi.org/10.3390/molecules18010735

**[111]** M. Haghighatlari, J. Hachmann, Advances of machine learning in molecular modeling and simulation, Curr. Opin. Chem. Eng., 23 (2019) 51-57. https://doi.org/10.1016/j.coche.2019.02.009

**[112]** C. Zhang, W. Wang, N. Xi, Y. Wang, L. Liu, Development and Future Challenges of Bio-Syncretic Robots, Engineering, 4 (2018) 452-463. https://doi.org/10.1016/j.eng.2018.07.005

**[113]** H. Tao, T. Wu, M. Aldeghi, T. Wu, A. Aspuru-Guzik, E. Kumacheva, Nanoparticle Synthesis Assisted By Machine Learning, Nat. Rev. Mater., 6 (2021) 701–716. https://doi.org/10.1038/s41578-021-00337-5

**[114]** O. Serradilla, E. Zugasti, C. Cernuda, A. Aranburu, J. Okariz, U. Zurutuza, Interpreting Remaining Useful Life estimations combining Explainable Artificial Intelligence and domain knowledge in industrial machinery, IEEE Int. Conf. Fuzzy Syst., 2020, 1-8. https://doi.org/10.1109/fuzz48607.2020.9177537

**[115]** C. Vlek, H. Prakken, S. Renooij, B. Verheij, A Method for Explaining Bayesian Networks for Legal Evidence with Scenarios, Artif. Intell. Law., 24 (2016) 285-324. https://doi.org/10.1007/s10506-016-9183-4

**[116]** M. Yeganejou, S. Dick, J. Miller, Interpretable Deep Convolutional Fuzzy Classifier, IEEE Trans. Fuzzy Syst., 28 (2020) 1407–1419. https://doi.org/10.1109/TFUZZ.2019.2946520

**[117]** M. Islam, D. Anderson, A. Pinar, T. Havens, G. Scott, J. Keller, Enabling Explainable Fusion in Deep Learning with Fuzzy Integral Neural Networks, IEEE Trans. Fuzzy Syst., 28 (2020) 1291-1300. https://doi.org/10.1109/TFUZZ.2019.2917124

**[118]** A. Jung, P. Nardelli, An Information-Theoretic Approach to Personalized Explainable Machine Learning, IEEE Signal. Process. Lett., 27 (2020) 825 - 829. https://doi.org/10.1109/LSP.2020.2993176

**[119]** Q. Zheng, H. Delingette, N. Ayache, Explainable Cardiac Pathology Classification on Cine MRI with Motion Characterization by Semi-supervised Learning of Apparent Flow, Med. Image Anal., 56 (2019) 80 - 95. https://doi.org/10.1016/j.media.2019.06.001

**[120]** R. Guidotti, A. Monreale, F. Giannotti, D. Pedreschi, S. Ruggieri, F. Turini, Factual and Counterfactual Explanations for Black Box Decision Making, IEEE Intel. Syst., 34 (2019) 14-23. https://doi.org/10.1109/MIS.2019.2957223

**[121]** V. Gatta, V. Moscato, M. Postiglione, G. Sperlì, CASTLE: Cluster-Aided Space Transformation for Local Explanations, Expert. Syst. Appl., 179 (2021) 115045. https://doi.org/10.1016/j.eswa.2021.115045

**[122]** J. Alonso, J. Toja-Alamancos, A. Bugarin, Experimental Study on Generating Multi-modal Explanations of Black-box Classifiers in terms of Gray-box Classifiers, IEEE Int. Conf. Fuzzy Syst., 2020, 1-8. https://doi.org/10.1109/fuzz48607.2020.9177770

**[123]** H. Cao, R. Sarlin, A. Jung, Learning Explainable Decision Rules via Maximum Satisfiability, IEEE Access, 8 (2020) 218180 -218185. https://doi.org/10.1109/ACCESS.2020.3041040

**[124]** M. Moradi, M. Samwald, Post-hoc Explanation of Black-box Classifiers using Confident Itemsets, Expert, Syst. Appl., 165 (2021) 113941. https://doi.org/10.1016/j.eswa.2020.113941

**[125]** C. Rubio-Manzano, A. Segura-Navarrete, C. Martinez-Araneda, C. Vidal-Castro, Explainable hopfield neural networks using an automatic video-generation system, Appl. Sci., 11 (2021) 5771. https://doi.org/10.3390/app11135771

**[126]** A. Mosavi, M. Salimi, S. Ardabili, T. Rabczuk, S. Shamshirband, A. Varkonyi-Koczy, State of the Art of Machine Learning Models in Energy Systems, a Systematic Review, Energies, 12 (2019) 1301. https://doi.org/10.3390/en12071301