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AI-Driven Advancements in Biomaterials Science: A Narrative Review

Sonali Patel, Akanksha Dwivedi and G.N. Darwhekar

ABSTRACT

INTRODUCTION

Biomaterials have emerged as a key component of contemporary medicine, propelling advancements in drug delivery, implants, and regenerative medicine. But conventional trial-and-error methods of finding new materials are sometimes cumbersome, resource-intensive, and ill-equipped to meet the demands of individual patients.

AI IN HEALTH CARE

By facilitating intelligent data analysis, diagnosis, and individualized therapy, artificial intelligence (AI), in particular, machine learning, deep learning, and data mining, has become a disruptive force in the health care industry. Its incorporation into biomaterials research opens up new avenues for clinical translation and innovation.

PREDICTIVE MODELING

AI systems are able to analyze sizable and intricate biological and material information in order to forecast attributes like mechanical strength, toxicity, biocompatibility, and in vivo response. These predictive skills enhance preclinical research ethics while speeding up the identification of biomaterials.

DESIGN AND DEVELOPMENT

AI makes it possible to create and modify biomaterials that are suited to a certain illness or a patient's unique circumstances. Targeted medication delivery systems, customized implants, and physiologically sensitive smart materials are a few examples of applications. Materials informatics and high-throughput screening drastically cut down on development time and expense.

FUTURE PROSPECTS

In spite of its potential, integrating AI into biomaterials presents difficulties, including the requirement for reliable data privacy frameworks, transparent algorithms, and standardized, high-quality datasets. To get over these obstacles, multidisciplinary cooperation between data scientists, physicians, materials experts, and regulators is crucial.

CONCLUSION

AI is changing the biomaterials industry by improving the accuracy and efficiency of material design, selection, and testing. AI will continue to play a key role in developing next-generation biomaterials for predictive and individualized health care with sustained improvements and cooperative efforts.

Keywords: AI-driven biomaterials design, Predictive biocompatibility modeling, Machine learning material informatics, Personalized implant customization, High-throughput in silico screening

Introduction

Biomaterials science, an important field of contemporary medicine, has developed at the nexus of biology, chemistry, and materials science.¹ The materials studied in this field—called biomaterials—have improved biological processes, made it possible to create new treatments, and helped replace and repair damaged tissue systems. Originally employed in early inventions like pacemakers, dental implants, and joint replacements, these biomaterials were made of basic, inert materials like metals, ceramics, and polymers. But as medical knowledge grew, so did the expectations placed on biomaterials, which today require higher levels of complexity, bioactivity, and flexibility.² In order to tackle difficult therapeutic problems, this naturally interdisciplinary field combines clinical medicine, chemistry, cell biology, and materials science. Patient care has changed dramatically as a result of recent advancements in tissue engineering scaffolds, medication delivery methods, and the developing field of bioelectronics. Notable developments include the creation of intelligent biomaterials that react dynamically to physiological stimuli, as well as resorbable scaffolds, biosensors, and drug-eluting stents.

The increasing prevalence of complicated illnesses, including diabetes, cancer, cardiovascular disease, osteoarthritis, and neurodegenerative diseases like Alzheimer's, is influencing the changing biomaterials environment.³ Biomaterials that are not only biocompatible and bioactive but also tailored to the specific requirements of each patient are needed to address these issues. Artificial intelligence (AI) has sparked innovation in this area in recent years. Its ability to assimilate data, recognize patterns, and model predictively provides a strong toolset for negotiating the complex interactions between biological systems and material features. The discovery of potential biomaterials from enormous chemical libraries has been greatly expedited by high-throughput screening and AI-driven materials informatics.⁴ Nowadays, complex information like proteomics, metabolomics, and physicochemical profiles is analyzed using machine learning (ML) algorithms, which improve material selection and uncover bioactivity processes.⁵ Additionally, AI is being used more and more to customize biomaterials according to a patient's genetic profile and the context of their ailment, which aids in the creation of customized implants and focused drug delivery systems. This individualized strategy has the potential to maximize treatment results and reduce side effects.⁶ Because biological systems are complex, AI is becoming more sophisticated, which is leading to new opportunities in

the study of biomaterials. The objectives of this review are to (i) give a thorough summary of how AI-powered approaches are changing the field of biomaterials research and (ii) predict potential advances that might result from this convergence of technologies. In order to do this, the paper starts with a basic introduction to biomaterials and then delves further into AI applications, backed up with case studies. It ends with a discussion of potential future paths for cooperative development between these two vibrant fields.^{7,8}

AI Integration in Health Care

Among the numerous areas that AI has the potential to affect is the health care sector. AI is revolutionizing health care by improving biomedical research, diagnosis, and therapy. The use of AI in medicine and its developing importance in the creation of biomaterials are summarized in this section.⁹ It addresses how biomaterials innovation is aided by AI to enhance medical device safety and customization. The development of intelligent computers that can mimic human cognitive processes is the aim of the computer science component of AI. AI integrates methods such as ML, deep learning (DL), and natural language processing (NLP) to replicate cognitive functions and analyze complex datasets. These advancements enable machines to collect and evaluate enormous volumes of data, identify trends, predict results, and react to new information. In the health care industry, AI has become a potent instrument that can address some of the most significant problems the industry is currently facing.¹⁰ AI's entry into the medical field has ushered in a new era of opportunities that will impact nearly every facet of the sector. Here, we look at some of the most significant applications of AI in health care:

AI has greatly advanced medical imaging and diagnostics, resulting in faster and more precise diagnoses. Machine learning algorithms can be applied to analyze pictures of medical conditions from computed tomography (CT), magnetic resonance imaging (MRI), and X-ray scans in order to identify anomalies and assist radiologists in making diagnoses. This ability enhances diagnosis and raises the precision of medical procedures. By finding potential therapeutic candidates, simulating medication interactions, and improving clinical trial designs, AI speeds up drug development.¹¹ Through data analysis and DL, AI can discover novel compounds and transform outdated drugs for new therapeutic applications. AI in personalized medicine utilizes clinical and generic data to customize therapies, enhancing results and reducing adverse effects. This makes it possible to tailor medical interventions to improve patient outcomes. Clinical decision support systems driven by AI offer evidence-based recommendations to physicians, assisting them in diagnosis and therapy planning. To assist physicians in making well-informed judgments, these systems make use of extensive health care databases and clinical advice.¹²⁻¹⁵ In the health care sector, AI enhances resource allocation, patient scheduling, and hospital administration. Hospitals may be able to better manage

resources and reduce patient wait times by employing predictive analytics to forecast patient admissions. Through the extraction of valuable information from unstructured electronic health records, NLP technologies facilitate the accessibility and usability of patient data. This enhances clinical documentation, boosts research capabilities, and encourages better patient care. AI-enabled wearables and sensors make it possible to continuously monitor a patient's health. These devices facilitate quick reactions and reduce readmissions to the hospital by detecting early warning signs.

Biomaterials are often used in tissue engineering, implants, and medical devices; they interact with physiological systems. Successful medical applications need the design and creation of biomaterials using certain properties, endurance, and biocompatibility. Conventional methods for finding new biomaterials are expensive and time-consuming. Algorithms driven by AI can predict material attributes, sift through massive material datasets, and identify deserving subjects for additional study.¹⁶ This makes it easier to find materials with the appropriate qualities. AI enables the creation of optimal biomaterials for certain design uses. By considering a number of variables, such as mechanical characteristics, biocompatibility, and degradation rates, AI may create designs that closely adhere to the requirements of medical equipment and implants.¹⁷ To prevent negative reactions when a biomaterial comes into contact with living tissues, it is crucial to evaluate its biocompatibility. Comprehensive *in vitro* and *in vivo* testing is not necessary since AI algorithms can predict a material's biocompatibility based on its chemical formula and structure. Biomaterials can be customized to match particular patient characteristics thanks to AI. This is particularly crucial in fields like tissue engineering, where patients' unique anatomy can be accommodated by personalized implants. Biomaterials research makes use of large databases that include biological interactions, experimental results, and material properties. Evidence-based decision-making is made easier by AI, which can efficiently aggregate and analyze this information to uncover hidden trends. AI can enhance the production processes for biomaterials, ensuring consistency and quality control. Automation and real-time monitoring can reduce error rates and increase production efficiency.¹⁸ Figure 1 depicts the impact of AI across various domains of health care.

Biomaterials Predictive Modeling in AI

Numerous fields of medicine, such as tissue engineering, medical equipment design, and regeneration medicine, depend heavily on biomaterials. The creation of biomaterials is essential to the progress of several health care domains. Predictive modeling powered by AI has proven useful for the design and study of biomaterials. The current work explores the connection between predictive modeling driven by AI and biomaterials. It looks at how various fields could cooperate to enhance the creation of biomaterials, explains their properties, and projects their effectiveness.¹⁹ Biomaterials are compounds designed to work with biological

Frequency

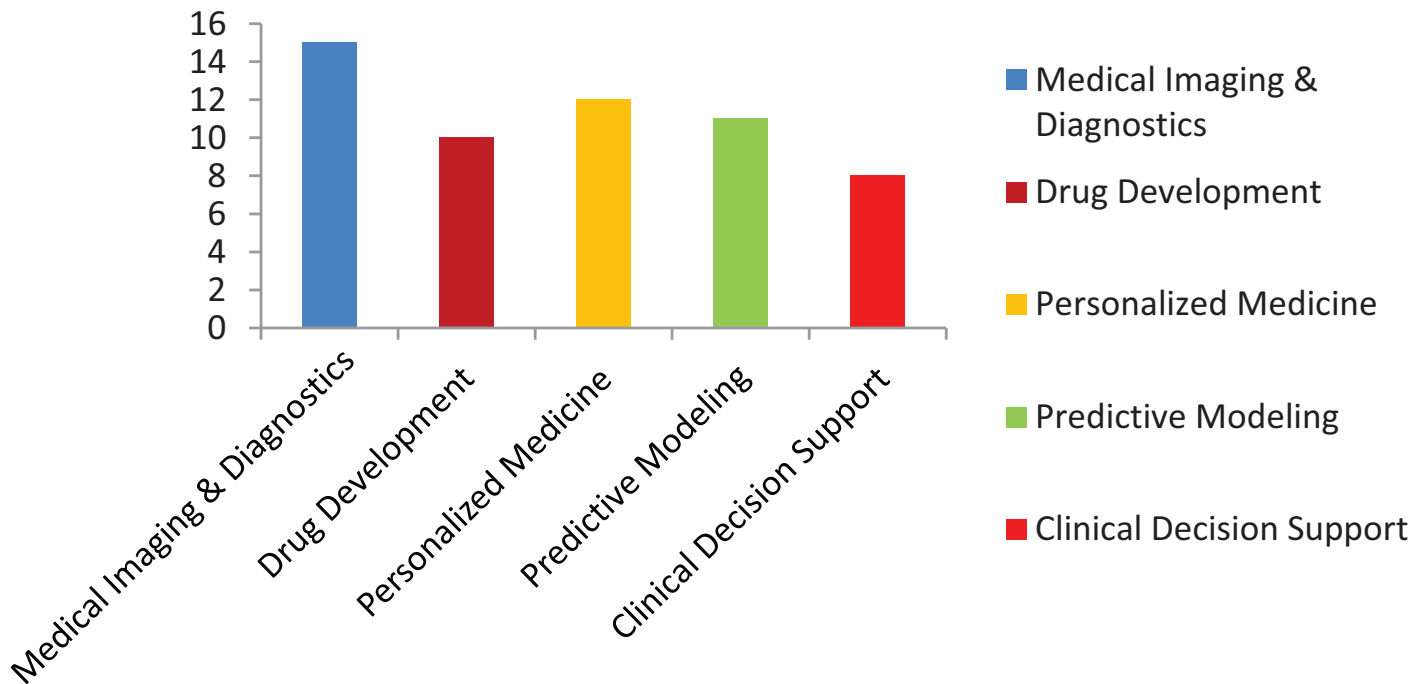


Fig 1 | Impact of AI in health care

systems for scientific, medicinal, or diagnostic reasons. They have been employed in several applications, including tissue scaffolds, medication routes, orthopedic implants, and medical procedures. They may be artificial or natural. Selecting and producing biomaterials is crucial to ensuring their appropriateness for biological environments and their ability to perform specific functions. The procedure has always been guided by actual experimentation and trial-and-error methods. However, the incorporation of AI into biomaterials research has resulted in a substantial change in the development and optimization of biomaterials.

AI is a general name encompassing a variety of computing techniques, including ML and DL, that are capable of analyzing intricate patterns in data and foreseeing outcomes based on enormous volumes of information. These methods are used in AI-driven predictive modeling for biomaterials to expedite the creation and review of biomaterials. Among AI's key benefits is its capacity to handle massive amounts of statistical data, which is very helpful when dealing with the complexity of biomaterials. Models of AI are able to identify relationships and trends in data on material properties that are not always apparent using conventional experimental methods.^{20–24}

Applications: From Prediction to Personalization

One essential application of AI in biomaterials is material property prediction. Conventional techniques examine properties including durability, biocompatibility,

and rates of deterioration in laboratory tests. These studies may be expensive as well as time-consuming. However, by using the data that is currently accessible, predictive algorithms based on AI can assess these properties for new biomaterials. For example, by using a dataset to learn known biomaterial properties, ML algorithms may forecast the physical properties of novel materials based on their structural traits and chemical makeup. This helps researchers analyze and prioritize potential biomaterials more efficiently, which in turn reduces development costs and timelines. One important use of AI in biomaterials is the optimization of material composition and structure.²⁵ In order to build biomaterials with specific properties and functions, it is often required to make iterative changes to their chemical composition and architecture. By building virtual prototypes and simulating their operation, AI can expedite this process. Simulations driven by AI can predict, for instance, how modifications to the surface chemistry of a biomaterial impact its interactions with cells or how modifications to the molecular structure of a polymer impact its mechanical characteristics. By determining the optimal biomaterial configurations and investigating a wider design space, these simulations assist researchers in saving time and money. AI can also help with patient-specific biomaterials customization. The increasing importance of individualized medicine in health care is also true for biomaterials. In order to customize biomaterials to every patient's unique needs, AI may evaluate information unique to each patient, including medical history and genetics. For example, AI

can help with the precise implant design for patients with orthopedic conditions, improving the incorporation of prosthetics and lowering the likelihood of issues. Likewise, in tissue engineering, AI can guide the creation of tailored scaffolds that promote tissue regeneration in a manner unique to each patient.

Predictive Model Evaluation and Challenges

Predictive modeling powered by AI can aid in the optimization, prediction, and performance assessment of biomaterials. Following implantation, biomaterials need to be observed in order to assess their long-term functionality and safety. In order to identify any anomalies or performance deteriorations, AI can analyze the data already available from implanted devices, such as sensors and other imaging devices. Early intervention and improved patient outcomes are possible results of proactive action.²⁶ AI can also be used to assess histologic and cellular responses to biomaterials, providing information on biocompatibility and tissue integration. These kinds of data can help optimize biomaterial designs and ensure their clinical viability. One noteworthy aspect of AI-driven predictive modeling in biomaterials is its capacity for continuous learning and adaptation. As the volume of open data increases and their knowledge of biomaterials advances, so does the predicted accuracy of AI systems. In the rapidly evolving biomaterials field, where new formulations and materials are continuously created, this self-improvement mechanism is advantageous. AI models are adaptable enough to change with the environment, incorporating new knowledge and insights into their predictions.²⁷ Despite the potential benefits of AI in biomaterials, a number of obstacles need to be removed before its full potential can be achieved. The availability of diverse, excellent, and well-annotated datasets is the most important component. The training and validation processes of AI algorithms heavily rely on data, and the accuracy and generalizability of the models are directly impacted by the integrity of the data. Researchers and institutions must collaborate to create and share extensive biomaterials databases in order to support AI-driven advancements in the field. AI simulations' accessibility in biomaterials has also drawn criticism. Among the numerous "black-box" AI

systems that make it difficult to understand how they generate their forecasts are DL models in particular. Comprehensible AI techniques, like examination of feature relevance and understandable AI methods, must be developed and incorporated into biomaterials research to improve the precision and utility of AI-driven predictions. It is necessary to address ethical issues when integrating AI into biomaterials research.^{28–30} Table 1 represents the role of AI-based predictive modeling in biomaterials.

Design and Development of Biomaterials Using AI

Evolving Role of Biomaterials in Modern Medicine

Biomaterials, carefully designed to function as medical or diagnostic procedures by interacting with biological systems and their different elements, have become essential components in the rapidly evolving field of medicine.³¹ The topic of biomaterials has seen exponential growth in interest and research over the last few decades, mainly because of their essential function in a variety of biomedical applications.³² The potential of biomaterials is to dramatically improve results for health care and the general quality of life as essential components of cutting-edge diagnostic and treatment systems. Biomaterials have historically been used as scaffolds for structural support, supporting and facilitating the healing and functional restoration of a variety of organs and tissues, including those used in the field of orthopedics, reconstructive, ophthalmology, dentistry, and cardiovascular operations.³³ But biomaterials now serve purposes beyond just providing structural support. These resources are widely used in advanced applications in biomedicine nowadays, such as biodegradable tissue engineering constructions, drug delivery systems, biosensors, and contrast agents for scanning.³⁴

Redefining Biocompatibility and Design Complexities

A comprehensive understanding of the intricate relationships that exist between the human body and biomaterials has always been essential. The comparatively low early implant success rates made this understanding a main emphasis more than 50 years ago. In order to understand the specific interactions between biomaterials and biological environments, both bio-

Table 1 | Role of AI-based predictive modeling in biomaterials

| Field/Area of Application | Role of AI | Outcome | References |
|--|--|--|------------|
| Prediction of material properties | Properties of new biomaterials estimated by predictive algorithms | Minimizes development timelines and expenses | 19–24 |
| Optimization of material composition | The iterative modifications to the architecture and chemical composition | Saves development time and money | 25 |
| Personalized care for every patient | Evaluates patient-specific information for customized biomaterials | Enhances prosthetic integration and minimizes problems | 26 |
| Extended functionality surveillance | Examines information from implanted devices | Better patient outcomes and early intervention | 26 |
| Evaluation of histologic and cellular response | Analyzes answers | Assures clinical viability | 26 |
| Consistent learning and adaptation | Incorporates fresh information into forecasts | Improves the accuracy of predictions | 27 |
| | Creating and releasing large databases | Supports developments promoted by AI | 28–30 |

chemical and biomechanical, a paradigm change has occurred since then. Defined as “biocompatibility,” this idea includes a variety of interactions and related characteristics, such as bio functionality, bioactivity, and bio stability.^{35,36} When designing and developing biomaterials for particular therapeutic or diagnostic purposes, it is crucial to ensure that any negative consequences, like systemic or local toxicity, fall under physiological thresholds that are acceptable.

The Three-Level AI Integration Framework in Biomaterials

A three-level conceptual framework that corresponds with practical biomedical applications may be used to coordinate the design and development of biomaterials utilizing AI. It is depicted in Figure 2.

AI-Driven Decision Toolbox for Biomaterials Design

The Table 2 summarizes the AI-driven decision toolbox for biomaterials design.

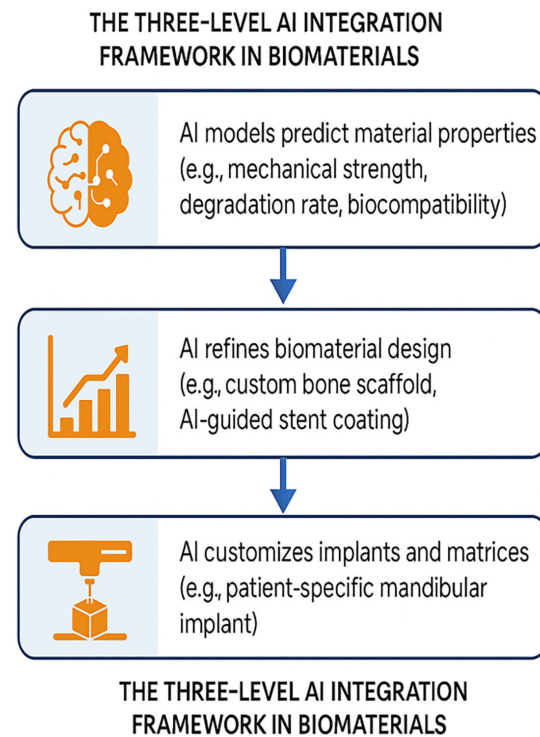


Fig 2 | The three-level AI integration framework in biomaterials

AI-Driven Transformations in Biomaterials Design

Biomaterials in clinical practice are frequently dynamic and essential elements that blend in perfectly with the native tissues rather than being essentially inert substances. Material screening, clinical and nonclinical safety assessments, testing for by-product releases, and stringent postmarket surveillance are all steps in the complex and multistage process of evaluating biomaterial interactions.⁴³ Strict regulatory requirements must be met by this complex review process, which calls for thorough evidence of compatibility for all biomaterials meant to come into contact with human tissue. For example, the lack of a precise and widely recognized definition of biocompatibility is a major obstacle in this discipline.⁴⁴ Despite this difficulty, the increased focus on biomaterials research and development has led to a rise in the amount of data and scientific publications about the interactions between biomaterials and cells. By expanding the criteria, tests, and data utilized to describe these intricate interactions, this comprehensive research seeks to achieve the best possible acceptance and incorporation of biomaterials into living systems. Although these definitions are crucial for defining basic elements, they frequently have significant flaws and restrictions because they are either too vague or too specialized, making universal quantification more difficult. Recognizing these shortcomings makes it clear that new definitions and improved ideas are required in order to attain a more thorough comprehension of the biomaterials sector.⁴⁵ The revised definitions could open the door to new methods of evaluating how biomaterials interact with living systems, improving stakeholder communication, and expediting the approval process for creative biomaterial uses.⁴⁶

A revolutionary opportunity exists while utilizing AI capabilities in the biomaterials industry. AI has the potential to transform the present manual procedures used in the literature by automating the data extraction from scientific publications into a structured format. In addition to greatly cutting down on the amount of time needed for information extraction, this revolutionary method makes it easier to establish standardized procedures, which guarantee stability and dependability in biomaterials discovery.⁴⁷

A deeper understanding of the complex relationships between biological systems and biomaterials can be gained thanks to AI’s skills in predictive analytics,

Table 2 | AI-driven decision toolbox for biomaterials design

| Problem | AI Technique | Example | References |
|---|---|--|------------|
| Predict degradation rate | Random forest (RF), support vector regression (SVR) | Modeling degradation behavior of PLGA, chitosan, and PCL scaffolds | 2,37 |
| Forecast immune/inflammatory response | DL and multiomics | Predicting immunogenicity of hydrogels and polymer-protein conjugates | 38 |
| Optimize strength and porosity | ML optimization, genetic algorithms (GAs) | AI-aided mechanical optimization in bone and cartilage scaffolds | 39 |
| Personalize implant design | DL and ML | Shape adaptation using 3D CT/MRI scans for implants and prosthetics | 40,41 |
| Discover new biomaterials from literature | NLP and ML | Literature mining for biomaterials function correlations (text embeddings) | 42 |

data mining, and ML. AI can improve our comprehension of cellular and molecular interactions by using massive datasets to find patterns and connections that conventional approaches might miss. AI can also help anticipate and simulate the performance of novel biomaterials, which can speed up the development process and eliminate the need for intensive *in vivo* testing. In conclusion, a major turning point in the history of biomaterials has been marked by the effort to create new biomaterials and redesign terminology and definitions in the domain. AI-assisted data extraction automation and updated advanced designs and definitions have great promise for sustained innovation, promoting teamwork in research, and accelerating the creation and introduction of new biomaterials to the market. By taking a comprehensive approach, biomaterials are guaranteed to satisfy the many and changing demands of contemporary medicine, which eventually enhances patient outcomes and advances the field of biomedical science. Table 3 summarizes the role of AI in biomaterials design and development.

Methodological Rigor and Systematic Approach

A systematic literature search was conducted using keywords associated with biomaterials and AI in PubMed, Scopus, and Web of Science (2004–2025). Publications numbering 1,332 were obtained after filters were applied and titles and abstracts were screened; these were then included based on their applicability to AI-driven biomaterials production, optimization, or prediction. Studies without AI components and editorials were not included. Figure 3 shows a Preferred Reporting Items for Systematic reviews and Meta-Analyses (PRISMA) flow diagram that describes the screening procedure. The Risk Of Bias In Systematic reviews (ROBIS) tool for included reviews and the Grading of Recommendations Assessment, Development and Evaluation (GRADE) approach for original research were used to evaluate the quality of the study. A decision toolset (Table 2) that aligns AI methodologies with biomaterials issues was added to a narrative synthesis.

AI's Innovating Role in Biomaterials

A sophisticated fusion of empirical methods and predictive modeling is needed to assess the interactions

between biomaterials and biological systems. Accurate evaluation is necessary for critical performance characteristics such as biodegradation, mechanical strength, corrosion resistance, and by-product release; yet, conventional numerical models frequently fail to reflect the complexity and unpredictability present in living systems.⁴⁷ A revolutionary remedy for these constraints is provided by AI. AI can model the behavior of biomaterials under various physiological situations by analyzing massive and complicated datasets using ML and DL approaches. By accurately predicting long-term performance and possible negative biological reactions, these models greatly speed up development cycles and improve material design. By combining sophisticated modeling with established standards, AI also improves the evaluation of biocompatibility. AI advances a more sophisticated and measurable comprehension of material-tissue interactions by dissecting important characteristics, including structural integrity, functional characteristics, and host tissue integration. Furthermore, AI-driven technologies improve the openness, interoperability, and usability of biomaterials research by embracing the Findable, Accessible, Interoperable, Reusable (FAIR) data principles.

These features have real-world applications: AI may help researchers identify toxicity hazards, improve formulations, and tailor materials for particular medical uses. Table 4 illustrates how AI's developing involvement in biomaterials research extends to processes for prediction, optimization, and intelligent design. Despite its potential, further research is needed to strengthen the model's resilience, answer open issues, guarantee algorithm openness, and ensure regulatory compliance. AI will advance the development of next-generation biomedical technologies by pushing the limits of biomaterials innovation with sustained interdisciplinary collaboration.⁴⁸

A systematic benchmarking framework is still missing, despite the fact that various studies have shown encouraging results when employing AI models to optimize or forecast biomaterials performance. Because datasets, modeling methodologies, and assessment measures vary, it is challenging to directly compare the predicted accuracy of various models. Additionally, a lot of research

Table 3 | Role of design and development of biomaterials using AI

| Characteristics | Traditional Approach | AI-Based Approach | Outcome | References |
|-------------------------|--|--|--|-------------|
| Applications | Structural scaffolds | Novel biomaterials performance simulation | Advancements in biomedical science | 31–34 |
| Biocompatibility | Understanding how biochemical and biomechanical processes interact | AI for predictive analytics and identification of patterns | Increased acceptance and integration of biomaterials | 35,36,45,46 |
| Material screening | A multiphase, intricate evaluation procedure | Automated integration and extraction of data | More rapid approval and development procedures | 44 |
| Regulatory requirements | Comprehensive compatibility proof required | Standardized practices to ensure consistency | Greater interaction with stakeholders | 3,45 |
| Research growth | Gradual improvements throughout time | Comprehensive examination of the dataset | Design innovation in biomaterials | 45,46,47 |
| Data extraction | Manual processes | Automated extraction from scientific papers | Effectiveness in finding novel biomaterials | 46 |

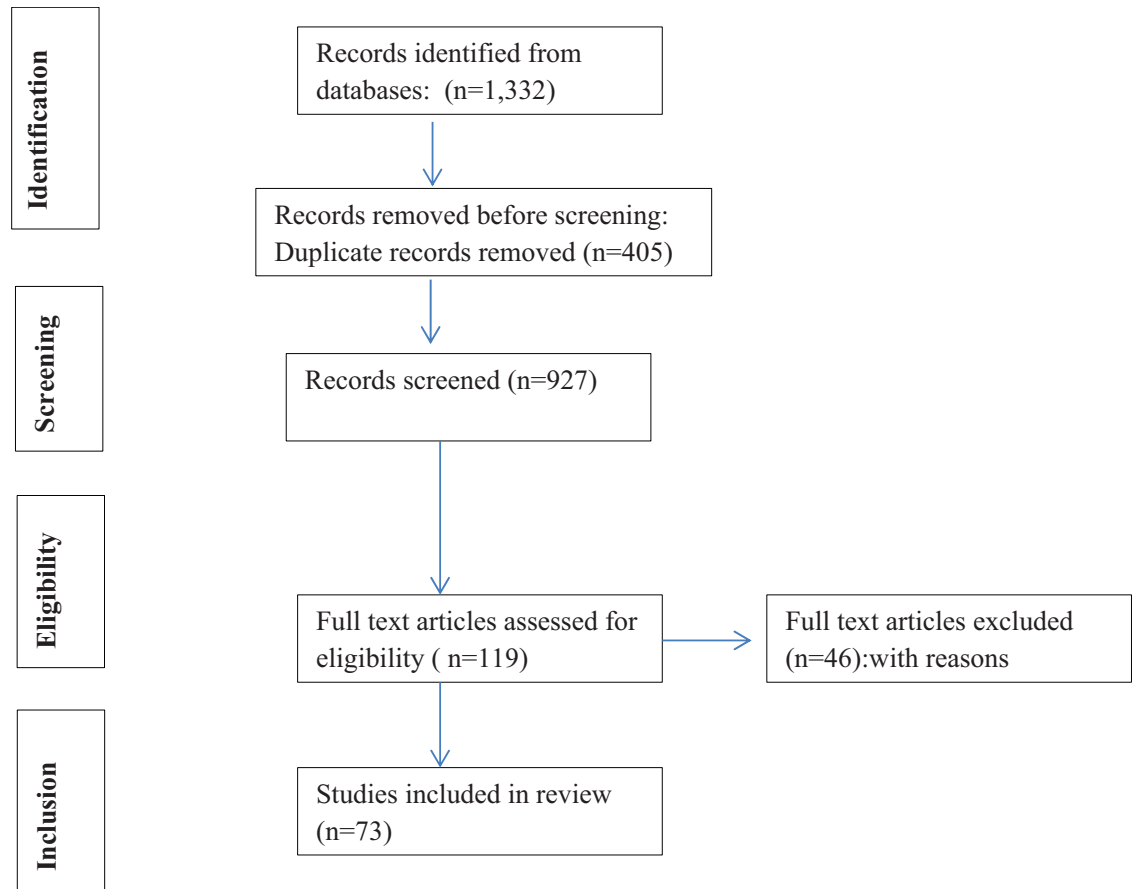


Fig 3 | PRISMA flow diagram for screening procedure

| Aspect | Description | References |
|---------------------------------------|--|------------|
| Traditional numerical models | Good for forecasting specific traits (such as biodegradation or mechanical load-bearing), but frequently unable to handle the intricacy and unpredictability of biological systems. | 48 |
| AI's role | Overcomes the drawbacks of conventional paradigms to revolutionize. Uses DL and ML to enable stochastic design concepts. Enhances biomaterials data usability and transparency while adhering to FAIR principles. | 49 |
| AI's predictive insights | Large datasets are used by AI models to simulate the behavior of biomaterials under varied circumstances, offering anticipated insights and improving the biocompatibility evaluation process. | 49 |
| Enhancing biocompatibility assessment | To offer a more thorough assessment of the ways in which biomaterials and biological systems interact, AI simplifies concepts from international norms and scientific literature by breaking them down to their most fundamental components. | 49 |
| Practical applications | AI helps develop complex algorithms for real-world issues, including anticipating long-term performance through analysis and simulation and identifying possible adverse reactions. | 49 |
| Future research | More research is required to solve open questions and advance existing models, increasing accuracy and reliability in synthesis, development, and assessments. | 49 |
| Potential | As AI develops, it may push the boundaries of biomaterials research and open up new possibilities for innovative biological uses. | 49 |

studies do not use standardized testing procedures or provide specific validation measures. In order to facilitate thorough and repeatable evaluation of AI models in biomaterials science, future research should concentrate on creating common datasets and reporting guidelines.

Designing a Promising Future in Biomaterials with AI

By providing cutting-edge equipment and approaches to improve procedures for design, development, and assessment, AI is transforming the biomaterials

industry. AI is being incorporated into biomaterials research in ways that go far beyond advancements.⁵⁰ It covers a broad spectrum of applications that advance the profession by addressing ethical issues, speeding up discovery, and optimizing material attributes. Large datasets, including omics data and high-throughput screening findings, can be analyzed thanks to AI-driven methods like ML and DL. These technologies aid in the discovery of correlations and patterns that

are essential for creating novel biomaterials with specific characteristics. AI algorithms, for instance, can forecast the exchanges between various biomaterials and biological systems, helping researchers choose the best materials for certain uses.^{51,52} AI greatly improves sophisticated *in vitro* models, such as organ-on-a-chip technologies, microfluidic devices, and models of 3D culture. These models offer comprehensive insights into the performance of biomaterials by more accurately simulating physiological conditions than conventional techniques. By processing and interpreting data from these models, AI can provide predictions about the behavior of biomaterials in actual biological contexts, facilitating more accurate evaluations of their safety and efficacy. Additionally, AI is essential for increasing the scalability and reproducibility of biomaterials research. AI lowers human error and guarantees consistency between investigations by automating data processing and experimental processes. This automation speeds up the investigation of novel materials and situations, enabling the completion of more thorough and in-depth studies in less time. AI also plays a key role in resolving the moral dilemmas raised by animal experiments. AI-powered predictive models and simulations can offer insightful information on interactions between biomaterials and possible outcomes, negating the necessity of using animal models and bringing research methods into compliance with moral guidelines. This change improves preclinical testing efficiency while simultaneously promoting ethical research practices.^{53–55}

AI Connects with Biomedical and Biomaterials

The advancement of AI technology has created numerous opportunities to effectively address numerous persistent issues in the contemporary biomedical domains.⁵⁶ AI, a concept that mimics human intelligence, has been used in the creation of biomaterials and medical research due to advancements in ML, particularly neural-network-based DL algorithms. AI applications include biomaterials design, drug target identification, disease prediction, and intervention.⁵⁷ Traditional clinical trials have long had challenges, including lengthy procedures, large equipment, the requirement for qualified workers, patient selection, and ethical issues.⁵⁸ Emerging AI technology can support biomaterials and biomedicine research by processing clinical data, matching patients with algorithms, and optimizing trials and decision-making, while addressing challenges and potential paths.⁵⁹ AI enhances medical diagnosis by integrating pathological and genetic information, enhancing efficiency and reducing inaccurate results, while traditional diagnosis relies on doctors' understanding of pathological tissues.⁶⁰ Biomedical data from biological multiomics, including transcriptomics, proteomics, metabolomics, epigenomics, and genomics, is integrated using advanced DL techniques like fully connected neural networks (FCNNs), convolutional neural networks (CNNs), recurrent neural networks (RNNs), graph neural networks (GNNs), deep neural networks (DNNs), and capsule neural networks

(CapsNets). These DL-based approaches offer adaptability, capturing complex interactions and nonlinear relationships, and providing accurate predictions. *In silico* vision-based AI can also connect clinical care and ML, enabling automatic processing and decoding of microscopy or medical imaging data, aiding disease diagnosis and treatment effectiveness.⁶¹

AI technology and patient analysis can enhance precision medicine, enabling personalized diagnosis and therapy, but current clinical trials struggle with inadequate medication responses and treatment-related side events.⁶²

Additionally, living biosamples can now be detected at single-cell levels.⁶³ High-throughput data processing and investigative techniques enable precise identification of individual cell actions, offering potential for individualized illness research. AI technology, particularly DL algorithms, improves computer-aided medication creation by improving design speed and internal performance. Recent efforts focus on optimizing biomaterials-based formulations, tracking pharmacological targets, and assessing *in vivo* responses.⁶⁴

Computational biomaterials is a field that uses AI to simulate and predict ideal architectures, physicochemical characteristics, and bioactivity of biomaterials. Biochemical laboratories construct libraries to investigate relationships between biomaterial systems. Proof-of-concept research uses ML models to understand the interaction between biomaterials and biosystems, such as peptide/protein biomacromolecules, for biomedical applications.⁶⁵

The fundamental constraints of AI approaches in biomedicine, particularly biomaterials, stem from their need for high processing capacity, which poses questions of accessibility and efficiency. The “black-box” aspect of many AI models is one of the main obstacles; it restricts model transparency and causes problems with nonrepeatability and nonreproducibility.⁶⁶ This limits the quick implementation of AI-generated suggestions in clinical contexts, where frameworks for logical decision-making grounded in practitioner knowledge are still crucial.⁶⁷ In order to improve interpretability and close the gap between clinical trust and predictive modeling, explainable AI (XAI) techniques like SHapley Additive exPlanations (SHAP), local interpretable model-agnostic explanations (LIME), and attention-based models are currently being investigated.⁶⁸ By promoting clear, credible connections between input data and results, these technologies aid in clarifying the reasoning behind AI predictions, boosting confidence, and easing regulatory approval. Furthermore, given persistent ethical issues about authorship, plagiarism, and copyright, human oversight is still essential in the context of generative AI to guarantee the dependability of outputs. In the end, when AI develops in biomedicine, strong, well-kept databases and professional prudence will be essential.⁶⁹

Conclusion

In summary, AI has a revolutionary impact on biomaterials research. It addresses ethical issues, increases

reproducibility, improves predictive accuracy, and permits exact material optimization. Researchers are opening the door for breakthroughs that could transform industrial and medicinal applications by incorporating AI into several facets of biomaterials development. This will provide fresh approaches and enhance results in a variety of domains. The development of biomedicine has benefited from the rise and advancements in AI technology in a number of areas, including drug discovery, imaging diagnostics, biochemical detection, and disease prediction. There is no question that AI will become more significant in the translational and clinical research domains, ranging from public health to clinical implementation, preclinical research, and clinical research. Even while biomaterials research has advanced significantly thanks to AI, there are serious ethical concerns with its application.

Transparency and accountability are two major problems. Due to their complex architecture, AI systems and intense learning models are typically known as “black boxes.” It could be challenging to understand how AI-driven material selections are produced because of this absence of transparency. When an AI model makes decisions that have unintended consequences, especially when such decisions hurt patients or the environment, ethical questions of accountability are raised. Researchers and authorities need to think about responsibility and liability in these situations. The grade and accessibility of data, which is the foundation of AI, can have a major impact on the effectiveness of AI-driven biomaterials design. In biomaterials research, obtaining superior, well-specified information can be a major obstacle. The biomedical data category, which is usually irregular and varied, includes details about the materials properties, clinical results, and biological responses. AI models require assistance in generalizing to a variety of new and unique circumstances, even while they perform well on a small amount of training data. Techniques for using expertise from related domains could help get over data limitations by using transfer learning and data augmentation strategies.

As AI integration in biomaterials advances, regulatory monitoring is becoming more and more crucial. Recent changes in international legislation highlight the growing need to integrate AI in health care—including the study and production of biomaterials—in a way that is moral, open, and risk-aware. Formally adopted in 2024, the European Union’s AI Act classifies AI systems used in digital health applications and medical devices as high-risk, imposing stringent requirements on them, including risk assessment, human oversight, robustness, and transparency throughout the AI lifecycle.^{70,71} This directly affects AI-powered biomaterials, particularly those used in therapeutic decision-making or implants, where traceability and interpretability of the model are essential. The U.S. Food and Drug Administration (FDA)’s 2024 Draft Guidance on AI/ML-Enabled Medical Devices, which emphasizes the importance of good ML practices (GMLP), real-world performance monitoring, and guaranteeing explainability of AI models used in medical decision support,

reflects parallel efforts in the United States. In addition to guaranteeing compliance, matching biomaterials research with these new regulatory frameworks will promote safety, trust, and translational viability in clinical settings.

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