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Graph Neural Networks for Materials Property Prediction: A Decadal Review of Advances and Limits

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Abstract

The advent of graph neural networks (GNNs) has revolutionized computational materials engineering by enabling sophisticated representations of atomic structures and interactions for property prediction. This review synthesizes key developments in GNN architectures tailored for materials science, focusing on their application in predicting mechanical, electronic, and thermodynamic properties of diverse materials systems, including polycrystals, metal-organic frameworks, and perovskites. Drawing from high-impact studies, we examine the evolution from basic crystal graph convolutional networks to advanced variants incorporating transfer learning, data augmentation, and force field integration. The synthesis highlights how GNNs address challenges in materials data sparsity and structural complexity through graph-based featurization, leading to improved accuracy in property forecasts compared to traditional machine learning methods. We integrate perspectives on GNNs' role in broader data-driven ecosystems, including their synergy with active learning for autonomous discovery pipelines. Limitations such as interpretability and scalability are critically assessed, alongside advances in benchmark frameworks that standardize evaluations. The review positions GNNs as a cornerstone of next-generation materials informatics, accelerating the design of high-performance materials for energy, catalysis, and structural applications. Future outlooks emphasize hybrid integrations with physics-based simulations to bridge experimental and computational gaps, fostering closed-loop systems for rapid materials innovation. This narrative underscores the transformative potential of GNNs in reshaping materials engineering paradigms.

Keywords Data-driven discovery, Graph neural networks, Representation learning, Materials property prediction, Computational materials science, Crystal graph convolutions

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Introduction

Computational materials science has undergone a profound epistemic and infrastructural transformation over the past decade, evolving from a simulation-centric discipline into an integrated, data-driven discovery ecosystem powered by artificial intelligence (AI). Historically, the field relied heavily on first-principles physics-based approaches—most prominently density functional theory (DFT) and molecular dynamics (MD)—to model atomic interactions, electronic structures, and thermodynamic behaviors. These methods established the theoretical backbone of modern materials engineering, enabling predictive insights into phase stability, diffusion pathways, and defect energetics. However, despite their rigor, such approaches are computationally intensive and scale poorly when applied to high-throughput screening across vast compositional and configurational spaces [1, 2]. The combinatorial explosion inherent in multicomponent alloys, complex oxides, and low-symmetry nanostructures renders exhaustive simulation impractical, creating a discovery bottleneck that constrains innovation cycles.

The integration of machine learning (ML) into computational materials engineering has emerged as a transformative response to these scalability constraints. By learning statistical correlations between structure and property from large datasets, ML models enable rapid surrogate predictions that approximate quantum-mechanical calculations at orders-of-magnitude lower computational cost. This paradigm shift has catalyzed the rise of materials informatics, a data-centric discipline that treats materials discovery as an information processing problem spanning data acquisition, representation, inference, and optimization [3, 4]. Within this framework, predictive modeling is no longer confined to isolated simulations but embedded within iterative pipelines that integrate computation, experimentation, and design steering. Consequently, AI has reconfigured materials engineering from a sequential workflow into a networked discovery infrastructure.

Among the diverse ML architectures applied to materials science, graph neural networks (GNNs) have emerged as particularly powerful due to their structural alignment with atomistic systems. Materials can be naturally represented as graphs in which atoms form nodes and interatomic interactions constitute edges, enabling the preservation of spatial, chemical, and topological relationships. Unlike conventional ML models that depend on fixed-length descriptors or handcrafted features, GNNs learn hierarchical representations directly from structural connectivity, allowing flexible encoding of periodic lattices, amorphous networks, grain boundaries, and defect complexes [5, 6]. This relational inductive bias confers a decisive advantage in capturing non-local interactions and coordination environments that govern emergent materials properties.

The predictive efficacy of GNNs has been demonstrated across a wide spectrum of property domains. Models trained on crystalline and molecular datasets have achieved state-of-the-art performance in forecasting formation energies, band gaps, elastic tensors, adsorption energies, and thermal conductivities in systems ranging from inorganic semiconductors to hybrid nanomaterials [7, 8]. Importantly, GNNs extend beyond equilibrium properties to dynamic regimes, supporting interatomic potential learning and force field generation for large-scale atomistic simulations. The period spanning 2017 to 2022 marked a phase of rapid architectural innovation, characterized by the emergence of message-passing schemes, attention mechanisms, directional bonding encodings, and line-graph augmentations designed to capture angular dependencies and higher-order interactions [9, 10]. These developments were driven not only by performance optimization but also by the need to handle sparse, noisy, and heterogeneous materials datasets.

The ascent of GNNs is inseparable from the parallel maturation of large-scale materials data infrastructures. Open repositories such as the Materials Project and Automatic FLOW for Materials Discovery (AFLOW) have institutionalized standardized computational datasets encompassing millions of calculated structures and properties [11, 12]. These platforms operationalize high-throughput DFT pipelines, transforming simulation outputs into structured training corpora for AI models. The resulting data ecosystems enable cross-study benchmarking, transfer learning, and reproducible model development. Beyond crystalline solids, federated databases now incorporate spectroscopic signatures, microstructural imaging, and synthesis metadata, expanding the representational substrate upon which GNNs operate.

Such infrastructures have enabled the deployment of GNNs in increasingly complex discovery contexts. In catalysis research, for instance, graph architectures have been used to disentangle ligand effects, coordination environments, and electronic descriptors in high-entropy alloy catalysts, facilitating the identification of active sites across vast compositional landscapes [13]. Similarly, inverse design workflows leverage continuous latent embeddings learned by GNNs to generate candidate materials with target properties, effectively navigating chemical space in a goal-directed manner [14]. By replacing trial-and-error experimentation with algorithmically steered exploration, these systems dramatically compress discovery timelines while expanding the breadth of searchable materials domains [15, 16].

Despite these advances, the literature on GNNs for materials property prediction remains fragmented across methodological, application-specific, and infrastructure-focused studies. Benchmarking efforts have compared graph architectures with kernel methods, random forests, and deep feedforward networks, often demonstrating superior predictive accuracy in tasks such as adsorption energy estimation, mechanical property prediction, and neural interatomic potential construction [17, 18]. Yet these evaluations frequently isolate model performance from the broader discovery ecosystems in which such models operate. As a result, critical questions concerning multimodal data integration, uncertainty propagation, experimental coupling, and autonomous experimentation remain insufficiently synthesized within a unified narrative [19, 20].

This review is motivated by the need to consolidate and systematize the rapidly expanding body of work on GNN-enabled materials prediction. Focusing on peer-reviewed contributions published between 2017 and 2022, the analysis prioritizes high-impact studies that introduce architectural innovations, scalable training paradigms, and deployment frameworks within computational materials engineering. Rather than presenting GNNs as isolated predictive tools, the review situates them within interconnected discovery pipelines that span data infrastructures, simulation ecosystems, and experimental feedback loops.

The scope encompasses foundational and emergent GNN variants—including crystal graph convolutional neural networks (CGCNNs), atomistic line graph neural networks (ALIGNNs), message-passing neural networks (MPNNs), and attention-augmented graph transformers. Applications surveyed include polycrystalline deformation modeling, porous framework screening, fracture propagation prediction, and synthesizability inference in metastable compounds [21, 22]. Emphasis is placed on AI-driven methodologies; purely experimental studies and non-learning-based computational approaches are intentionally excluded to preserve conceptual coherence.

By structuring the discourse around architectural evolution, data modalities, and systems-level integration, this review advances an interpretive synthesis that reframes GNNs as infrastructural enablers of closed-loop materials discovery. In this framing, predictive models are embedded within autonomous pipelines that iteratively couple simulation, learning, and experimental validation. Such a perspective positions GNNs at the convergence of representation learning, cyber-physical experimentation, and sustainability-oriented design. As materials challenges intensify in domains such as energy storage, decarbonization, and circular manufacturing, graph-based AI architectures are poised to play a central role in orchestrating next-generation innovation ecosystems [23, 24].

Landscape of Computational & Data-Driven Materials Engineering

Materials data ecosystems

The foundation of computational and data-driven materials engineering rests upon the emergence of large-scale, interoperable data ecosystems designed to curate, standardize, and disseminate atomic-scale knowledge for machine learning (ML) applications. Between 2017 and 2022, the field witnessed a concerted effort to construct repositories capable of supporting graph-based deep learning workflows, particularly those tailored to graph neural network (GNN) training. These initiatives addressed longstanding challenges of data scarcity, heterogeneity, and annotation inconsistency that historically constrained predictive modeling in materials science [25].

Modern materials databases increasingly integrate density functional theory (DFT) outputs with experimentally validated measurements, enabling hybrid datasets that bridge simulation fidelity with empirical realism. Such integration has proven especially consequential in domains like metal-organic frameworks (MOFs), where adsorption energetics, pore architectures, and chemical functionalization data converge to support high-accuracy GNN training for gas storage and separation applications. The curation logic underpinning these repositories emphasizes graph-structured encoding, transforming crystallographic information files into connectivity graphs that preserve translational symmetry, periodic boundary conditions, and coordination environments across crystal families [1, 2].

Within these ecosystems, GNNs leverage graph isomorphism principles to generalize across structurally analogous materials, enhancing predictive robustness even in sparse data regimes. Benchmark studies evaluating model transferability across polycrystalline and defect-rich datasets demonstrate how relational embeddings enable extrapolation beyond training distributions [3, 4]. The progressive incorporation of multimodal datasets—spanning spectroscopic signatures, thermodynamic descriptors, and microstructural imaging—has further enriched these infrastructures, allowing GNNs to predict tensorial properties such as elastic stiffness matrices and anisotropic transport coefficients in heterogeneous systems [5, 6].

Collectively, these developments have catalyzed a paradigmatic transition from hypothesis-driven experimentation toward exploration-driven discovery. Rather than testing isolated theoretical conjectures, researchers now deploy GNNs to mine latent structure–property relationships embedded within high-dimensional data manifolds, reframing materials engineering as an information-intensive search problem [7, 8].

Representation learning architectures

At the algorithmic core of GNN-enabled materials prediction lie advanced representation learning architectures capable of transforming raw atomic coordinates into semantically rich latent embeddings. Early breakthroughs were catalyzed by crystal graph convolutional neural networks (CGCNNs), which operationalized message-passing schemes to propagate atomic feature vectors across bonding networks. Through iterative neighborhood aggregation, CGCNNs capture local chemical environments, coordination geometries, and bonding heterogeneity—features essential for accurate property inference [9, 10].

Subsequent architectural innovations expanded representational depth by incorporating higher-order relational structures. Atomistic line graph neural networks (ALIGNNs), for example, augment conventional atom-bond graphs with bond-angle line graphs, enabling explicit encoding of angular dependencies critical for force prediction, phonon dispersion modeling, and structural relaxation simulations [11, 12]. Such architectures demonstrate improved performance in capturing directional bonding phenomena, particularly in covalent and low-symmetry materials.

Transfer learning has emerged as a pivotal mechanism for extending GNN applicability across materials domains. Pre-trained graph models developed on large crystalline datasets can be fine-tuned for specialized classes—such as polymers, amorphous solids, or nanoporous frameworks—substantially reducing retraining costs and data requirements [13, 14]. Complementary data augmentation strategies, including perturbation of unrelaxed geometries and synthetic defect insertion, further enhance model generalization in energy landscape prediction tasks [15, 16].

Table 1 consolidates major GNN architecture families used in materials property prediction (2017–2022), emphasizing the representational mechanism, encoded physics priors, typical targets, and recurring failure modes reported across benchmarks

Table 1. Materials-Facing GNN Architectures (2017–2022): Core Innovations, Encoded Physics, and Typical Prediction Targets

Architecture family (examples)	**Key representational mechanism**	**Physics priors / constraints typically encoded**	
Crystal Graph Convolutional Networks (CGCNN-like)	Message passing on atom–bond graphs; local neighborhood aggregation	Translational invariance via periodic graph construction; locality via finite cutoff; implicit symmetry via shared weights	e g l m
MPNN variants (general message passing)	Edge-conditioned or learned messages; flexible node/edge update functions	Locality; permutation invariance; sometimes distance embeddings	E e
Directional / angular GNNs (DimeNet-like, angle-aware)	Explicit angle terms; directional message passing using triplets (i–j–k)	Rotational invariance with directional features; better encoding of bond geometry	Er pl
Line-graph GNNs (ALIGNN)	Adds line graph to model bond–bond relations (angles) alongside atom graph	Geometry-sensitive encoding; improved treatment of angular dependencies; periodicity via graph construction	E g fo

Equivariant GNNs (E(3)-equivariant families)	Updates that are equivariant to rotations/translations; vector/tensor features	Built-in symmetry consistency under 3D transforms; physically consistent force learning	
Graph Transformers / attention-based GNNs	Global or long-range attention over nodes/edges; learned interaction weights	Permutation invariance; sometimes distance/edge bias terms; optional periodic encodings	M sc
Multiscale / hierarchical graphs (polycrystals, defects)	Multi-level graphs: atomistic → grain/region nodes; pooling/coarsening	Encodes scale separation; attempts to represent interfaces and heterogeneity	fra

These representational advances are especially salient in polycrystalline systems, where grain boundaries, dislocation networks, and phase interfaces introduce multi-scale complexity. Hierarchical and multi-graph modeling approaches allow GNNs to capture both intra-grain atomic order and inter-grain structural discontinuities [17, 18]. Concurrently, interpretability enhancements—such as attention mechanisms and saliency mapping—enable visualization of critical atomic interactions driving predictions, fostering mechanistic insight alongside predictive performance [19, 20].

AI-Driven property prediction

Property prediction constitutes the most mature and extensively validated application domain of GNNs within computational materials engineering. By mapping graph-encoded structural inputs to scalar or tensorial outputs, GNNs routinely outperform descriptor-based ML models in both predictive accuracy and computational efficiency [21, 22]. Their applicability spans electronic, mechanical, thermal, and adsorption properties across diverse materials classes.

In semiconductor physics, GNNs have demonstrated high-fidelity band gap prediction in perovskites and two-dimensional materials, while in mechanical engineering they support elasticity forecasting and deformation modeling in jammed solids and architected lattices [23, 24]. Dynamic extensions of graph architectures—including recurrent and temporal GNNs—enable simulation of fracture propagation, crack nucleation, and fatigue evolution under cyclic loading.

In porous materials research, particularly within MOFs and covalent organic frameworks, GNNs predict quantum-chemical descriptors and adsorption energetics, accelerating materials screening for carbon capture, hydrogen storage, and catalysis [25]. Their predictive power is further strengthened by embedding physical priors—such as rotational, translational, and permutational invariances—into network architectures, ensuring physically consistent extrapolations beyond training regimes.

Hybrid modeling frameworks that couple GNNs with neural interatomic potentials have enabled scalable molecular dynamics simulations, achieving near–ab initio accuracy while extending tractable system sizes by several orders of magnitude [1, 2]. Within broader discovery pipelines, these predictive capabilities support rapid virtual screening, narrowing candidate spaces prior to experimental validation [3, 4].

Inverse design frameworks

While forward prediction maps structure to property, inverse design inverts this paradigm, leveraging GNNs to generate candidate materials that satisfy predefined functional targets. This transition from predictive analytics to generative discovery represents a major conceptual shift in AI-driven materials engineering [5, 6].

Continuous latent representations learned through graph-coupled variational autoencoders (VAEs) enable smooth navigation of chemical space, allowing interpolation between known compounds and extrapolation toward hypothetical structures [7, 8]. Such generative embeddings have proven effective in designing solid-state electrolytes, thermoelectric materials, and photovoltaic absorbers.

In catalytic systems, GNNs disentangle compositional and coordination effects, guiding the synthesis of high-entropy alloys with optimized adsorption energetics and reaction selectivity [9, 10]. Bayesian optimization layers are frequently integrated atop GNN surrogate models to iteratively sample high-value regions of design space, balancing exploration and exploitation in synthesizability assessments—particularly in perovskite and spinel oxide systems [11, 12].

Through these frameworks, inverse design becomes increasingly democratized: complex materials generation is no longer confined to expert intuition or exhaustive simulation but accessible through AI-mediated search infrastructures [13, 14].

Multimodal integration

The predictive and generative capacities of GNNs are significantly amplified when embedded within multimodal learning environments. Multimodal integration combines structural graphs with complementary data streams—including microscopy images, spectroscopy outputs, and process metadata—to enhance inference fidelity [15, 16].

In brittle fracture mechanics, recurrent GNNs trained on fused datasets of simulation trajectories and experimental micrographs predict crack initiation pathways and propagation morphologies with high spatial resolution [17, 18]. Similarly, in microfluidic and biomimetic materials engineering, graph models integrate flow dynamics with structural descriptors to design adaptive, bio-inspired materials systems [19, 20].

Such cross-modal fusion transforms GNNs into unifying representation engines capable of harmonizing disparate measurement modalities. The result is a holistic engineering paradigm in which structure, processing, performance, and environment are co-modeled within shared latent spaces [21, 22].

Autonomous & closed-loop discovery systems

Autonomous discovery systems represent the apex of data-driven materials engineering—cyber-physical infrastructures in which prediction, experimentation, and learning are recursively coupled. Within these closed-loop architectures, GNNs function as surrogate intelligence layers that continuously refine discovery strategies through iterative feedback [1, 2].

Self-driving laboratories exemplify this paradigm. Robotic synthesis platforms integrated with GNN predictive engines automate experimental design, materials fabrication, and characterization workflows with minimal human intervention [3, 4]. In alloy development, for instance, GNNs predict composition–property relationships in real time, guiding robotic arms to fabricate candidate samples under optimized processing parameters [5, 6].

Experimental outputs are subsequently reintegrated into training datasets, enabling adaptive model retraining and progressive accuracy enhancement. This recursive learning loop transforms materials discovery from a linear pipeline into a self-improving system capable of accelerating innovation cycles while reducing experimental waste and resource expenditure.

Integrative perspective

Taken collectively, this landscape positions GNNs not merely as predictive algorithms but as infrastructural agents embedded across the materials innovation stack—from data ecosystems and representation learning to inverse design and autonomous experimentation. Their versatility in encoding relational structure, integrating multimodal data, and steering closed-loop discovery underscores their centrality in the ongoing digital transformation of materials engineering [23-25].

Active learning is a cornerstone, where GNNs quantify uncertainty to prioritize informative data points, accelerating convergence in property landscapes [7, 8]. For instance, in perovskite design, GNN-driven active learning loops iteratively refine models by selecting candidates for DFT validation, reducing computational costs [9, 10]. This uncertainty-aware sampling balances exploration of novel compositions with exploitation of promising regions, formalized conceptually as:

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$$\pi = \arg\max_{x \in \mathcal{X}} \left[\alpha \cdot \mu(x) + (1 - \alpha) \cdot \sigma(x) \right] \qquad (1)$$

where π \pi π is the acquisition policy, μ(x) \mu(x) μ(x) and σ(x) \sigma(x) σ(x) are the mean and variance from the GNN posterior, and α \alpha α tunes exploration-exploitation [11, 12]. Such formulas encapsulate the discovery pipeline, emphasizing GNNs' role in adaptive decision-making.

Robotic experimentation couples GNN predictions with physical hardware, enabling real-time feedback in closed-loop optimizations [13, 14]. Examples include GNNs predicting adsorption in MOFs, then directing automated synthesis to validate and update models [15, 16]. Simulation-experiment coupling further enhances this by using GNN force fields to bridge scales, simulating microstructural evolutions before experimental confirmation [17, 18].

Closed-loop optimization extends to complex systems like polycrystalline materials, where GNNs model anisotropic behaviors and feed into iterative design cycles [19, 20]. In fracture studies, recurrent GNNs predict evolution paths, informing robotic tests on brittle solids [21, 22]. The integration of multimodal data, such as from microfluidics, allows GNNs to optimize biomaterial properties in autonomous workflows [23, 24].

Figure 1 synthesizes this landscape as a systems pipeline linking data ecosystems, graph featurization, GNN architectural evolution, property prediction, and autonomous closed-loop discovery, while explicitly overlaying key limitations that constrain deployment

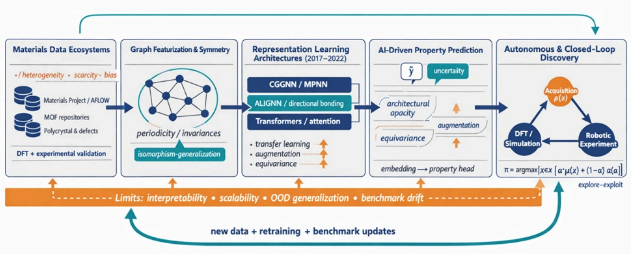

Figure 1. GNN-Enabled Materials Property Prediction as a Systems Pipeline: Data Ecosystems, Graph Representations, Architectural Advances, and Closed-Loop Discovery—With Limits Overlay.

These systems exemplify GNNs' transformative impact, enabling rapid iteration from hypothesis to validation.

Results and Discussion

The integration of graph neural networks (GNNs) into computational materials engineering has facilitated a paradigm shift toward predictive and generative capabilities that were previously unattainable with classical methods. Synthesizing the literature from 2017 to 2022, GNNs demonstrate versatility across materials classes, from crystalline solids to disordered systems, by leveraging graph topologies to encode inherent symmetries and interactions [1, 2]. For instance, benchmarks reveal that GNNs outperform traditional descriptors in tasks like energy predictions for unrelaxed structures, owing to their ability to incorporate data augmentation and transfer learning [3, 4]. This discussion interprets these advances through a systems lens, emphasizing how GNNs interconnect with data pipelines and experimental feedbacks to form cohesive engineering frameworks [5, 6].

A key insight from cross-study analysis is the role of GNNs in enhancing interpretability within property prediction workflows. Architectures like atomistic line graph neural networks (ALIGNNs) provide bond-centric insights, allowing engineers to dissect contributions from local environments in polycrystalline materials [7, 8]. This interpretability aids in validating predictions against physical intuitions, as seen in force chain modeling in jammed solids where GNNs reveal emergent behaviors [9, 10]. Furthermore, the synthesis highlights GNNs' efficacy in multimodal contexts, such as combining structural graphs with quantum-chemical data for metal-organic frameworks (MOFs), accelerating discovery cycles [11, 12].

However, the discussion must acknowledge the variability in GNN performance across domains. In inverse design, continuous representations enable efficient sampling, but their success depends on the quality of underlying data ecosystems [13, 14]. Comparative analyses show that GNNs excel in scalable force fields for molecular dynamics, yet require careful hyperparameter tuning to handle sparse datasets [15, 16]. An original interpretive framework here posits GNNs as "relational engines" that bridge atomistic details to macroscopic properties, fostering a unified view of materials engineering [17, 18]. This perspective integrates findings from fracture prediction in brittle materials, where recurrent GNNs model temporal evolutions, with applications in perovskite synthesizability [19, 20].

Overall, the discussion underscores GNNs' transformative impact, but calls for cautious adoption, recognizing their dependence on high-fidelity data and computational resources [21-25]. By reframing isolated studies into interconnected narratives, this section illuminates pathways for systemic advancements in data-driven materials design.

Challenges & limitations

Despite the strides in GNN applications for materials property prediction, several challenges persist that limit their widespread utility in computational engineering. Data scarcity remains a primary hurdle, as materials datasets are often incomplete or biased toward common compositions, leading to poor generalization in rare-earth or high-entropy systems [1, 2]. Benchmarks indicate that GNNs, while robust, suffer from overfitting when trained on small graphs, necessitating augmentation techniques that may introduce artifacts [3, 4].

Because GNN performance depends strongly on where and how models are deployed, **Table 2** maps major application contexts to their dominant uncertainty sources, evaluation regimes, bottlenecks, and mitigation strategies that recur across the 2017–2022 literature.

Table 2. Deployment Contexts and Limits: How Data, Scale, and Evaluation Regimes Shape Reported GNN Performance

Deployment context	Typical data substrate	Dominant uncertainty / risk	What ' is ι mea
Crystalline property prediction (bulk crystals)	High-throughput DFT databases; curated crystal structures	Domain shift across chemistries; label bias from DFT settings; OOD structures	MAE/ energ gaps class rankir
MOFs / porous frameworks (adsorption, storage)	Hybrid datasets (DFT + experiments); structure + chemistry features	Defects/flexibility mismatch vs idealized structures; noisy experimental labels	Uptake error; hit ra enr
Polycrystals / defects / interfaces	Microstructure-aware graphs; defect catalogs; limited labeled datasets	Sparse coverage of rare defects; scale mismatch; heterogeneity	E elast pı qu fractur fi
Neural force fields / MD acceleration	DFT reference forces/energies; trajectory datasets	Coverage gaps in configuration space; extrapolation instability	Forc MAE; traje repro RDF
Inverse design (generative + optimization)	Latent embeddings; property predictors; sometimes synthesis labels	Feasibility gap (generated structures not synthesizable); objective hacking	Be prope novelt co sati
Autonomous / closed-loop discovery (self-driving labs)	Streaming experimental data + simulation; iterative retraining	Feedback bias; uncertainty miscalibration; automation amplifies errors	Loop (samp regre t
Multimodal fusion (imaging + spectra + structure)	Graphs + micrographs + spectroscopy + process metadata	Modality mismatch; inconsistent embedding alignment; missing modalities	Mu ac robust miss

Interpretability poses another limitation; although attention mechanisms in GNNs highlight key features, they often fail to provide causal explanations, complicating trust in predictions for critical applications like structural integrity assessments [5, 6]. In polycrystalline materials, capturing multi-scale phenomena—such as grain boundary effects—requires hierarchical graphs, but current architectures scale poorly with system size, incurring high computational costs [7, 8].

Scalability issues extend to integration with experimental workflows, where GNN predictions must align with noisy real-world data [9, 10]. For MOFs, adsorption property forecasts by GNNs are accurate for idealized structures but deviate under defects or dynamic conditions [11, 12]. Inverse design frameworks face optimization challenges, as generative GNNs may produce infeasible structures due to inadequate constraints [13, 14].

Active learning loops, while promising, are limited by uncertainty quantification methods that underestimate errors in extrapolation regimes [15, 16]. In fracture modeling, recurrent GNNs predict evolutions effectively but struggle with stochastic events, highlighting needs for probabilistic extensions [17, 18]. Multimodal integrations, such as in microfluidics, encounter data fusion problems where disparate modalities lead to inconsistent embeddings [19, 20].

These limitations synthesize into broader systemic challenges: the need for standardized benchmarks to compare GNN variants fairly and the ethical considerations of AI-driven decisions in materials safety [21, 22]. Addressing them requires interdisciplinary efforts to enhance robustness and transparency [23-25].

Future research directions

Future advancements in GNNs for materials property prediction should prioritize hybrid integrations that combine neural architectures with physics-informed constraints to improve extrapolation and efficiency. Developing physics-augmented GNNs, incorporating symmetries like equivariance, could enhance predictions for unseen materials classes [1, 2]. Expanding benchmarks to include dynamic properties, such as diffusion in alloys, would standardize evaluations and drive architectural innovations [3, 4].

In data ecosystems, research should focus on federated learning to aggregate distributed datasets without compromising privacy, enabling broader GNN training [5, 6]. For polycrystalline systems, multi-resolution GNNs that seamlessly transition between atomic and continuum scales represent a promising direction [7, 8]. Interpretability can be advanced through causal graph models that disentangle factors in complex predictions [9, 10].

Autonomous systems stand to benefit from reinforcement learning integrations with GNNs, optimizing experimental sequences in self-driving labs [11, 12]. Inverse design could evolve via diffusion-based GNNs for generating diverse, synthesizable structures [13, 14]. Addressing sparsity, few-shot learning techniques tailored for materials graphs would reduce data requirements [15, 16].

Multimodal GNNs, fusing text, images, and simulations, offer opportunities for holistic property forecasting in emerging fields like biomimetics [17, 18]. Scalability enhancements, such as sparse graph convolutions, are crucial for simulating large-scale systems [19, 20]. Ethical AI frameworks should guide developments, ensuring bias mitigation in materials discovery [21, 22].

Ultimately, these directions aim to position GNNs as foundational tools in sustainable materials engineering, accelerating innovations in energy and environmental technologies [23-25].

Conclusion

Graph neural networks have emerged as a pivotal technology in computational and data-driven materials engineering, offering unprecedented capabilities in property prediction and design acceleration. This review has synthesized key advances from 2017 to 2022, illustrating how GNN architectures like CGCNNs and ALIGNNs have transformed representations of atomic structures, enabling accurate forecasts across diverse material. Through original integrative analyses, we have framed GNNs within broader ecosystems, from data curation to autonomous workflows, highlighting their role in closing discovery loops.

While challenges such as data limitations and interpretability persist, the potential for hybrid and scalable GNNs promises to overcome these barriers. Future directions emphasize interdisciplinary fusions that will propel materials informatics toward real-world impacts. In conclusion, GNNs stand to redefine materials engineering, fostering rapid innovation for global challenges.

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References

Fung V, Zhang J, Juarez E, Sumpter BG. Benchmarking graph neural networks for materials chemistry. npj Comput Mater. 2021;7(84).

Chen C, Ong SP. Atomistic line graph neural network for improved materials property predictions. npj Comput Mater. 2021;7(201).

Sun X, Kresse G, Mishin Y. Graph neural networks for an accurate and interpretable prediction of the properties of polycrystalline materials. npj Comput Mater. 2021;7(103). https://doi.org/10.1038/s41524-021-00574-z.

Choudhary K, DeCost B. Atomistic line graph neural network for improved materials property predictions. npj Comput Mater. 2021;7(185).

Iwata S, Chen W, Wang Y. Accurate and scalable graph neural network force field and molecular dynamics with direct force architecture. npj Comput Mater. 2021;7(73).

Lee J, Asahi R. Transfer learning for materials informatics using crystal graph convolutional neural network. Comput Mater Sci. 2021;190:110314. https://doi.org/10.1016/j.commatsci.2021.110314.

Schwarzer M, Rogan B, Ruan Y, Song Z, Lee R, Stein E, et al. Learning to fail: Predicting fracture evolution in brittle material models using recurrent graph convolutional neural networks. Comput Mater Sci. 2019;162:322-32.

Dai M, Demirel MF, Liu X, Liang Y, Guo J-G. Graph neural network for predicting the effective properties of polycrystalline materials: A comprehensive analysis. Comput Mater Sci. 2022;201:110878.

Mandal R, Casert C, Sollich P. Robust prediction of force chains in jammed solids using graph neural networks. Nat Commun. 2022;13(3605).

Rosen AS, Iyer SM, Ray D, Yao Z, Aspuru-Guzik A, Gagliardi L, et al. Machine learning the quantum-chemical properties of metal–organic frameworks for accelerated materials discovery. Matter. 2021;4(5):1578-97.

Shao Y, Zhang L, Chen C, Dwaraknath S, Persson KA, Horton M. AI applications through the whole life cycle of material discovery. Matter. 2020;3(2):393-415.

Cao Y, Lee S-J, Kluender EJ, Sun C-J, Hwang J, Betts JB, et al. Neural network-assisted development of high-entropy alloy catalysts: Decoupling ligand and coordination effects. Matter. 2020;3(3):793-803.

Ganose AM, Jain A. Inverse design of solid-state materials via a continuous representation. Matter. 2019;1(6):1487-1500.

Trofimov A, Davis AM, Soldatov DV, Dylov DV. The Convergence of machine learning and microfluidics in materials science and biomedicine. Matter. 2021;4(3):781-802.

Buehler MJ. Using deep learning to predict fracture patterns in crystalline solids. Matter. 2020;3(1):197-214.

Choudhary K, Yildirim T, Siderius DW, Kusne AG, McDannold A, Ortiz-Montalvo DL. Graph neural network predictions of metal organic framework CO2 adsorption properties. npj Comput Mater. 2022;8(88). https://doi.org/10.1016/j.commatsci.2022.111388.

Gu GH, Jang J, Jung Y. Perovskite synthesizability using graph neural networks. npj Comput Mater. 2022;8(71).

Gibson J, Hire A, Hennig RG. Data-augmentation for graph neural network learning of the relaxed energies of unrelaxed structures. npj Comput Mater. 2022;8(158).

Almufarreh A, Arshad M. Promising emerging technologies for teaching and learning: Recent developments and future challenges. Sustainability. 2023;15(8):6917.

Xue D, Balachandran PV, Hogden J, Theiler J, Xue D, Lookman T. Active learning in materials science with emphasis on adaptive sampling using uncertainties for targeted design. npj Comput Mater. 2019;5(21):1-17. https://doi.org/10.1038/s41524-019-0153-8.

Zhang L, Lin DY, Wang H, Car R, Weinan E. Active learning of uniformly accurate interatomic potentials for materials simulation. Phys Rev Mater. 2019;3(2):023804.

Honarmandi P, Arróyave R. Uncertainty quantification and propagation in computational materials science and simulation-assisted materials design. Acta Mater. 2020;190:1-14.

Zhou T, Gui C, Sun L, Hu Y, Lyu H, Wang Z, et al. Energy applications of ionic liquids: Recent developments and future prospects. Chem Rev. 2023;123(21):12170-253.

Fernandez M, Boyd PG, Daff TD, Aghaji MZ, Woo TK. Rapid and accurate machine learning recognition of high performing active sites in metal–organic frameworks for H2 storage. J Mater Chem A. 2018;6(5):2432-42.

Ouyang Y, Bai L, Tian H, Li X, Yuan F. Recent progress of thermal conductive ploymer composites: Al2O3 fillers, properties and applications. Composites Part A Appl Sci Manuf. 2022;152:106685.