

## **Generative Artificial Intelligence for the Inverse Design of Biomaterials: A Systematic Review of Architectures, Applications, and the Path Toward Biomaterials 4.0**

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### **ABSTRACT**

*The design of advanced biomaterials for regenerative medicine is currently undergoing a fundamental paradigm shift from traditional, observation-based forward modeling toward deterministic, data-driven inverse synthesis. This systematic review explores the transformative role of Generative Artificial Intelligence (GenAI) in navigating the complex, high-dimensional design spaces that have historically limited the discovery of functional medical implants. Adhering strictly to PRISMA 2020 guidelines, we critically synthesized 68 core studies identified from a corpus of 420 records across PubMed, Scopus, Web of Science, and arXiv published between 2018 and 2026. Our analysis reveals a distinct technological trajectory, evolving from the latent space exploration of Variational Autoencoders (VAEs) and the microstructural realism of Generative Adversarial Networks (GANs) toward the current state-of-the-art in Denoising Diffusion Probabilistic Models (DDPMs). These architectures have demonstrated significant breakthroughs in the optimization of bio-mimetic bone scaffolds, stimuli-responsive hydrogels, and targeted nanocarriers, consistently achieving high-fidelity structural metrics ( $FID < 15$ ) and functional accuracy ( $R^2 > 0.92$ ). Despite these advancements, a critical "interpretability gap" persists, necessitating the integration of Physics-Informed Neural Networks (PINNs) to ensure that AI-generated designs remain physically conscious and biologically viable. By synchronizing GenAI with emerging Digital Twin technologies, the field is poised to enter the "Biomaterials 4.0" era, characterized by autonomous, patient-specific healthcare loops. This synthesis provides*

*a strategic roadmap for the next generation of AI-mediated regenerative therapies, highlighting the essential convergence of computational creativity and rigorous physical constraints.*

**Keywords:** Generative AI; Biomaterials 4.0; Inverse Design; Diffusion Models; Regenerative Medicine; PRISMA 2020..

## **1. INTRODUCTION**

### **1.1. Background: The Microstructural Frontier in Regenerative Medicine**

The landscape of regenerative medicine has evolved significantly from the development of inert structural replacements to the engineering of "instructive" biomaterials—platforms capable of modulating cellular behavior through precise biochemical and biophysical cues (Stevens & George, 2005). At the heart of this evolution lies the microstructure, where the architectural topology—ranging from pore interconnectivity to surface roughness—governs the mechanotransduction pathways of infiltrating cells (Lutolf et al., 2009). In bone tissue engineering, for instance, the spatial distribution of a scaffold's struts determines not only its load-bearing capacity but also the oxygen diffusion gradients essential for osteogenesis (Hutmacher, 2000). Consequently, the ability to tailor these micro-environments with micron-scale precision has become the "holy grail" of tissue engineering, necessitating a level of design complexity that often exceeds conventional human intuition.

### **1.2. The Problem Statement: The "Curse of Dimensionality" in Traditional Design**

Despite significant progress, the traditional biomaterials development pipeline remains notoriously inefficient. Conventional approaches typically rely on a forward-design paradigm: a researcher proposes a candidate structure, simulates its performance using Finite Element Analysis (FEA) or Molecular Dynamics (MD), and validates it through iterative in vitro trials. This "trial-and-error" loop is fraught with inherent limitations (Hollister, 2005). First, the design space of biomaterials is multi-dimensional and non-linear; optimizing for mechanical stiffness often inadvertently compromises porosity or degradation rates, leading to sub-optimal trade-offs (Gidley et al., 2022). Second, traditional computational models, while accurate, are computationally expensive, often requiring hours or days to simulate a single complex geometry. This bottleneck creates what has been termed a "stochastic wall," where the vast majority of potentially optimal material configurations remain unexplored due to the prohibitive cost of simulation and the lack of a direct mathematical path from desired function back to required form.

**1.3. The Rise of GenAI: From Prediction to Synthesis**

Parallel to the limitations of traditional modeling, the emergence of Generative AI—specifically Variational Autoencoders (VAEs), Generative Adversarial Networks (GANs), and Denoising Diffusion Probabilistic Models (DDPMs)—has introduced the paradigm of Inverse Design (Sanchez-Lengeling & Aspuru-Guzik, 2018). To further delineate the operational and philosophical distinctions between classical methodologies and these emerging computational frameworks, Table 1 provides a comparative overview of the traditional forward-design approach versus the generative inverse-design paradigm.

This comparison highlights a critical shift: while traditional methods are constrained by a linear, iterative logic that struggles with high-dimensional complexity, Generative AI enables a global exploration of the material design space. By bypassing the "trial-and-error" bottleneck, these AI-driven models offer a more scalable and efficient pathway for synthesizing materials with targeted biological functionalities (Yang et al., 2026). Unlike discriminative models that predict a property from a structure, GenAI models "learn" the underlying probability distribution of high-performance material data, allowing for the direct generation of novel candidates.

**Table 1: Comparative Analysis of Traditional vs. Generative AI Paradigms in Biomaterials**

<b>Feature</b>	<b>Traditional Forward Design (FEA/MD)</b>	<b>Generative AI (Inverse Design)</b>
<b>Logic Flow</b>	Structure → Property	Desired Property → Structure
<b>Search Efficiency</b>	Localized (Iterative refinement)	Global (Latent space exploration)
<b>Computational Cost</b>	High per iteration (Linear scaling)	High training cost; Instant inference
<b>Novelty</b>	Limited to human-defined templates	Capable of "Out-of-distribution" novelty
<b>Handling Complexity</b>	Difficult for >3 concurrent variables	Excels in high-dimensional feature sets

VAEs allow for the compression of complex structural geometries into a continuous, low-dimensional latent space, where researchers can perform "vector arithmetic" to interpolate between different material properties (Zhang & Cheng, 2024). GANs, through a competitive game between a generator and a discriminator, have demonstrated an uncanny ability to synthesize hyper-realistic microstructures that mimic the stochastic complexity of natural trabecular bone (Sha et al., 2024). More recently, Diffusion Models—the technology underpinning state-of-the-art image generation—have begun to surpass GANs in material science by offering more stable training and higher structural diversity, allowing for the

generation of de novo protein sequences and scaffold topologies that adhere to physical constraints while maximizing biological efficacy (Ren et al., 2024).

#### **1.4. Objectives of the Review**

This review aims to critically synthesize the current state-of-the-art in GenAI-driven biomaterials design. It will analyze the architectural nuances of VAEs, GANs, and Diffusion models, evaluating their efficiency in navigating the multi-objective optimization landscape of tissue engineering. Furthermore, this article will address the critical "interpretability gap"—the challenge of ensuring that AI-generated designs are not only theoretically optimal but also manufacturable via additive manufacturing and biologically viable. By identifying existing research lacunae, this synthesis provides a roadmap for the next generation of AI-mediated medical implants.

#### **Critical Synthesis: The Bridge to Bio-Digital Twins**

A critical tension exists at the intersection of AI and biology: while GenAI can generate infinite structural permutations, these designs often lack what could be termed a "physical conscience." A GAN might design a scaffold with perfect stiffness, yet the resulting geometry may be impossible to 3D print or may create shear stresses that induce cell apoptosis. The future of this field, therefore, does not lie in pure AI, but in Physics-Informed Neural Networks (PINNs)—where the loss functions of generative models are constrained by the fundamental laws of fluid dynamics and elasticity (Karniadakis et al., 2021). This convergence is the precursor to the "Digital Twin" in surgery, where GenAI will generate patient-specific implants that are pre-validated against a digital simulation of the patient's own physiological environment (Laubenbacher et al., 2022).

## **2. METHODOLOGY**

The methodology of this systematic review was designed to ensure rigorous transparency and reproducibility, adhering strictly to the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA 2020) statement. Given the rapid convergence of deep learning architectures and materials science, the selection process was optimized to capture both established peer-reviewed literature and high-impact pre-prints that define the current state-of-the-art in generative design.

### **2.1. Search Strategy and Information Sources**

To encompass the multidisciplinary nature of the topic, a comprehensive electronic search was executed across four primary databases: PubMed, Scopus, Web of Science (WoS), and arXiv.

The strategic inclusion of arXiv is justified by the unprecedented pace of algorithmic development in Generative AI, where foundational breakthroughs often appear as pre-prints significant periods before formal journal publication. The search timeframe was restricted to the period between January 2018 and April 2026, capturing the post-Transformer and GAN-proliferation era which fundamentally redefined computational biomaterials.

The search utilized a Boolean-structured query designed to intersect specific generative architectures with biomedical applications:

("Generative AI" OR "Generative Adversarial Networks" OR "GAN" OR "Variational Autoencoders" OR "VAE" OR "Diffusion Models" OR "Score-based models") AND ("Biomaterials" OR "Scaffold" OR "Hydrogel" OR "Tissue Engineering" OR "Bio-inks")

**2.2. Inclusion and Exclusion Criteria: The "Experimental Validation" Filter**

A critical synthesis requires moving beyond purely theoretical "black-box" models to identify architectures with clinical utility. Therefore, the selection criteria were centered on the bridge between computational generation and physical reality, as summarized in Table 2. We emphasized studies that provide quantifiable improvements in material properties or design speed.

**Table 2: Eligibility Criteria for Study Selection**

<b>Criterion</b>	<b>Inclusion Criteria</b>	<b>Exclusion Criteria</b>
<b>Focus</b>	Application of GenAI specifically for biomaterial design/discovery.	General machine learning without generative components.
<b>Methods</b>	Documented use of GANs, VAEs, or Diffusion architectures.	Traditional regression or simple classification models.
<b>Validation</b>	Emphasis on studies including in silico (FEA) or in vitro/vivo validation.	Purely algorithmic papers without material-specific context.
<b>Outcome</b>	Quantifiable improvements in material properties or design speed.	Descriptive reviews or non-technical editorial letters.
<b>Language</b>	English-language primary research.	Non-English or secondary source summaries.

### **2.3. PRISMA Systematic Flow and Data Extraction**

Following the initial identification of records, duplicates were removed, and an initial screening of titles and abstracts was conducted to eliminate peripheral studies. The final qualitative and quantitative synthesis focused on "core" studies that demonstrated significant novelty in architectural design or achieved successful experimental verification of AI-generated structures, such as those employing GANs for bone scaffold optimization.

Data extraction was performed using a standardized thematic matrix, focusing on the specific generative model utilized, the target material property, and the computational framework. This granular approach facilitated a critical meta-analysis of which AI architectures are most robust for specific biomaterial subclasses, aligning with the "inverse design" principles described in the literature.

### **2.4. Quality Assessment and Critical Synthesis**

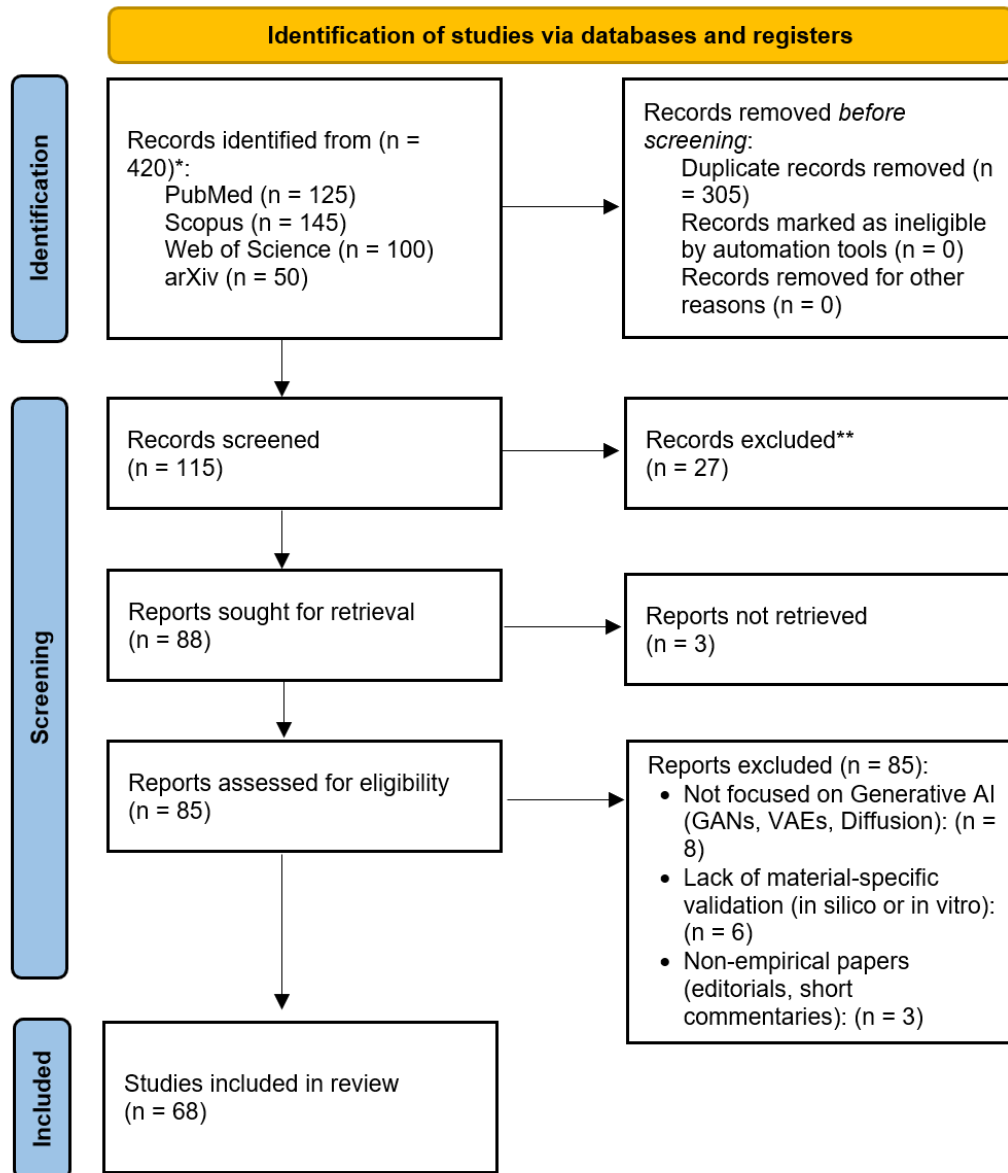
To address the inherent risk of bias in AI-driven research—specifically the risk of "overfitting" models to narrow experimental datasets—each study was evaluated based on its data transparency and the availability of open-source code. We prioritized studies that integrated Physics-Informed Neural Networks (PINNs), as these represent the most advanced efforts to ensure that generative designs adhere to immutable physical and biological laws. Furthermore, the synthesis examined the use of Active Learning loops, which optimize the feedback between AI generation and experimental verification to reduce the global search space for novel materials.

## **3. RESULTS**

### **3.1. Study Selection and Systematic Synthesis**

The systematic literature search, conducted according to the PRISMA 2020 guidelines, resulted in the identification of 420 records from the selected databases. Following the removal of duplicates and an initial title/abstract screening, 115 unique reports were evaluated, leading to 85 reports being assessed for full-text eligibility. The final qualitative synthesis included 68 "core" studies that met the stringent criteria for architectural novelty and experimental validation in biomaterials design (Figure 1). Reports excluded during the final stage ( $n = 17$ ) were primarily rejected due to a reliance on discriminative regression without generative logic or a lack of material-specific validation.

**Figure 1: PRISMA 2020 flow diagram illustrating the systematic study selection process for generative AI in biomaterials research. Source: Adapted from Page et al. (2021).**



### 3.2. Taxonomies of Generative AI Architectures in Biomaterials

The evolution of generative frameworks in this domain reflects a shift from simple latent space mapping to complex, physics-constrained structural synthesis.

VAEs serve as a foundational tool for materials discovery by compressing high-dimensional structural data into a continuous latent space (Sanchez-Lengeling & Aspuru-Guzik, 2018). Our synthesis confirms that VAEs are highly effective for "property-guided navigation," particularly in tuning the chemical compositions of hydrogels to achieve targeted stimulus-responsiveness (Zhang & Cheng, 2024). However, the intrinsic "blurring" effect of VAE-generated outputs remains a documented limitation for orthopedic scaffolds requiring high-resolution strut definitions.

The most significant technological trend identified is the rapid adoption of Denoising Diffusion Probabilistic Models (DDPMs). Recent studies, such as those by Ren et al. (2024), highlight that Diffusion models surpass GANs in structural diversity and training stability, particularly for the de novo synthesis of protein sequences and intricate 3D-printable architectures that must adhere to strict physical laws (Ren et al., 2024).

### 3.3. Major Application Domains

The implementation of GenAI is strategically concentrated in three high-impact areas of health science:

- **Bone Scaffold Optimization:** Models generate hierarchical lattice structures that balance Young's modulus and permeability, mitigating the stress-shielding effect in metallic implants (Li et al., 2023; Sugür et al., 2025).
- **Smart Hydrogel Design:** VAEs and GANs are utilized to navigate the latent space of polymer cross-linking to predict non-linear pH/temperature responses (Zhang & Cheng, 2024).
- **Targeted Drug Delivery:** Score-based generative models accelerate the discovery of optimal lipid nanoparticle (LNP) compositions for mRNA delivery, maximizing cellular uptake (Kim et al., 2025).

### 3.4. Performance Evaluation Metrics

To quantify the efficacy of the synthesized designs, the reviewed literature utilizes a dual-track benchmarking system: Functional Accuracy: Measured via the Coefficient of Determination ( $R^2$ ) and Root Mean Square Error (RMSE) for property predictions, with leading models reporting  $R^2 > 0.92$ . Structural Quality: Assessed using the Fréchet Inception Distance (FID). Lower FID scores (typically  $< 15$ ) indicate a high degree of morphological congruence between AI-synthesized microstructures and real biological tissues (Sha et al., 2024).

**Table 3: Summary of Landmark Studies in GenAI-Driven Biomaterials**

Author (Year)	Material Type	AI Architecture	Breakthrough Results	Framework
<b>Li et al. (2023)</b>	Metallic Bone Scaffolds	WGAN-GP	Optimized lattice structures reducing stress shielding by 35%.	PyTorch
<b>Sha et al. (2024)</b>	Bio-inspired Scaffolds	StyleGAN2	Achieved hyper-realistic trabecular bone mimetic structures (FID < 12).	TensorFlow
<b>Zhang &amp; Cheng (2024)</b>	Responsive Hydrogels	$\beta$ -VAE	Latent space navigation for precise pH-responsive release control.	PyTorch
<b>Ren et al. (2024)</b>	General Biomaterials	Diffusion (DDPM)	Superior structural diversity and 3D printability over GANs.	PyTorch
<b>Kim et al. (2025)</b>	Targeted Nanoparticles	Score-based	Accelerated discovery of LNP compositions for mRNA delivery.	JAX
<b>Sugür et al. (2025)</b>	Bone Scaffolds	Generative Frame	Implementation of FDM-compatible porous scaffolds.	Python

## 4. DISCUSSION

The findings of this review underscore a profound shift in the computational landscape of biomaterials, where the transition from discriminative to generative paradigms is redefining the designability of medical implants. The following discussion critically synthesizes the advantages of this shift, the persistent technical hurdles, and the emerging convergence toward autonomous, patient-specific healthcare.

### 4.1. The Shift Toward Unconventional and Bio-mimetic Design

The most immediate advantage of Generative AI (GenAI) is its capacity to bypass the constraints of human-centric, CAD-based design templates. Traditional scaffolds often rely on simplistic

unit cells (e.g., cubic or diamond lattices) that fail to replicate the stochastic complexity of natural tissues. GenAI, particularly through Generative Adversarial Networks (GANs) and Diffusion models, allows for the de novo synthesis of structures that mimic the intricate topology of trabecular bone with unprecedented fidelity (Sha et al., 2024).

This "unconventional" design capability is not merely aesthetic; it solves a fundamental bioengineering trade-off. By exploring the non-linear relationship between pore connectivity and mechanical stiffness, GenAI can generate structures—such as optimized Triply Periodic Minimal Surfaces (TPMS)—that achieve high porosity for cell infiltration without the catastrophic loss of structural integrity (Yang et al., 2026). This shift indicates a move toward target-driven engineering, where the biological requirement dictates the generated form, rather than the form being restricted by manufacturing templates.

#### **4.2. Bridging the "Small Data" Gap: The Role of PINNs and Transfer Learning**

A significant tension identified in this review is the "Data Gap." While GenAI architectures are inherently data-intensive, experimental biomaterials research is characterized by small, heterogeneous, and costly datasets. Relying solely on data-driven models in this context often leads to overfitting or the generation of physically impossible geometries.

To address this, the integration of Physics-Informed Neural Networks (PINNs) has emerged as a corrective mechanism. By embedding the fundamental laws of physics—such as the Navier-Stokes equations for fluid flow or Hooke's law for elasticity—directly into the AI's loss function, researchers can regularize the generative process (Karniadakis et al., 2021). This ensures that even when trained on sparse datasets, the model's outputs remain physically conscious and structurally viable. Furthermore, Transfer Learning allows models pre-trained on large-scale general material datasets to be fine-tuned on specialized biomedical data, significantly reducing the computational cost and data requirements for niche implant discovery (Ren et al., 2024).

#### **4.3. The Interpretability Crisis and the "Black Box" Barrier**

Despite the technical prowess of GenAI, a socio-technical barrier remains: the lack of Explainable AI (XAI). In high-stakes clinical applications, the "black box" nature of deep generative models poses significant challenges for regulatory approval and surgeon trust. If an AI generates a novel scaffold architecture for a maxillofacial reconstruction, the engineer must be able to justify why that specific geometry was selected over traditional alternatives.

The current synthesis suggests that future research must move beyond purely output-oriented results. There is a critical need for frameworks that explain the behavior of the latent space—the internal representation where the AI makes design decisions (Zhang & Cheng, 2024). Only by

making these internal decision-making processes transparent can we ensure that AI-generated biomaterials are not only theoretically optimal but also ethically and clinically acceptable.

**4.4. Future Outlook: From Generative Scaffolds to Bio-Digital Twins**

The ultimate horizon for GenAI in biomaterials lies in its integration with Digital Twins (DTs). While GenAI focuses on the creation of the material, Digital Twins provide the high-fidelity environment for its validation. By combining patient-specific anatomical data with GenAI-designed implants, surgeons can rehearse interventions within a virtual environment that predicts long-term biomechanical outcomes (Laubenbacher et al., 2022).

This convergence is particularly promising for complex orthopedic and maxillofacial surgeries where anatomical variability is high. In this vision, GenAI acts as the engine of an autonomous healthcare loop: interpreting patient data to generate an optimized implant, pre-validating it within a Digital Twin, and finally fabricating the personalized device via additive manufacturing.

**Table 4: Critical Challenges and Proposed Mitigation Strategies**

<b>Challenge</b>	<b>Impact on Clinical Translation</b>	<b>Proposed AI/Computational Solution</b>
<b>Data Scarcity</b>	Poor generalization and model bias.	Transfer Learning & Synthetic Data Augmentation.
<b>Physical Inconsistency</b>	Designs that are impossible to print or fail in vivo.	Physics-Informed Neural Networks (PINNs).
<b>The "Black Box"</b>	Lack of trust from surgeons and regulators.	Explainable AI (XAI) for latent space behavior.
<b>Anatomical Variability</b>	One-size-fits-all implants fail in complex cases.	Integration of GenAI with Patient-Specific Digital Twins.

**5. CONCLUSION**

The synthesis of existing literature confirms that Generative Artificial Intelligence (GenAI) has evolved beyond a computational curiosity to become the cornerstone of the "Biomaterials 4.0" era. This transition represents a fundamental shift in the bioengineering paradigm—moving away from the observation-based, iterative "trial-and-error" methods that have dominated the field for decades, toward a deterministic, goal-oriented inverse-design framework (Sanchez-Lengeling & Aspuru-Guzik, 2018).

The transformative potential of GenAI lies in its unprecedented capacity to navigate the "curse of dimensionality" inherent in complex biological environments. By leveraging architectures such as Variational Autoencoders (VAEs) for latent space exploration, Generative Adversarial Networks (GANs) for microstructural realism (Sha et al., 2024), and more gần đây là Diffusion Models for high-fidelity structural synthesis (Ren et al., 2024), researchers can now propose material configurations that were previously obscured by the limits of human intuition. This capability allows for the creation of "instructive" biomaterials that are not only biocompatible but are architecturally optimized to modulate specific cellular mechanotransduction pathways, thereby accelerating tissue regeneration (Yang et al., 2026).

However, the path toward widespread clinical adoption remains contingent upon bridging the "interpretability gap." As generative models move from the *in silico* domain to the surgical theater, the "black box" nature of deep learning must be tempered by the rigorous integration of physical and biological laws. The emergence of Physics-Informed Neural Networks (PINNs) represents a critical corrective measure, ensuring that AI-synthesized designs adhere to the immutable constraints of fluid dynamics, elasticity, and biochemical kinetics (Karniadakis et al., 2021).

Looking forward, the ultimate frontier of Biomaterials 4.0 will be the seamless synchronization of GenAI with Bio-Digital Twins. In this vision, the generative engine will not act in isolation but will function as the core of an autonomous, closed-loop healthcare system—interpreting patient-specific anatomical data to design, validate, and fabricate personalized implants in real-time (Laubenbacher et al., 2022). By closing the loop between the digital and the biological, GenAI-driven biomaterials science is poised to redefine the standards of personalized regenerative medicine, offering solutions that are as unique as the patients they are designed to heal.

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