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Artificial intelligence integration in materials science

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Abstract

The pervasive integration of Artificial Intelligence (AI) in materials science has transformed the design, functionality, properties and structures of innovative, as well as traditional molecules and crystalline. The new AI-powered laboratories promise to address persistent problems facing humans such cost reduction and productivity improvement in research and development. AI accelerates the discovery of resilient and durable chemical structures capable of providing humans with quality lasting products. More importantly, AI allows researchers to devise new bioactive materials making drugs more potent and affordable. The present research offers readers a succinct comprehensive overview of the progress in Ai application within materials science. Findings demonstrate that AI has improved chemoinformatics, imaging and drug discovery. Moreover, the implementation of AI has resulted in advancing additive manufacturing through transforming 3D printing design and optimization processes. The study documents an increasing trend in developing specific AI tools for advancing materials science such as ChatMOF, MatKG, BioinspiredLLM, MatterGen, and SpectATNet. Notwithstanding the progress in AI's implementation within materials science, there are important limits to the process represented by data quality, availability and accessibility. Future directions of research in the discipline include developing autonomous research assistant models and laboratories, improving the flexibility and responsiveness of AI systems to mimic human decision-making, and advancing interdisciplinary collaborations to enhance AI-enabled materials discovery.

Keywords Artificial intelligence, Materials science, Additive manufacturing, ChatGPT, Chemoinformatics

1 Introduction

Artificial Intelligence (AI) is the science and practice of developing smart autonomous systems capable of taking independent decisions [1–3]. In the past decade, the proliferation of Machine learning algorithms (ML) and Generative AI tools using Large Language Models (LLMs) and supervised training data have transformed human lives in many respects [4–6]. More than 2000 peer-reviewed articles featured machine learning as a core topic in materials science research in 2023 alone. The growth of ML materials research is exponentially increasing at a 1.67 annual rate for the past decade [7]. AI



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enabled research in materials science resulted in a 44% increase in new materials discovery and 39% rise in patent applications in 2024. AI enabled research in materials science resulted in a 44% increase in new materials discovery and 39% rise in patent applications in 2024 [8].

Notwithstanding the prevalence of ML and AI tools integration into materials science research, little systematic research has articulated the ways in which scientists applied such tools in the discipline [9–12]. Further, existing research on the subject typically covers one domain in the field ignoring other equally important applications [4, 9, 13]. For instance, a great proportion of AI studies in materials science concentrated on chemoinformatics without emphasizing the tools value in advancing imaging or bioactive structures [4, 14, 15]. Comprehensive coverage of AI tools contributions to materials science are lacking in the literature especially in recognition the main AI assistants used in enhancing drug discovery and additive manufacturing [16, 17].

Early research on AI and materials science concentrated on machine learning or deep learning techniques [4, 10, 18–20]. Such an agenda prioritized rudimentary aspects of AI integration into materials discovery like the availability of sufficient large data, the accuracy of models, the use of data processing software and the incorporation of autonomous statistical models in predicting and refining results [9, 21–23]. While this literature added valuable insights into how AI could assist scientists achieve new knowledge, it fails to capture the full breadth of how AI truly transformed materials discovery in the advent of Generative AI [24, 25]. In the past two years, the use of Generative AI in materials science transcended the traditional implementation of machine learning into the increasing reliance on AI assistants to perform complex reasoning and experimentation [9, 26–28]. The rise in AI's utilization within materials science calls for an immediate assessment of how such systems have impacted the design, optimization and use of new or existing materials.

The documentation of Generative AI implementation in materials discovery is limited and has not received adequate attention in the materials science literature [29, 30]. For instance, success stories of discovering new metal alloys with attractive properties used in the aerospace industry because of Generative AI innovative use by researchers at the University of Toronto have received little to no recognition across public media outlets [31]. Recently, many specific materials science AI tools have been developed to help practitioners screen materials, predict results and even design new structures with realistic test simulations [32, 33]. Up-to-date, little systematic commentary or reflection on the rapid development of Generative AI tools in materials discovery surfaced across the main outlets of the discipline [9, 25, 34].

The primary objective of the current analysis is to survey the most recent applications of AI models or systems in materials science. Within such an aim, the paper documents AI achievements in advancing chemoinformatics, imaging, biological structures and additive manufacturing. Moreover, the analysis highlights a few AI tools gaining popularity among material scientists such as ChatMOE, MatKG, BioinspiredLLM, MatterGen, and MechGPT. The main research question underlying this investigation is how have materials scientists used AI platforms and models to enhance the design, optimization and functionality of new or existing materials? Similarly, the analysis attempts to answer what are the most recent developments in AI tools for materials scientists use? Answering such questions provide material scientists with the appropriate knowledge of

how AI is being employed in the field to stimulate further conducive application of the technology.

The first section of the paper presents AI tools contribution to chemoinformatics. Within the section a discussion on how AI has transformed chemists statistical work, as well as imaging capabilities is introduced. Second, the paper delves into how scientists deployed AI in the manufacturing of materials processes. The advancements of AI technology in additive manufacturing, as well as the design of products are thoroughly examined. In the third section, the paper offers an overview of popular key platforms in the materials science space demonstrating AI empowered tools value to materials science. Finally, the paper highlights how material scientists impacted the biological aspects of new and known materials.

2 AI advances in chemical materials science

The purpose of this section is to provide readers with a high-level overview of AI applications in chemical materials discovery. The section covers AI's use in imaging, chemoinformatics and key areas of materials enhancement and testing. Chemical materials science concerns the composition, structure and interactions of elements [35, 36]. The field investigates the reactionary of elements to a variety of conditions like bonding or amalgamation [36]. AI tools allow researchers to simulate chemical processes discovering how comments react to certain conditions based on training data fed to the systems by chemists and other experts [37]. AI algorithms, platforms and agents have heavily improved the chemical analysis and enhancement of molecules structures in the drug discovery process [6, 38]. On the one hand, researchers have identified multiple targets components to ameliorate drugs functioning in the optimization phase [4, 9, 39]. On the other hand, scientists have better information on the potential efficiency and effectiveness of linking certain molecular structures together because of AI system's capabilities to furnish readily instant available information [38, 40]. Further, AI models have facilitated spectroscopic and microscopic chemical analyses of molecules leading to optimal materials selection [18, 41]. Relatedly, AI has enabled chemists to perform accurate advanced statistical analyses on the content used to improve materials saving a tremendous amount of time and effort [42–44].

2.1 Drugs discovery and chemoinformatics

The process of identifying new treatments to illnesses constitutes a major component of drug discovery [45]. The research, analysis, testing and reporting of trial findings on the efficacy of new or traditional treatments is another face of drug discovery [46]. The initial identification of chemical or biological pathways linking components to interact in certain. Ways benefiting treatments of diseases formulated another domain of drug discovery [47]. Today, scientists across the board utilize AI tools at every stage of the process throughout the drug discovery journey.

The application of statistical and probability models to the study of chemical features presents the main application of chemoinformatics [48, 49]. Traditionally, scientists collected information on chemical elements or processes using laboratory equipment and human observation. Then, scientists used computer software to analyze data manually. Today, AI systems allow researchers to collect and analyze data automatically without human interventions [50]. Advances in chemoinformatics enabled through AI models

have not only ameliorated materials structures or molecules but also improved the quality of life for humans around the world [38, 40]. Djoumbou-Feunang et al. [38] demonstrated how AI generative and predictive models improved the testing and optimization of bioactive molecules in the pesticides industry. The authors argued that AI has revived the stagnant research on pest control through the use of virtual laboratories incorporating autonomous chemoinformatics [38]. Evidence suggests the improvement of chemical materials produced in pesticides in the past decade enabled by large AI-based models capable of performing chemoinformatics efficiently and effectively [38, 40]. Such results led to higher yields, which translates into better food security metrics around the world [38].

One of the promising frontiers of AI potential impact lies within drug discovery [39, 51]. Scientists at the University of California San Diego designed POLYGON to help chemists and toxicologists identify multiple targets components in the early phases of drugs testing [51]. The platform performs instant searches for suitable links between molecules to optimize drugs' conducive properties [51]. The AI tool not only saves time and experimentation resources, but also accurately pinpoints the desirable characteristics of materials making useful drugs like those treating cancer [39, 51].

Researchers at Massachusetts Institute of Technology (MIT) developed an AI algorithm that helps identify cost-effective molecules, as well as optimal properties streamline drug discovery [6]. The AI tool improves Synthesis Planning and Rewards-based Route Optimization Workflow (SPARROW) [6]. The tool estimates the cost of identified molecules aiding drug developers in determining whether the combined candidates batch meet their expected budgets [6]. On another level, the model selects optimal molecules with the desired properties suiting the needs of drug developers in a very short time [6].

AI models incorporate the molecular design sorting procedure outlined in Fig. 1. Similar to traditional methods, models build a set of candidate designs with appropriate elements based on the data at hand. Second, the AI systems test the candidate designs using recommended parameters in the databases used as input for the systems. Based on the results of tests and specified outcomes, the AI platforms then generate optimal designs containing desired elements and molecular structures.

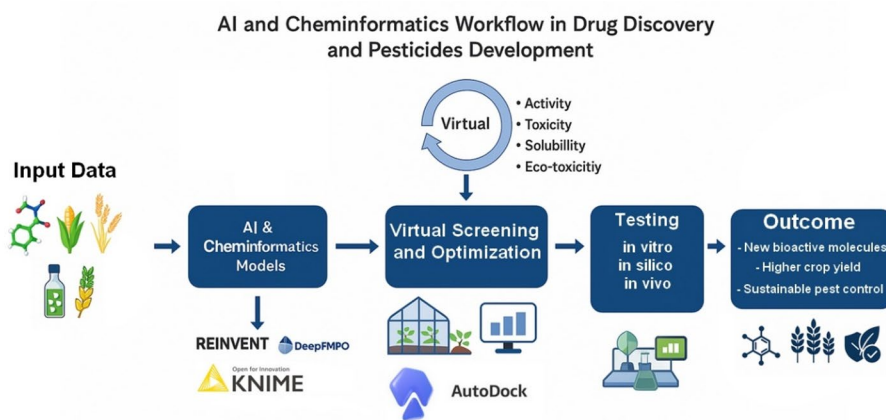


Fig. 1 AI-driven workflow for drug and pesticide development, from molecular input to optimized compound generation

2.2 Spectroscopic analysis

Spectroscopy is an essential process informing scientists about the fundamental elements, structure and composition of materials [43, 52]. Spectroscopic methods heavily rely on data analysis techniques [53, 54]. The primary objective of spectroscopy is the identification of recognizable or regular patterns within the data [18, 41]. Traditionally, applying data analysis techniques such as chemometrics requires the analyst to perform many procedures such as Principal Component Analysis (PCA) or Discriminant Analysis (DA) to understand patterns or dimensional structures within the data [42, 55]. Further, the analysis may also utilize Structural Equation Modelling or Regression to predict an anomaly within the data, which consume a tremendous amount of time and necessitates advanced expertise in the use of applied statistics [56, 57]. The recent advent of AI platforms has transformed spectroscopy and chemometrics practice in materials science [42–44].

The rapid development of AI tools and ML applications have accelerated materials scientists' discovery, testing and refining of new and existing materials [4, 9, 58, 59]. For instance, laboratory teams deploy a series of innovative tools to aid in performing classification, measurement and pattern recognition procedures part of the spectroscopic analysis [60, 61]. Cowger et al., used ML techniques to classify microplastics quickly, which helped the researchers identify new patterns in the data without much effort [62]. SpectATNet constitutes a popular architecture platform allowing materials scientists to generate data efficiently to perform advanced chemometrics analyses without extensive manual work [42, 63]. The advent of XAI platforms has provided material scientists with a repertoire of tools that provide deep reasoning leading to the output generated based on the spectroscopic analysis [44, 64]. Unlike traditional AI tools that only supply users with predictions, XAI platforms aid users with detailed description of the logic used to reach the presented conclusions accompanied with thorough explanations [65, 66].

2.3 Imaging

With respect to materials science, imaging refers to the utilization of instruments to inspect chemical elements or substances visually [67]. The instruments could be microscopes or spectrometers, as well as other equipment [68]. The examination of materials concerns elements attributes, properties or defects [69]. AI tools have evolved in the past few years offering scientists valuable opportunities to perform imaging in labs and beyond.

The adoption of AI and ML applications has increasingly penetrated synchrotron facilities [70, 71]. Such facilities generate radiographic materials essential for the analysis and discovery of molecules structures and composition of materials [4, 72]. AI tools allow scientists to perform unsupervised data screening, processing, reduction, interpretation and transformation in rapid and accurate forms saving colossal personnel and materials costs [22, 73, 74].

Recently, materials scientists have incorporated AI tools in X-Ray micro spectroscopy aiding in the processing and interpreting of the millions of Spectra resulting from the analysis [44, 72, 75]. A notable gain from AI use is the speed and accuracy of diffraction output based on the classification of crystalline systems and space groups [15, 76]. Using large simulation datasets, AI platforms could rapidly identify the structure and composition of a symmetric [15, 77, 78]. A second growing use of AI in synchrotronic

experiments is the reconstruction of images tomography. Wang et al. [79] demonstrated how AI tools reduce noise and the effects of missing data on the tomographic output of image-to-image reconstruction models [78]. One example on AI algorithms in processing images reconstruction is Noise2Inverse, which saves scientists a tremendous amount of computational power in addressing noise challenges in datasets [80, 81].

Noise2Inverse follows the process outlined in Fig. 2. First, the system recognizes a pattern and then reconstructs the trend into a meaningful product relying on machine learning. Finally, the system learns autonomously, and the AI agent acts as the lead point for making or analyzing elements using Noise2Inverse.

3 AI applications in manufacturing

Traditionally, material scientists convene in laboratories to engineer structures fulfilling specific functions satisfying safety requirements for products' usage [82, 83]. Structures represent certain architectures of components and materials that facilitate the performance of expected tasks for products withstanding natural forces causing failures [84, 85]. For instance, experts would come together and design commercial or industrial products that hold against fatigue, extended use and prove to be strong and tolerant [86]. Such a process consumes a colossal amount of time and may require prohibited costs because of the iterative optimization procedures involved to generate the final design [84, 87]. Generative AI applications have emerged as a resourceful tool for materials scientists not only to save time and cost, but also to produce architecture and designs escaping incompatibility and achieving high mechanical functional and safety levels [84].

3.1 Design

One of the recent applications of generative AI models in improving design and mechanical functioning is Wang's BEGAN algorithm [78]. The model heavily draws on deep learning methods mining large datasets full of images deploying the power of GANs. The results of the AI model were compared with 3D printed materials, as well as Fused Filament Fabrication (FFF) demonstrating the superiority of the AI designs on innovation, functionality and design properties [78]. In a similar AI application, Challapalli et al. (2021) utilized inverse design data-driven algorithms to investigate the load capacity of lettuce unit cells. The authors designed light-weight cells using AI models that demonstrated better load capacities when compared with the traditional octet cells. The computer aided design advanced algorithm achieved desirable properties and mechanical functionality much faster than previously [88].

Summary of the main application of AI in synchrotron facilities.

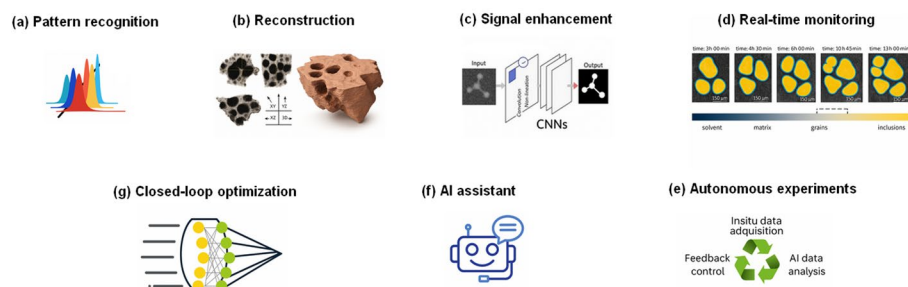


Fig. 2 Key AI applications in synchrotron facilities, from pattern recognition to autonomous experiments

Researchers at Virginia Institute of Technology (Virginia Tech) have enhanced the strength of Multiple Principal Element Alloys (MPEA) using AI tools and frameworks [89]. MPEAs possess a great deal of durability, strength and resilience against external stress or pressure [89]. They are versatile and used across many applications such as medical bone plates, as well as aerospace industry parts [89]. Using explainable AI systems that uncover the black box procedures the AI tool uses, the researchers developed a new MPEA characterized with stronger resistance and superior mechanical functionality to other MPEAs [89]. The explainable AI model furnished the principles used to improve the alloy benefiting researchers through uncovering the knowledge utilized to construct the new material [89].

Today, many teams across the globe partake in cutting-edge research attempting to overcome the cubic scaling challenge in building structures [90]. For instance, scientists from the Upper Peninsula at Michigan Technological University have collaborated with the University of California Los Angeles research teams to advance the generation of electronic structures based on Kohn-Sham Density Functional Theory [90]. Traditionally, a colossal amount of resources involving repeated experimentation requiring a great deal of time and cost are needed to scale material structures appropriate for industrial applications [90]. Machine learning models allowed the researchers to predict optimal structures using minimal resources [90].

Figure 3 illustrates the network architecture of the BEGAN algorithm used for generating innovative structures through deep learning. The generator, shown in (a), acts as a decoder that reconstructs images from random noise using a fully connected layer followed by convolution and up-sampling layers. The discriminator, shown in (b), functions as an autoencoder, compressing input images via convolution and sub-sampling layers into an embedded feature vector, then reconstructing the image from that vector, enabling effective adversarial training.

The use of AI applications to improve structural and functional designs has offered scientists superior results when combined with unsupervised simulations platforms. Argilaga (2023) incorporated GAN AI models with FEA simulations to generate optimal elastic properties for materials [92]. The infusion of AI and simulations generated a

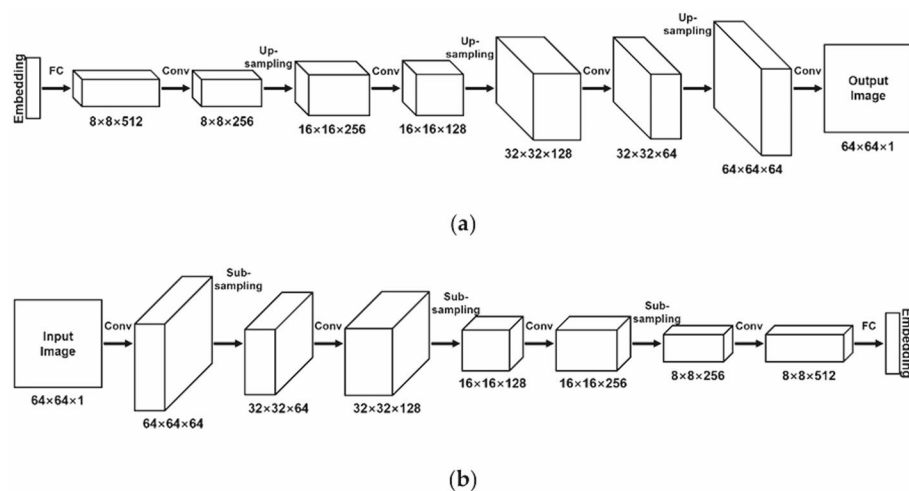


Fig. 3 Network architecture for the generator and discriminator. Adapted from [91], licensed under CC BY 4.0

large number of images with identical properties compared with real images of the same designs and materials. The combined use of AI and unsupervised simulation techniques not only save time and cost but also generate accurate results capable of serving as models for real materials design [93].

3.2 Additive manufacturing

Additive manufacturing refers to the construction of products using digital platforms [94]. The process involves adding layers on top of each other to create the final object [95]. Like other systems, manufacturing digital tools have evolved and incorporated with AI tools [96]. Today, designers utilize AI at every stage of the additive manufacturing process. The use of AI in materials science has influenced 3D printing of new structures improving the strength and durability of products [97]. A research team at Arizona State University received funding from the National Science Foundation to generate an AI-based platform that ameliorates stainless steel properties [97]. The team proposed the use of a naval metal propeller to optimize the size of the metal grain during the 3D printing process [97]. The use of AI in additive manufacturing has become a more common application of the technology in sophisticated industries such as the military industrial complex [97].

AI advancements have allowed manufacturers the opportunity of creating titanium alloys to be used in aerospace industries or medical equipment [98, 99]. While sophisticated 3D printing technology led to the development of desirable titanium alloys, the process still consumes a great deal of time and resources [98]. Concentrating on Ti-6Al-4 V, a low weight highly strong titanium, researchers at the Applied Physics Lab, as well as the School of Engineering at John Hopkins University discovered faster printing and better duality because of AI models deployment [98]. The authors suggested that AI not only resulted in accurate desirable properties but also challenged long-held assumptions about processing procedures [98]. AI suggested that manufacturers could change parameters perceived as unchangeable by many materials scientists [98, 99]. Thus, AI proved to open new avenues within additive manufacturing spaces resulting in optimizing metals or other industrial components [100–106].

4 Large Language models (LLMs) AI-based tools and materials science

The increasing development of Large Language Models and chat-based AI tools have largely impacted the Materials science discipline [107, 108]. For instance, new tools such as ChatMOF has gained some popularity among students and practitioners [109]. ChatMOF allows users to generate structures predict features and retrieve data related to metal-organic frameworks [109]. The tool achieved high accuracy rates on searching, prediction and generation metrics [109]. ChatMOF relies on ChatGPT platforms aiding experts in designing and optimizing structures [109]. The Fig. 4 illustrates a schematic representation of ChatMOF's interactive workflow, where human queries are processed by an AI agent that selects appropriate tools to generate or retrieve answers related to MOFs.

Another illustration of AI tools in materials science is MatKG [110]. The knowledge graph is based on the available scientific evidence containing information on materials, polymers, synthetic structures, properties, entities and relationships [110]. The platform

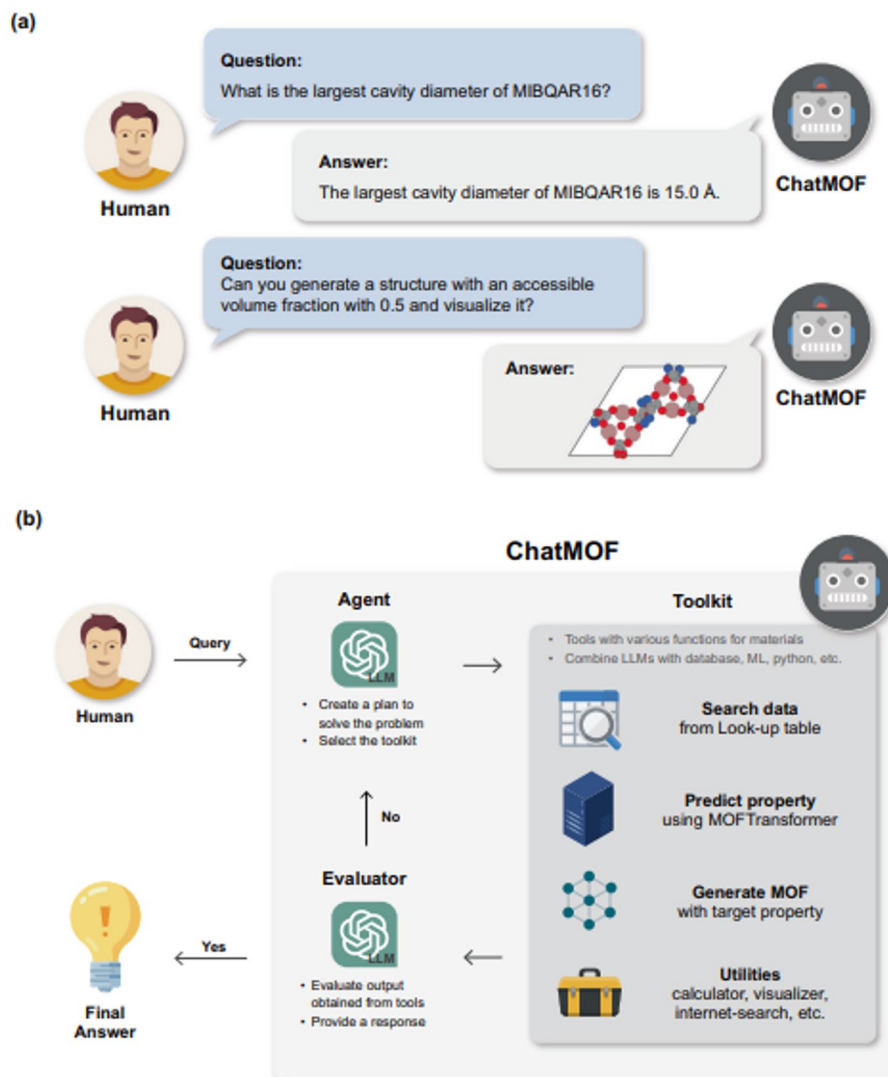


Fig. 4 Conceptual and schematic overview of ChatMOF. (a) A conceptual illustration showing ChatMOF's ability to respond to user queries about MOF properties and generate new MOFs based on user-defined conditions. (b) A schematic representation of ChatMOF's architecture, composed of three main components: an agent that formulates a plan, a toolkit that generates outputs, and an evaluator that refines the results into the final response. Adapted from [109], licensed under CC BY 4.0.

utilizes natural language processing to mine information on more than 70,000 components and 5.4 million triples [110].

Another increasingly popular development is the construction of interactive LLMs for special uses [111]. BioinspiredLLM illustrates such a reality by functioning as an engineer that assists researchers or practitioners in optimizing biomaterials [112]. The model relies on more than 1000 peer-reviewed articles containing data and information on bio inspired materials [111]. The platforms' accuracy for information retrieval, features selection and data generation are high [111, 112]. The model is able to generate hypotheses regarding new materials that have not been tested previously [112]. BioinspiredLLM is expected to serve as a valuable tool for materials scientists in the bioengineering field and industry [112].

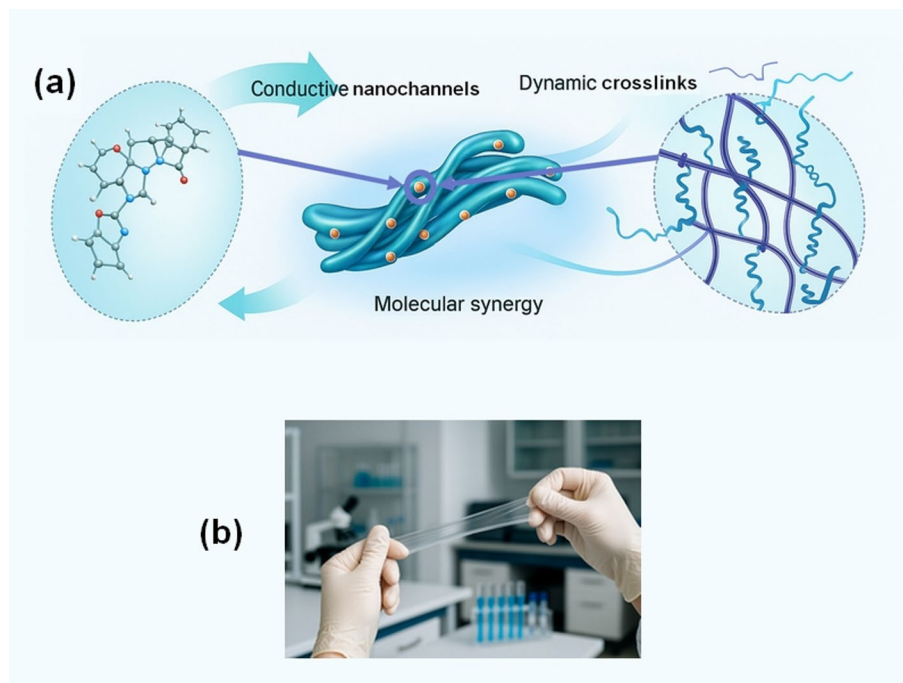


Fig. 5 (a) Schematic representation of a hydrogel's molecular structure with conductive nanochannels and dynamic crosslinks. (b) Photograph showing the hydrogel's stretchability during a stretch-release process

A Microsoft research team has recently built a generative AI model that optimizes inorganic stable materials based on diffusion methods [113]. The model is referred to as MatterGen [113, 114]. MatterGen does not utilize the common image-based diffusion models relying on Gaussian properties. The model incorporates a new diffusion method that depends on the symmetry of materials, as well as the periodic Table [114]. Throughout the output generation process of desirable properties, the model introduces labeled datasets to fine-tune the selection and prediction processes at each stage of the construction [113, 114].

5 AI and biomedical materials

Biomedical engineers have utilized AI tools in advancing the design, optimization and application of important materials for medical usage [28, 115]. For instance, AI utilization has accelerated the discovery of new and refined hydrogels [115, 116]. Hydrogels contain a large amount of water and possess unique properties [116, 117]. Traditionally, a tremendous amount of trial and error, as well as time are required to reach the optimal design and characteristics desired to be present in hydrogels [28, 117, 118]. Recently, AI-powered systems allowed researchers to identify the necessary additives, linking agents and polymers via machine learning algorithms mining large datasets autonomously [28, 115]. In other words, AI has enabled scientists to generate hydrogels with appropriate strength, porosity, chemical profiles and versatility allowing for wider applicability in Biomedicine [116–118].

Figure 5 illustrates the molecular structure and stretchability of an AI-optimized hydrogel used in biomedical applications. As seen in panel (a), the design incorporates conductive nanochannels and dynamic crosslinks that enhance mechanical flexibility and molecular synergy. Panel (b) displays a laboratory demonstration of the

hydrogel's stretch-release behavior, showcasing its potential for soft robotics and tissue engineering.

Another less popular, yet emerging, application of AI in materials science is the development of drug nanocarriers, as well as nanomedicinal components [32, 33]. AI tools help physicians and researchers provide personalized treatments via the use of genetic and patient data [32, 34]. AI platforms assist material scientists predict appropriate properties compatible with drug materials, as well as patient needs [33, 34]. While ethical challenges still face developers of nanomaterials in medicine, the discipline is gaining popularity as AI applications penetrate nanomedicinal materials discovery and refinement [34].

5.1 Medication development

Artificial intelligence (AI) has significantly accelerated the development and refinement of medications [52, 119]. Research teams have increasingly relied on AI systems to design hydrogels and develop personalized treatments using complex datasets mined by intelligent machine learning models [120, 121]. Similarly, medical scientists have leveraged AI to examine protein structures and optimize drug discovery and delivery processes [122, 123]. In recent years, biomedical research has incorporated various AI tools and frameworks to expedite therapeutic innovations, capitalizing on the growing availability of data and the predictive power of machine learning [124, 125].

5.2 Protein design and structure

AI tools have revolutionized the prediction of protein structures, as well as the design of new biomaterials [126]. Research teams at the University of Washington were able to generate protein molecules efficiently and effectively when using AI tools [126]. Based on amino acid sequences datasets, the researchers utilized the AlphaFold and RoseTTAFold AI algorithms to predict the design of natural proteins [126]. The AI tools incorporate generative AI tools such as DALL-E, as well as advanced machine learning autonomous algorithms to produce accurate representations to new protein molecules [126].

Recent machine learning advancements have proved useful in improving inverse protein folding methods [127]. British research teams from Sheffield and South Hampton universities developed machine learning algorithms that outperformed laboratory techniques for inverse protein folding [127]. The AI framework begins with predicting appropriate amino acids to eventually build a 3D protein structure [127]. The AI tools compare and contrast different folding combinations quickly to reach the optimal solution for the given scenario at hand [127]. Inverse folding is a critical step in identifying the optimal structure generating the desired function for the protein [127].

6 Limitations

The most pressing challenge facing material scientists advocating and heralding AI use in the discipline is explaining the black box phenomenon [128, 129]. The journey of a material scientists is replete with explainable phases including the prediction of properties, the choice of molecular structures and experimental conditions or outcomes [128, 129]. To inform scientists that AI models generated a host of decisions without explaining the how or the why behind such selections proves to be a difficult endeavor [128,

[129]. Thus, progress toward uncovering the black box phenomenon in AI's implementation constitutes a priority for future research [128, 129].

A constant challenge for AI applications in materials science lies in the new materials' replicability, validation and utility. Many highlighted that much of today's progress in AI enabled materials discoveries pertains to highly specific domains lacking appropriate universal application [91]. Similarly, the new AI tools are still in the developing phase requiring further rigorous testing for making a real impact on industrial applications [91]. Most importantly, data, as well as information quality remains a top challenge for any AI or machine learning model [91].

Scalability remains to be considered one of the challenges facing AI's implementation in materials sciences. To apply AI frameworks on a large scale, a great deal of computational processing power is needed [130]. Access to quality cloud-based computation, high-performing computers and distributive systems is untenable to many labs or enterprises around the globe limiting implementation [130]. While the advent of new AI models has made significant strides in advancing materials science discoveries today, computational barriers remain important in scaling up AI's integration into materials scientists' daily work [130].

A salient limitation in the application of AI to accelerate new materials discovery is the scarcity of actual empirical testing, validation or modification. In many cases of AI implementation, researchers rely on machine learning algorithms power to mine datasets [131]. The output or results of the models are theoretical and conceptual in nature. Across several experiments, scientists demonstrated that the AI expectation or prediction did not hold on to cereal materials were used in laboratories [131]. The hypothesized relationships in AI models did not translate into reality once real materials replaced AI filled components.

One of the crucial limits of AI synthetic generated data is model collapse [132, 133]. Many experts reported the failure of LLMs to generate expected results because of collapse caused by a variety of reasons [132]. A more important limit is fidelity to realistic characterizations of materials [134]. Such a limit is especially significant in niche manufacturing sectors [133]. One of the main challenges is the dearth of quality training datasets on rare materials [132, 133]. Scalability and reliability are important considerations that are compromised when AI models are used in AM contexts [135]. One illustration of AI limits in data generation applications within materials science is DALL-E inability to truly autonomously produce accurate images without human intervention [136, 137]. Niche manufacturing applications indeed require human involvement when DALL-E or other AI platforms are invoked to advance materials resilience or functionality characteristics [136, 137]. The reason for driving is that DALL-E may not provide valid knowledge representations of different elements.

7 Emerging discoveries of AI and materials science

The deployment of AI in advancing polymers discovery has led to the development of a new rubber-like materials more quickly and easily compared with traditional materials [138]. Researchers (i.e., Olexandr Isayev, Frank Leibfarth, and Dylan Anstine) at Carnegie Mellon University and The University of North Carolina at Chapel Hill created a strong flexible polymer using machine learning algorithms [138]. Oftentimes, material scientists create stiff polymers when applying strength processes to flexible materials

generating a challenge [138]. The process begins with determining desired design properties for the polymers. The AI tool provides recommendations on the necessary tests. Scientists perform the experiments using software and the AI tools. Then, the output helps in refining the construction of the final material. Researchers at both institutions have shown significant excitement on developing specialized polymers resolving some of the intransigent problems facing materials science in the past.

The advancement of electronic polymers is facilitated through AI tools deployment. Electronic polymers are special materials that possess the flexibility of plastics and properties of metals [78]. They could be used to carry out energy (electricity) from one point to the next [139]. Despite the desirable properties electronic polymers have, making them is time consuming and costly [139]. The University of Chicago and Argonne National Laboratory researchers have developed machine learning approaches to advance the creation of electronic polymers [140]. The researchers developed a fully functioning AI tool, Polybot, to help in the creation of electronic polymers thin films. The tests proved useful results noting the ability of AI in helping scientists create stronger materials in affordable fashion [139, 140].

The strengthening of Multiple Principal Elements Alloys (MPEA) is facilitated through the use of AI tools today. Such alloys are used in the aerospace and biomedical industries found in many parts like bone plates [141, 142]. Using Large amounts of data, researchers at Virginia Tech developed a new MPEA alloy with stronger properties compared to previous types [143, 144]. The researchers utilized an AI model generating predictive output. The team utilized SHAP (SHapley Additive exPlanations) method to interpret the results. The discovery culminated in the identification of a stronger MPEA that is versatile and could be used across several industries.

The rapid evolution of AI tools has allowed research teams to design novel architecture assisting scientists in materials discovery work [9]. Researchers at John Hopkins University Applied Physics Lab developed Autonomous Researcher for Materials Discovery AI platform [145]. The tool helps researchers in three phases: the identification of structures, the synthesis of elements and the measurement of properties. The tool also performs tests to validate the output generated by the system. The research team at the University developed new materials capable of withstanding extreme heat conditions.

One of the increasingly popular materials science AI tools prevalent in industrial settings is Citrine. The tool provides users with a friendly workflow canvass requiring little to no coding. Citrine uses statistics and probability models to identify desirable characteristics of materials. The tool is capable of performing virtual experiments. Plastics and polymers manufacturers utilize Citrine to identify green materials to be used in sustainable demands put forth by clients [146, 147].

The Munich-based AI platform ExoMatter facilitates research and development in materials science. Alloys and Metals producers utilize the platform to identify the most relevant materials for the specified applications [148]. Similarly, Kebotix is another research and development AI tool for materials discovery. British Petroleum (BP) used Kebotix to test many chemical structures hoping to generate new materials.

7.1 Quantitative metrics on AI integration to materials science application

Materials science AI platforms have received a great deal of investment in the past two years noting their industrial significance. The National Science Foundation partnered

with Intel to invest \$20 million in Cornell University's AI Materials Institute. The NSF continued commitment to AI and materials science culminated in funding five national labs around the United States with more than \$100 million [149]. Periodic Labs, a newly founded AI materials science firm, announced a drive to raise \$200 million in 2025 [150]. Economists expect the AI and materials science market to grow exponentially in the present decade. Many startups like Exomatter raised a few million during the founding years to lay out their products and services in the marketplace.

Despite the bleak evidence facing AI projects success across all sectors, emerging AI successes in materials science points to promising future in the field. In a report MIT published earlier in the year, Sheryl (2025) concluded that 95% of AI pilots in companies have failed [151]. In another report, AI integrations thus far did not carry intended return on investments [152]. In fact, 42% of AI projects generated no return on investments. Nevertheless, funding for AI materials science investment has grown significantly in the past few years. The number of patents registered with respect to new materials facilitated by AI has also increased signaling innovation in the field. More materials manufacturers are adopting AI platforms to facilitate their work signaling a general acceptance to the technology. Experts suggest that it is too early to evaluate the success of AI in materials science.

7.2 Future research directions

Recent developments in AI Applications across materials science points to the increasing interest in the creation of autonomous research assistant models [11, 153]. Recently, Cornell University researchers developed knowledge distillation AI models that condense large amounts of information in seconds, generating new useful output on materials properties [153]. Corollary to such endeavors are the efforts geared to establish autonomous laboratories performing scientists' work without human intervention [11, 153]. The aforementioned progressively developing trends points to the general construction of independent AI systems capable of performing humans' cognitive demanding tasks autonomously [153]. Future researchers need to perform further testing of such independent models to determine viability and functionality.

A growing complex application of AI in materials science is the production of quantum materials using autonomous robots. University of Chicago researchers have developed a robot that makes thin superconducting materials [154]. The research effort aims at enhancing the Molecular Beam Epitaxy (BME) process necessary in building materials layers [154]. Future researchers are urged to explore similar frontiers intersecting AI systems, as well as quantum materials.

The constant need to improve AI's models or systems performance represents a primary area of research for future work [57]. AI is still developing and fails to perform every task a scientists performs in or out of the laboratory. AI' systems are less flexible compared to human protocols making them less responsive when needs arise to modify or change parameters. Thus, future researchers are encouraged to improve the flexibility and responsiveness of autonomous robots and AI assistants to perform scientific tasks in a manner similar to human scientists in their real-world settings.

The growth of interdisciplinary teams collaborating to advance AI application in materials science is expected to rise in the next decade. For instance, Pennsylvania State University secured National Science Foundation to establish The Institute for AI-Enabled

Materials, Discovery, Design, and Synthesis (AIMS). Communities of practice intersecting materials science and computer science are appearing rapidly on college campuses across the United States, as well as other countries [155]. Future researchers are encouraged to pursue interdisciplinary research agendas prioritizing collaborations among teams from different fields.

8 Conclusion

The present research has demonstrated the prevalent incursions of AI into materials science. New tools, platforms, and programs such as DALL-E, ExoMatter and Citrine have penetrated the variety of processes involved in the materials design and development paradigm. The use of AI in materials science has advanced contributions in chemoinformatics, additive manufacturing, drug discovery, alloys, plastics, polymers and metals. The past few years witnessed the discoveries of new materials across academic laboratories and industrial plants around the world.

Investments in AI and materials science are on the rise. Governments and companies alike have allocated hundreds of millions to refine the research and development of existing and new materials. The number of AI platforms for materials science has significantly increased signaling serious commitment in the advancement of the field.

The exponential growth of AI platforms helped material scientists to design, refine and consolidate innovative functional substances that address serious and complex problems facing the world. During the past decade, the applications of AI in materials sciences have not only grown in quantity or quality, but they have also transcended new areas of research and development such as autonomous laboratory simulation systems or robotic experimental settings. With such rapid developments in academia and industry, a parallel focus on the enhancement of scientists training has emerged concentrating on skills covering data analytics, computer programming, machine learning and applied statistics.

Like other disciplines and domains, materials science has increasingly witnessed unprecedented levels of AI integration in the past five years. One of the main application areas of AI deployment in materials science is the discovery of innovative materials or the refinement of already known materials. Scientists have incorporated AI tools that utilize machine learning algorithms in furthering the development of materials for laboratories, as well as industrial applications. For instance, the use of AI methods and applications led to the identification of new solid electrolytes making lithium-ion batteries safer.

AI tools will not immediately replace the role of material scientists in labs or the academy. However, learning the tools provide an edge for new, as well as experienced material scientists. AI platforms or applications offer scientists a valuable leverage in improving the efficiency of their work. While expertise is still a prerequisite to quality products, material scientists who employ AI tools are expected to be more productive, as well as effective compared to their peers who do not learn or use AI. Therefore, graduate programs preparing scientists need to incorporate AI training in their curriculum and instructional.

Another significant development in materials science is the revolutionary evolution of self-driving laboratories especially in chemical industries. The advent of machine learning, the availability of large quality data and the present of intelligent systems have

allowed experts to develop autonomous labs performing scientists work with little to no human intervention. Notwithstanding such sophistication, many challenges still face the normalization of self-driving laboratories. On the one hand, most current models are highly complex and costly. On the other hand, replications are scarce because of proprietorship. Increasing access to information and data facilitates the democratization of self-driving laboratories construction globally.

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M.A.-S. conceived and designed the study, conducted the literature review, wrote the manuscript, and prepared all figures and tables. The author reviewed and approved the final manuscript.

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Declarations

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