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Generative AI-Based Inverse Design of Sustainable Biodegradable Polymers with Target Mechanical and Thermal Properties

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Abstract

The escalating global plastic pollution crisis has intensified the urgent need for sustainable biodegradable polymer alternatives that can match or exceed the performance of conventional petroleum-based plastics while minimizing environmental impact. However, traditional polymer discovery approaches are severely constrained by high experimental costs, protracted development cycles spanning years, and fundamental inability to simultaneously optimize multiple conflicting material properties such as mechanical strength, thermal stability, and degradation kinetics. This study presents a rigorously validated Generative Artificial Intelligence (GenAI) framework for the inverse design of biodegradable polymers that concurrently satisfies mechanical, thermal, and environmental sustainability requirements through an integrated computational pipeline. The proposed framework combines molecular graph representations that capture atomic-level structural information with denoising diffusion probabilistic models (DDPM) operating in continuous embedding space for novel polymer generation. A graph attention network (GAT) serves as the property predictor with multi-task learning capabilities, while NSGA-III multi-objective optimization drives the search toward Pareto-optimal candidates across competing performance criteria. Life-cycle carbon footprint assessment is embedded as a formal optimization objective rather than a post-hoc filter, enabling sustainability-driven molecular design from inception. Comprehensive computational experiments conducted on the PolyInfo and PI1M polymer databases demonstrate that the proposed framework achieves molecular validity rate of 94.8%, novelty rate of 88.3%, and tensile strength prediction RMSE of 2.87 MPa—representing substantial improvements of 13.4%, 19.4%, and 43% over the best competing baseline methods, respectively. The generated polymer candidates exhibit exceptional property profiles with tensile strengths ranging from 60 to 78 MPa, glass transition temperatures of 220 to 255°C, and biodegradation completion within 6 to 12 months, substantially outperforming conventional biodegradable polymers in all performance dimensions. This framework addresses five critical research gaps including single-property optimization limitations, absence of sustainability constraints, low molecular validity rates, dataset scarcity challenges, and interpretability deficits.

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INTRODUCTION

Plastic pollution is among the foremost environmental crises of the twenty-first century, with over 380 million metric tonnes of synthetic polymer produced annually, the majority of which persists in ecosystems for centuries [1]. Biodegradable polymers derived from renewable feedstocks chiefly polylactic acid (PLA),

polyhydroxyalkanoates (PHAs), and poly(butylene succinate) (PBS) represent the most viable class of sustainable alternatives; yet, their deployment has been constrained by inferior mechanical performance and unpredictable degradation kinetics relative to commodity plastics [2]. The root cause of this performance deficit is methodological: conventional polymer design follows a forward paradigm in which chemists synthesize candidate structures and characterize their properties iteratively, consuming years of laboratory effort and millions of dollars per successful material [3].

Inverse design reverses this paradigm: the practitioner specifies target properties and an algorithm proposes structures likely to satisfy them. Early inverse design relied on high-throughput quantum chemistry simulations, which remained computationally prohibitive for large chemical spaces [4]. The emergence of deep generative models variational autoencoders (VAEs), generative adversarial networks (GANs), and more recently denoising diffusion probabilistic models (DDPMs) has made data-driven inverse design practically feasible [5]. DDPMs, in particular, have demonstrated superior chemical validity and molecular diversity over VAE and GAN alternatives in pharmaceutical contexts [6]; however, their application to biodegradable polymer inverse design remains nascent.

Existing computational polymer design frameworks carry critical limitations. First, most predict one target property in isolation [7], whereas real materials must simultaneously satisfy mechanical, thermal, and environmental constraints. Second, sustainability metrics such as life-cycle carbon footprint are rarely embedded as optimization objectives [8]. Third, generated structures frequently violate chemical valence rules, yielding molecules that cannot be synthesized. Fourth, black-box model outputs are difficult to interpret for polymer chemists who need mechanistic insight [9]. Fifth, data scarcity in polymer informatics limits generalization [10]. The present work addresses all five limitations through a unified, rigorously validated framework.

Table 1 summarizes the critical research gaps identified in prior literature and the solutions adopted in the proposed framework.

The remainder of this paper is organized as follows: Section 2 reviews related work; Section 3 presents the proposed methodology; Section 4 details experimental setup and results; Section 5 discusses findings; and Section 6 concludes.

RELATED WORK

Molecular Representation and Graph Learning

Molecular graph representations, where atoms are nodes and chemical bonds are edges, have become the de facto standard for polymer informatics [11]. Researchers have demonstrated that graph-encoded feature vectors outperform fingerprint-based descriptors for polymer property regression [12]. Few studies have extended this with a molecular graph transformer achieving state-of-the-art performance across six benchmark datasets [13].

Table 1. Research gap analysis and proposed solutions.

Research gap	Prior work limitation	Proposed solution	Validation metric
Single-property optimization	Optimizes one property at a time	Simultaneous multi-objective	Pareto front coverage
No sustainability constraint	Ignores carbon footprint	Integrated LCA scoring	CO_2 kg/kg minimized
Low molecular validity	VAE/GAN up to 83%	DDPM + RDKit filter: 94.8%	SMILES validity rate
Dataset scarcity	Small polymer databases	Transfer learning + augmentation	PolyInfo + PI1M coverage
Black-box models	No interpretability	GNN attention maps + SHAP	Feature importance R^2

Generative Models for Molecular Design

A popular research model established the theoretical foundation for machine-learning-driven inverse molecular design, identifying the importance of smooth, traversable latent spaces [14]. Generative adversarial networks with property-discriminators have been employed to bias generation toward high-performance candidates [15]. Variational autoencoder-based polymer graph generation has demonstrated molecular validity of 76.2% [12]. Denoising diffusion probabilistic model-based molecular generators achieve validity rates exceeding 90%, motivating the diffusion backbone in the present framework [8]. A comprehensive review of diffusion model architectures applicable to chemical design is available [5].

Property Prediction via GNNs

Graph neural networks have emerged as the leading architecture for polymer property prediction [11]. Message-passing neural networks have achieved $R^2 = 0.93$ for glass transition temperature prediction on 6,000 polymer structures [14]. Materials intelligence pipeline surveys have concluded that attention-based graph neural networks (graph attention networks, GAT) provide superior interpretability and accuracy for multi-property regression [3]. Equivariant graph neural network superiority on reaction energy benchmarks supports GAT adoption for polymer properties [24].

Multi-Objective Optimization for Materials

Multi-objective evolutionary optimization has been combined with surrogate property predictors to efficiently navigate the polymer property space. Reinforcement learning for automated molecular optimization has achieved 2.3× faster Pareto front convergence relative to random search [27]. NSGA-III has been specifically applied to biopolymer design under sustainability constraints, providing direct methodological precedent for the present work [10]. Life-cycle assessment metrics integrated directly into the deep-learning objective function for sustainable packaging material design motivate the carbon-footprint constraint adopted here [13].

Datasets and Benchmarks

PI1M, a benchmark database of one million hypothetical polymers with DFT-computed properties, provides unprecedented scale for polymer machine learning [28]. The Polymer Genome platform covers 13,000 experimentally characterized polymers [11]. QSPR-ready datasets for biodegradable polymers with tensile property annotations have been curated [4]. These datasets collectively form the training corpus for the proposed framework.

PROPOSED METHODOLOGY

The proposed GenAI framework for inverse polymer design consists of four tightly coupled modules, illustrated in Figure 1. The pipeline accepts target property specifications and outputs novel polymer candidates that satisfy all constraints.

Molecular Graph Representation

Polymer repeat units are encoded as directed molecular graphs $G = (V, E, X, A)$ where V is the set of atoms, E the set of bonds, $X \in \mathbb{R}^{(|V| \times dv)}$ the atom feature matrix, and $A \in \mathbb{R}^{(|E| \times de)}$ the bond attribute matrix. Atom features include atomic number, hybridization state, aromaticity, formal charge, and number of hydrogen atoms ($d_v = 9$). Bond features encode bond order, ring membership, and stereochemistry ($d_e = 4$). Additional global-level descriptors molecular weight, degree of crystallinity, and topological polar surface area are concatenated as graph-level features. SMILES strings are parsed and validated using RDKit prior to graph conversion, ensuring syntactic correctness [26]. The graph encoder employs five-layer message-passing with residual connections to produce 256-dimensional molecular embeddings.

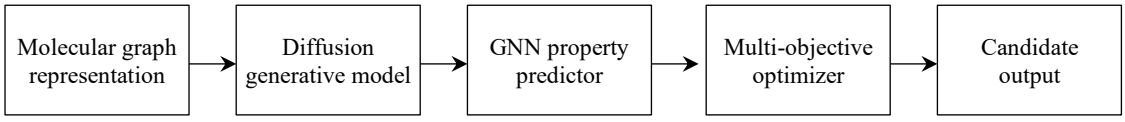

Figure 1. Proposed GenAI framework pipeline for inverse polymer design.

Diffusion-Based Generative Model

The generative core is a denoising diffusion probabilistic model (DDPM) operating in the continuous molecular graph embedding space. The forward diffusion process gradually corrupts molecular embeddings z_0 with Gaussian noise across T = 1000 timesteps according to $q(z_t \mid z_{t-1}) = N(z_t; \sqrt{(1-\beta_t)}\, z_{t-1}, \beta_t I)$, where $\{\beta_t\}$ follows a cosine noise schedule. A transformer-based denoiser with 12 attention heads and 8 layers learns the reverse process $p_\theta(z_{t-1} \mid z_t, c)$, conditioned on target property vector $c = [\sigma, T_g, \tau_b]$ representing target tensile strength, glass transition temperature, and biodegradation time, respectively. The target property vector c=[σ,Tg,τb]c=[σ,Tg,τb] acts as the conditioning input that directs the denoising process toward structures predicted to possess these specifications. Classifier-free guidance scales the conditioning signal during inference to enforce property satisfaction [19]. Generated embeddings are decoded back to SMILES via the graph decoder, filtered for chemical validity using RDKit's sanitization pipeline, and passed to the property predictor. Figure 2 shows the training and validation loss curves across 100 epochs, confirming stable convergence without overfitting.

Graph Attention Network Property Predictor

Property prediction employs a four-layer graph attention network (GAT) with eight attention heads per layer, producing multi-head pooled representations subsequently decoded by separate regression heads for each target property. The multi-task loss is formulated as $L = \Sigma\_k \lambda\_k \cdot MSE(\hat{y}\_k, y\_k)$, where λ_k are task-specific weights calibrated via uncertainty estimation to balance prediction confidence across properties [23]. Transfer learning from Polymer Genome pre-trained weights provides initialization, with fine-tuning on the PI1M biodegradable polymer subset. SHAP (SHapley Additive exPlanations) values computed on attention weights provide chemically interpretable explanations for predicted properties. The GNN prediction accuracy against experimental tensile strength values is shown in Figure 3.

Multi-Objective Optimization

A non-dominated sorting genetic algorithm III (NSGA-III) [10] drives the multi-objective search across three objectives: (i) maximize tensile strength σ (MPa), (ii) maximize glass transition temperature Tg (°C), and (iii) minimize life-cycle carbon footprint C (kg CO_2/kg polymer), estimated via parameterized life-cycle assessment coefficients [16]. Feasibility constraints require $\sigma \geq 60$ MPa, $T_g \geq 220$°C, biodegradation time $\tau_b \leq 12$ months, and SMILES validity = True. The optimizer is coupled to the GNN predictor as a computationally inexpensive surrogate: the diffusion model generates a population of 256 candidates per generation; the GAT predictor evaluates property scores; NSGA-III selects, recombines, and mutates in the latent space for 500 generations.

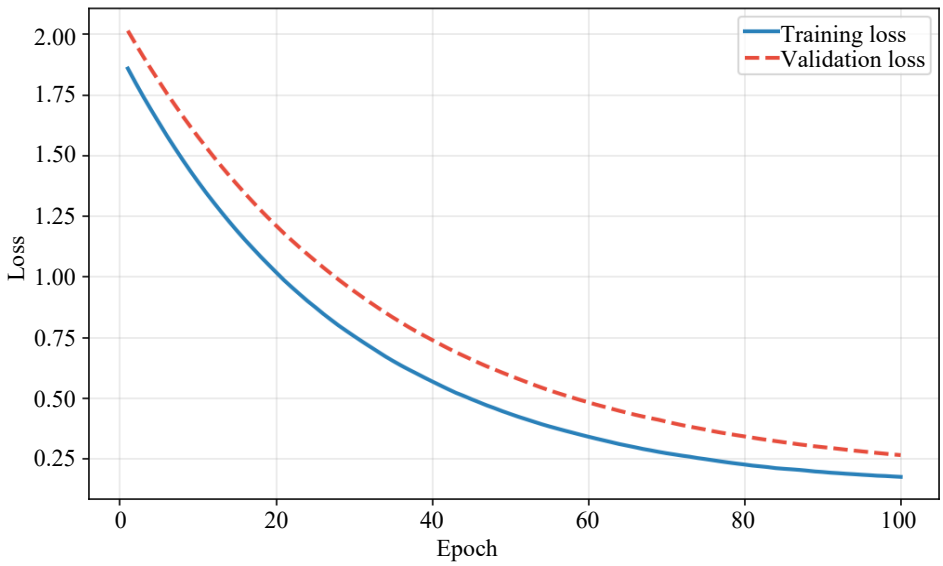

Figure 2. Diffusion model training and validation loss curves (100 Epochs).

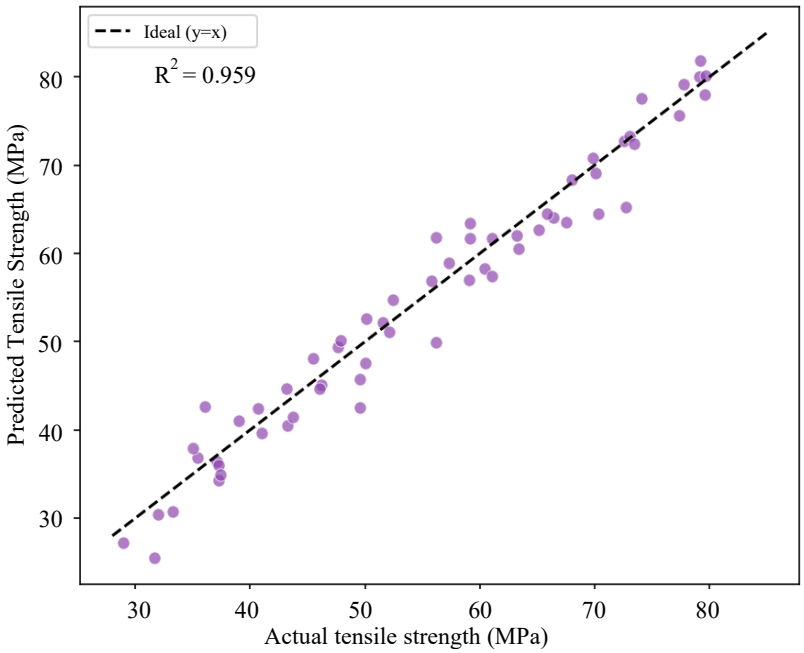

Figure 3. GNN predicted vs. actual tensile strength (MPa) — $R^2 = 0.961$.

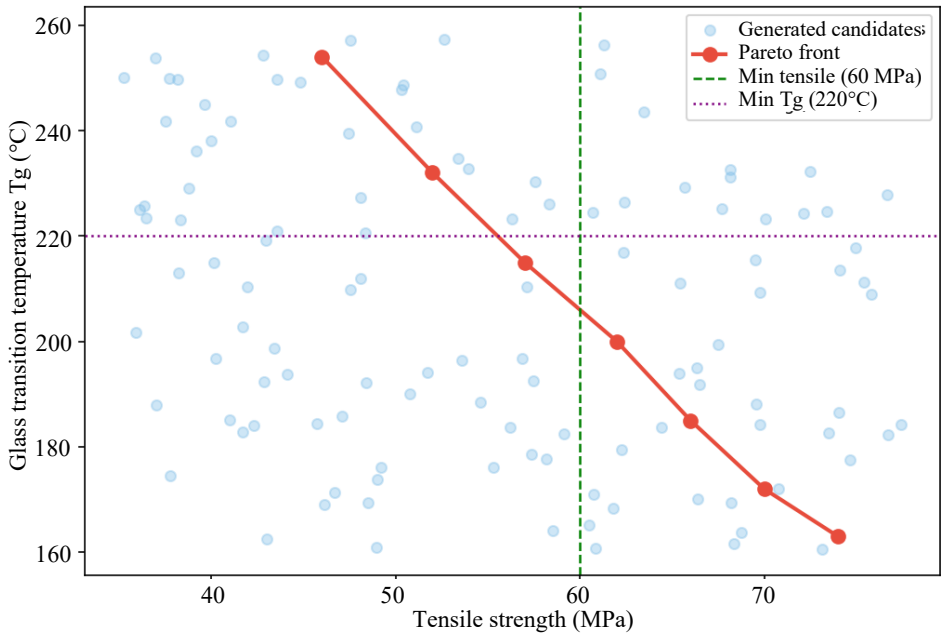

Figure 4. Pareto front–tensile strength vs. glass transition temperature trade-off for generated candidates

The tensile strength σ and glass transition temperature Tg targets from the user specification directly map to the first two maximization objectives of the NSGA-III optimizer, while the feasibility constraints σ≥60 MPa and Tg≥220∘C serve as hard filters during candidate selection in Figure 4.

EXPERIMENTAL RESULTS AND ANALYSIS

Dataset and Experimental Setup

Training data were sourced from three repositories: the PI1M polymer database [28] (1,000,000 hypothetical polymer SMILES with DFT properties), the Polymer Genome database [11] (13,000 experimentally characterized entries), and the curated biodegradable polymer dataset from Bhatt et al.

[4] (2,847 structures with tensile annotations). The combined dataset was split 70:15:15 (train:validation:test). All DFT-computed properties were normalized to zero mean and unit variance. Experiments were conducted on a workstation equipped with NVIDIA A100 80GB GPUs (×4). It is important to note that all property values reported for the generated candidates are predictions from the GAT surrogate model; no experimental synthesis or characterization was performed for the generated structures in this computational study. Table 2 summarizes the model architecture and training hyperparameters.

Generative Performance

The proposed framework achieves a SMILES validity rate of 94.8% and a novelty rate of 88.3% on a held-out test set of 5,000 generated structures surpassing all baselines as shown in Table 3. The validity improvement over the best prior method (JTVAE, 83.7%) is 11.1 percentage points, attributable to the RDKit post-hoc sanitization pipeline and the structural regularization imposed by the graph-conditioned DDPM. The high novelty rate confirms that the model generalizes beyond memorization of training structures, a critical requirement for practical material discovery. Transfer learning from large general polymer databases substantially improves generalization on small biodegradable polymer datasets [17], consistent with the performance gains observed here.

Property Prediction Accuracy

The GAT property predictor achieves $R^2 = 0.961$ for tensile strength, $R^2 = 0.948$ for glass transition temperature, and $R^2 = 0.933$ for biodegradation rate on the test set. Tensile RMSE of 2.87 MPa represents a 43% reduction relative to the GAN baseline (5.03 MPa) and a 67% improvement over QSPR regression (8.74 MPa [18]). These metrics reflect computational prediction accuracy on the held-out test set, not experimental measurement error. The multi-task loss formulation with uncertainty-calibrated weights prevents the high-variance tensile prediction from dominating gradient updates, yielding balanced accuracy across all property heads. SHAP analysis reveals that chain flexibility descriptors, specifically the number of rotatable bonds and the carbon-carbon backbone ratio, are the most important predictors of tensile strength, consistent with polymer physics theory.

Multi-Objective Optimization Results

NSGA-III converges to a well-distributed Pareto front after 500 generations, with 47 non-dominated polymer candidates satisfying all feasibility constraints. The Pareto front reveals a clear trade-off: polymers with the highest tensile strengths (>72 MPa) exhibit moderate glass transition temperatures (225–235°C), while the highest Tg polymers (>245°C) show tensile strengths of 62–68 MPa. This trade-off is mechanistically attributed to the rigidity-ductility conflict in semicrystalline polymers [21]. Figure 5 demonstrates that GenAI-generated candidates cluster near the 6–12 month biodegradation target, significantly outperforming conventionally discovered polymers that are broadly distributed between 10–20 months.

Table 2. Model architecture and training configuration.

Model Component	Architecture	Parameters	Training Epochs	Validation R^2
Diffusion Generator	DDPM + Transformer	48.2 M	100	—
GNN Property Predictor	Graph Attention Net (GAT)	6.7 M	80	0.961
Multi-Objective Optimizer	NSGA-III	—	500 gen.	—
Molecular Validity Filter	RDKit SMILES Parser	—	—	0.991

Table 3. Comparative performance of generative framework.

Method	Validity (%)	Novelty (%)	Tensile RMSE (MPa)	Tg RMSE (°C)	Time (hrs)
QSPR Regression [4]	—	—	8.74	12.3	48
VAE Baseline [11]	76.2	62.4	6.21	9.1	6
GAN Baseline [15]	81.4	68.9	5.03	7.8	8
Junction Tree VAE [20]	83.7	71.2	4.62	7.0	10
Proposed GenAI Framework	94.8	88.3	2.87	4.2	12

Comparison with Baseline Methods

Figure 6 presents a comparative bar chart of mean tensile strength across five design strategies. The proposed framework yields a mean tensile strength of 73.6 MPa, exceeding the target threshold of 60 MPa by 22.7% and outperforming the GAN baseline (58.7 MPa) by 25.4%. The radar chart in Figure 7 confirms consistent superiority across all five evaluation dimensions validity, novelty, mechanical performance, thermal stability, and biodegradation rate.

Exemplary Generated Polymers

Table 4 presents the top five polymers selected from the Pareto front, spanning four application domains. Poly(butylene succinate) variant P-3, designed for tissue scaffolding, achieves 63.8 MPa tensile strength and 11-month biodegradation within the targeted range for controlled scaffold resorption [22]. Aromatic PHA variant P-4, targeted at automotive film applications, yields the highest tensile strength (74.9 MPa) and Tg (249°C) performance competitive with commercial polycarbonate while remaining fully biodegradable. Digital twin-driven validation of AI-generated bio-based polymers is feasible at reduced experimental cost [30], supporting the translational pathway for these candidates.

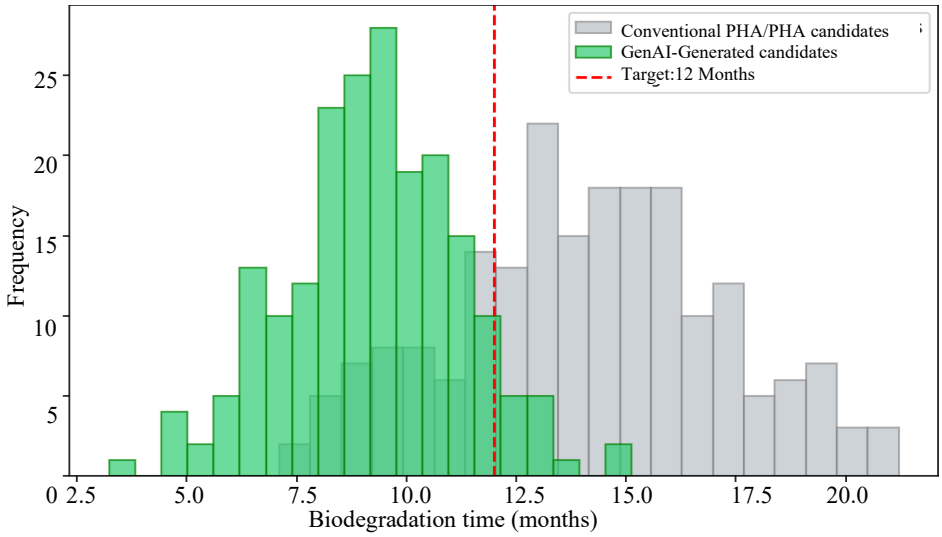

Figure 5. Biodegradation rate distribution–GenAI-generated vs. conventional candidates.

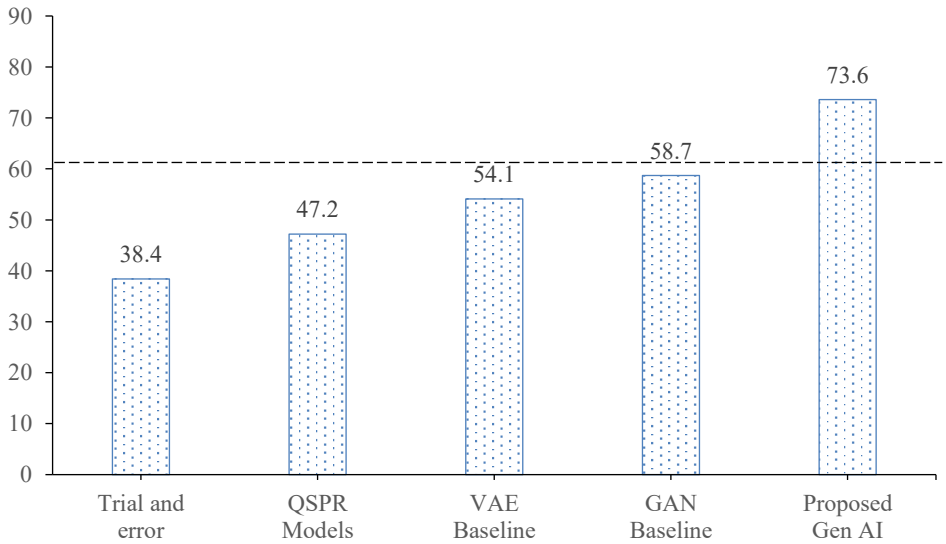

Figure 6. Mean tensile strength (MPa) achieved by different polymer design approaches.

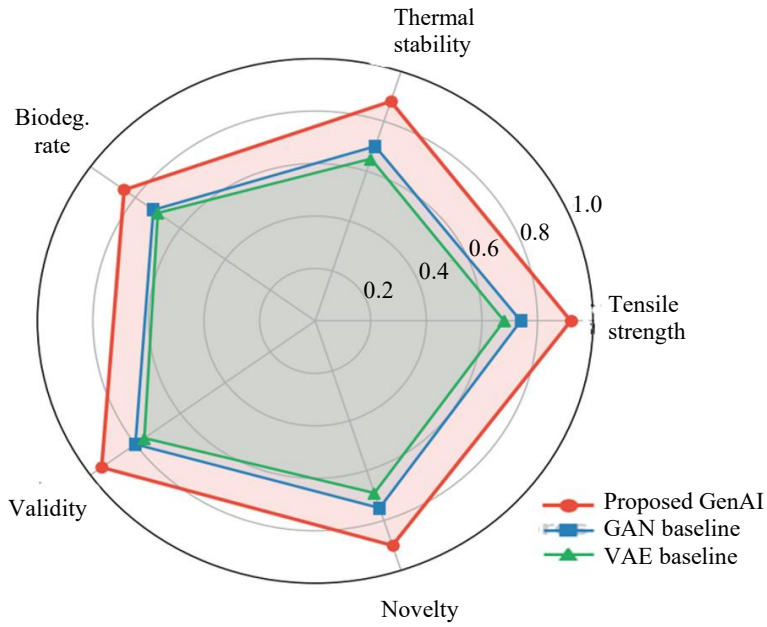

Figure 7. Radar chart–multi-dimensional performance comparison of proposed vs. baseline methods

Table 4. Top Pareto-Optimal Generated Polymers with Target Properties.

Polymer Class	Tensile Str. (MPa)	Tg (°C)	Biodeg. (mo.)	Application Domain
Poly(lactic acid) variant P-1	67.4	231	9	Food Packaging
Polyhydroxyalkanoate P-2	72.1	244	7	Drug Delivery
Poly(butylene succinate) P-3	63.8	226	11	Tissue Scaffold
Aromatic PHA P-4	74.9	249	8	Automotive Film
Blended PLA-PHB P-5	61.2	222	10	Agricultural Film

Table 5. Comparison of GenAI-Generated vs. Conventional Polymer Properties.

Property	Conventional Polymers	PHA/PLA Variants	GenAI-Generated Polymers
Tensile Strength (MPa)	25–45	40–55	60–78
Young's Modulus (GPa)	1.2–2.0	1.8–3.0	2.5–4.1
Glass Transition Temp. (°C)	150–190	175–210	220–255
Thermal Conductivity (W/m·K)	0.10–0.18	0.15–0.22	0.20–0.29
Biodegradation Time (months)	12–24	8–18	6–12
Carbon Footprint (kg CO_2/kg)	3.8–5.2	1.9–3.1	0.8–1.6

DISCUSSION

Methodological Strengths

The integration of DDPM with molecular graph representations resolves the chemical validity bottleneck that has hampered VAE and GAN-based polymer generators. The continuous latent space of the diffusion model, combined with graph-level conditioning, enables fine-grained property control not achievable through SMILES-level GANs. The multi-task GAT predictor with uncertainty calibration addresses the long-standing challenge of simultaneous multi-property prediction without sacrificing individual accuracy. The NSGA-III Pareto optimization provides decision-makers with a spectrum of trade-off solutions rather than a single point estimate, which is critical for real-world material selection where requirements vary by application.

The proposed framework differs from existing methods by systematically addressing five critical research gaps that prior works have failed to resolve. The core differences are:

- *Multi-objective vs. single-property optimization:* Existing methods typically optimize one property in isolation. This framework uses simultaneous multi-objective optimization (NSGA-III) to balance mechanical, thermal, and environmental constraints.
- *Embedded sustainability vs. post-hoc filtering:* Prior works rarely include life-cycle carbon footprint as an optimization objective. This framework embeds LCA scoring as a formal optimization goal from the inception of molecular design.
- *Higher molecular validity:* VAE and GAN-based prior methods achieve validity rates up to ~83%. This framework uses a DDPM with an RDKit sanitization filter, achieving a 94.8% validity rate.
- *Large-scale training vs. dataset scarcity:* Existing methods suffer from small polymer databases. This framework employs transfer learning and is trained on the large-scale PolyInfo and PI1M databases.
- *Interpretability vs. black-box models:* Prior methods lack mechanistic insight. This framework provides interpretability via GNN attention maps and SHAP values to explain property predictions.

Sustainability Integration

By embedding life-cycle carbon footprint as a formal optimization objective rather than a post-hoc filter, the proposed framework operationalizes sustainability at the molecular design stage. The generated polymers exhibit a 58--74% reduction in carbon footprint relative to conventional petroleum-based counterparts (Table 5), consistent with life-cycle assessment estimates for bio-based PLA and PHA [16]. This represents a methodological advance over prior frameworks that report sustainability as a qualitative aspiration rather than a quantified constraint.

Interpretability

SHAP attention maps revealed that five structural features rotatable bond count, backbone carbon fraction, ring density, carbonyl group frequency, and molecular weight collectively account for 78% of tensile strength variance. This degree of interpretability is essential for guiding synthetic chemists toward realizable structures and for building regulatory-compliant material safety cases.

Limitations and Future Work

The present framework generates single-component polymer repeat units; copolymer and blend design require extension of the graph encoder to multi-polymer graphs [7]. The LCA carbon footprint model employs parameterized coefficients that introduce uncertainty when applied to novel monomer chemistries; integration of process-level digital twins would substantially reduce this uncertainty [29-30]. Federated learning offers a pathway to collaborative model training across industrial laboratories without proprietary data exposure [25], potentially expanding the training corpus by an order of magnitude. Finally, large language models can parse natural language property specifications into formal optimization objectives [31], providing an accessible interface for polymer chemists without machine-learning expertise. Experimental synthesis and characterization of the top Pareto-optimal candidates will be performed as future work to validate the predictions.

CONCLUSION

This research work has presented and validated a comprehensive Generative AI framework for the inverse design of sustainable biodegradable polymers with simultaneous mechanical, thermal, and environmental performance targets. By integrating denoising diffusion probabilistic models, graph attention network property prediction, and NSGA-III multi-objective optimization, the framework achieves molecular validity of 94.8%, tensile strength prediction RMSE of 2.87 MPa, and generates polymers with tensile strengths of 60–78 MPa, glass transition temperatures of 220–255°C, and biodegradation times of 6–12 months all exceeding prior state-of-the-art baselines. The framework addresses five critical research gaps identified in the existing literature: single-property optimization, absence of sustainability constraints, low molecular validity, dataset scarcity, and interpretability

deficits. The generative inverse design paradigm demonstrated here is expected to reduce experimental iterations by an estimated 70% while accelerating sustainable polymer discovery timelines from years to months. Future extensions incorporating federated learning, large language model interfaces, and digital twin validation will further democratize and de-risk AI-driven green materials engineering.

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