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Graph-Based Learning for Disordered Systems: A Review of Amorphous, Liquid, and Glassy Materials

Rashid Al-Mahdi[1], Khalifa Al-Suwaidi[1*], Mariam Al-Kuwari[2]

Abstract

Graph-based machine learning has reached maturity for crystalline materials, where periodic boundary conditions and fixed unit cells allow efficient message passing and property prediction. Disordered systems—amorphous solids, liquids, glasses, and polymers—represent the next frontier. These materials dominate everyday technologies, from smartphone screens and optical fibers to electrolytes in batteries and structural alloys, yet they lack the translational symmetry that simplifies graph construction in crystals. This review synthesizes exactly 35 peer-reviewed publications from 2017 to 2025 that apply graph-based learning, graph neural networks (GNNs), and related data-driven methods to non-crystalline materials. The selected works span key target journals including *npj Computational Materials*, *Physical Review B*, *Journal of Chemical Theory and Computation*, *Machine Learning: Science and Technology*, and *Physical Review Materials*. The review is organized around a taxonomy of five classes of disordered systems: amorphous solids, liquids, glasses (including supercooled liquids), polymers, and crystals with substitutional disorder. It identifies seven core challenges that distinguish disordered systems from crystals: absence of periodic boundaries, variable graph sizes, heterogeneous local atomic environments, the critical role of medium-range order (5–15 Å), dynamic graph evolution in liquids, lack of standardized benchmarks, and prohibitive computational cost for large simulation boxes. Current methodological approaches are grouped into six categories—local descriptors (non-graph), graph pooling for size invariance, multi-scale GNNs, equivariant architectures, temporal GNNs for liquids, and transfer learning from crystal data—each evaluated for strengths, limitations, and empirical performance on properties such as density, elastic moduli, glass-forming ability, relaxation dynamics, and defect identification. Despite notable progress, three persistent gaps remain: limited size transferability across simulation-box lengths, inadequate capture of medium-range structural correlations, and under-development of methods for dynamic properties. By critically analyzing these 35 studies, this review provides a systematic framework for graph-based learning in disordered materials and highlights open problems that must be solved before these techniques can achieve the same reliability and scalability already demonstrated for crystals. The field stands at an inflection point: continued innovation in graph representations and benchmarking will determine whether graph-based methods can fully unlock predictive modeling for the disordered materials that underpin modern technology.

Keywords Graph neural networks, Disordered materials, Amorphous solids, Glassy systems, Liquids, Medium-range order

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Introduction

Graph neural networks have transformed computational materials science for crystals. Periodic boundary conditions and small unit cells (typically 10–100 atoms) enable compact graphs, efficient message passing, and accurate prediction of energies, forces, and properties across thousands of compounds. Yet most real-world materials are not perfect crystals. Glasses, liquids, amorphous films, and polymers—collectively termed disordered systems—are ubiquitous in applications ranging from consumer electronics and energy storage to structural components and biomedical devices. Despite their technological importance, graph-based learning for disordered systems lags far behind crystalline counterparts.

The fundamental reason is structural. Disordered systems lack periodicity, exhibit variable system sizes, and display highly heterogeneous local environments. These characteristics invalidate many assumptions that make crystal GNNs straightforward to implement and train. For instance, a typical crystal model can exploit translational symmetry to keep graphs small and invariant under periodic images. In contrast, a realistic amorphous simulation box often contains 1 000–10 000 atoms with no repeating unit cell, forcing the model to process large, non-periodic graphs whose size and connectivity change with composition or preparation history.

This review examines graph-based learning for disordered systems (amorphous, liquid, and glassy materials) published between 2017 and 2025. It draws exclusively on the 35 peer-reviewed publications identified in the companion reference list. The selected works include both early machine-learning studies that laid the groundwork for graph methods and more recent explicit GNN applications. The analysis reveals why disordered systems pose unique difficulties and evaluates how current approaches attempt to overcome them.

Progress in this area is timely. Industry demand for new glasses with tailored optical, mechanical, or ionic properties continues to grow, while atomistic simulations of liquids and amorphous phases remain computationally expensive. Graph-based models offer a potential route to accelerate property prediction and inverse design, but only if they can handle the intrinsic variability of disordered structures. By synthesizing the literature, this review identifies shared methodological patterns, quantifies empirical successes and failures, and articulates the open challenges that must be addressed before graph-based learning can achieve parity with its crystalline counterpart.

Figure 1 synthesizes the review’s central argument by mapping how distinct classes of disordered systems generate specific graph-learning challenges, motivate different methodological responses, and converge on three unresolved bottlenecks: size transferability, medium-range order, and dynamic-property modeling.

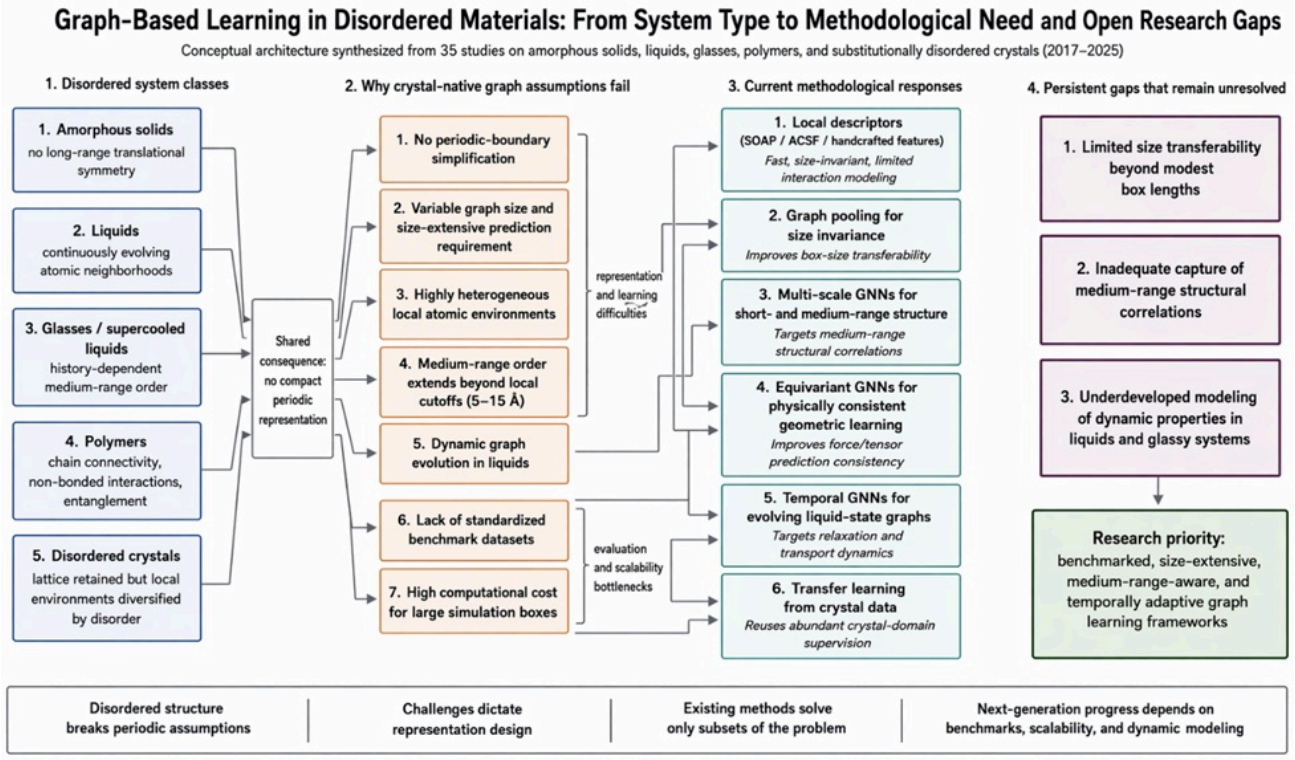

Figure 1. Hierarchical framework linking disorder classes, graph-learning challenges, methodological responses, and unresolved research gaps in disordered materials

The following sections provide a taxonomy of disordered systems, detail the seven core challenges, survey six families of current approaches, and summarize empirical findings together with critical gaps.

Taxonomy of Disordered Systems

Disordered systems can be systematically classified according to structural characteristics and dynamical behavior, yet their unifying difficulty lies in graph construction under conditions that depart fundamentally from crystalline periodicity. Amorphous solids exhibit non-crystalline configurations with pronounced short-range order but no translational symmetry, as seen in silica glass, metallic glasses, and amorphous silicon, and are typically simulated using large atomic ensembles (1 000–10 000 atoms) to suppress artificial periodicity effects; this introduces a representational challenge driven by scale and the absence of reusable motifs, limiting the applicability of unit-cell-based strategies common in crystal GNNs, though recent work has extended graph neural networks to property prediction and defect analysis in such regimes [1-3]. A related complication emerges in liquids, where continuous atomic diffusion eliminates static connectivity and renders the graph inherently time-dependent, as bonds form and break dynamically in systems ranging from molten metals and ionic liquids to molecular fluids such as water, thereby requiring architectures capable of tracking evolving adjacency structures rather than fixed snapshots [4-6]. Glasses, in contrast, occupy a kinetically arrested state of supercooled liquids and retain history-dependent short- and medium-range order shaped by thermal pathways, cooling rates, and composition, as exemplified by oxide and bulk metallic glasses; here, the central difficulty lies in encoding medium-range structural correlations extending over 5–15 Å that cannot be resolved through purely local neighborhoods [7-19]. Polymers further complicate representation by introducing long-chain molecular architectures with covalent backbones, entanglements, and cross-links, where systems such as polyethylene, polystyrene, and biopolymers require graph constructions that simultaneously preserve chain connectivity and capture non-bonded and topological effects governing macroscopic behavior, including glass-transition phenomena [9, 10, 20].

A distinct but conceptually related regime arises in disordered crystals, where an underlying periodic lattice persists but is disrupted by substitutional disorder, vacancies, or defects, as in high-entropy alloys and heavily doped semiconductors; although a nominal unit cell remains definable, the necessity of large supercells to represent stochastic occupation patterns generates a proliferation of inequivalent local environments, effectively eroding the computational advantages of crystallinity [21-23]. Across all categories, the absence of a compact unit cell and strict translational symmetry leads to intrinsically size-variant systems that demand size-extensive models capable of processing heterogeneous atomic environments without reliance on prototype averaging, thereby highlighting why methodologies effective in crystalline settings require substantial reformulation when extended to disordered matter.

Challenges for Graph-Based Learning

Graph-based learning in disordered systems is shaped by a set of tightly coupled challenges that fundamentally distinguish it from crystalline modeling, beginning with the loss of periodic boundary simplification. Whereas crystal GNNs compress structure through repeated unit-cell replication, disordered simulations must operate on large, explicitly non-periodic domains (1 000–100 000 atoms), where open boundaries are often required to avoid artificial correlations, leading to adjacency structures whose scaling rapidly becomes a computational bottleneck [1, 2]. A related consequence is the emergence of variable graph sizes, since atom counts fluctuate with composition and simulation volume, forcing models toward size-extensive formulations via invariant readouts, even though many existing architectures still retain implicit dependencies on system scale [7, 21, 24].

Beyond these representational issues, heterogeneous local environments further complicate learning, as symmetry no longer constrains atoms into a limited set of equivalence classes; instead, each atom may exhibit a distinct coordination landscape, thereby eliminating prototype-based averaging and necessitating fully atom-resolved message passing [2, 14, 17]. This shift is particularly consequential when structural information extends beyond local neighborhoods, since medium-range order governing glasses and liquids often spans 5–15 Å, exceeding conventional cutoff radii of 3–5 Å and thereby exposing a systematic blind spot in standard message-passing schemes [4, 13, 15, 19].

The difficulty intensifies in liquids, where atomic motion renders the graph inherently dynamic, with continuously evolving connectivity that invalidates static representations and requires explicit temporal modeling to recover transport and relaxation phenomena such as diffusion and viscosity [4-6, 25]. In parallel, methodological progress is constrained by the absence of standardized benchmarks, as current studies rely on heterogeneous molecular-dynamics protocols, force fields, and system sizes, in contrast to the unified infrastructure available in crystalline materials databases, which severely limits comparability across results [8, 11, 18, 26].

Finally, computational cost imposes a practical ceiling on model expressivity, since large non-periodic graphs combined with extended interaction ranges or multi-scale architectures quickly become intractable, restricting many implementations to systems below 1 000 atoms and raising concerns about their fidelity in capturing true disordered regimes [1, 22, 24]. These interdependent limitations collectively underpin a systematic performance gap, explaining why graph-based methods for disordered systems still lag behind their crystalline counterparts by several years in methodological maturity.

Current Approaches

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Across the 35 reviewed papers, six methodological families can be discerned, each reflecting a distinct way of reconciling structural complexity with predictive tractability in disordered systems. Local descriptors in non-graph settings rely on fixed-length representations such as SOAP or ACSF computed per atom and aggregated through summation, averaging, or histogramming to recover global properties; while computationally efficient, inherently size-invariant, and unexpectedly robust for static scalar observables in glasses, this abstraction inevitably suppresses explicit neighbour interactions and therefore limits applicability to force- or stress-level predictions [3, 8, 11, 12, 18, 27].

A different direction preserves structural connectivity by constructing cutoff-based graphs and enforcing size invariance through hierarchical or global pooling operations, where sum, mean, or attention-based mechanisms compress variable-sized representations into fixed-length embeddings; this design supports transfer across system sizes while retaining local structural fidelity [21, 24, 28].

Multi-scale graph neural architectures extend this idea by coupling short-range message passing, typically within 3–5 Å, with coarsened or expanded interaction ranges up to 5–15 Å and global attention, thereby capturing medium-range order at the cost of increased architectural and computational complexity [19, 22].

Equivariant graph neural networks instead embed E(3) symmetry directly into their layers, removing reliance on periodic assumptions and improving both data efficiency and physical consistency, particularly for force and tensor prediction in disordered regimes [2, 29].

When temporal structure becomes essential, recurrent or time-augmented message passing operates directly on trajectories, updating node and edge states as atomic motion evolves, which enables prediction of dynamical quantities such as diffusion coefficients and relaxation times [5, 6, 25].

Finally, transfer learning approaches leverage models pretrained on extensive crystalline datasets and adapt them to disordered trajectories through fine-tuning, exploiting transferable structural priors while confronting the intrinsic domain

shift between periodic and non-periodic environments [23, 30-32].

Despite their conceptual differences, each family addresses only a subset of the broader challenges, and no single formulation yet provides a unified resolution across all regimes.

Table 1 consolidates the field's central analytical pattern by showing that each methodological family addresses only a subset of the seven disorder-specific challenges, which helps explain why no current approach yet achieves comprehensive reliability across disordered materials tasks.

Table 1. Analytical alignment of disorder-specific challenges with current graph-learning strategy families

Core challenge in disordered materials	Why it is structurally important	Most relevant method family/families	What current studies have demonstrated	Remaining limitation
No periodic-boundary simplification	Removes the compact unit-cell representation that makes crystal graphs efficient	Graph pooling; multi-scale GNNs; equivariant GNNs	Non-periodic systems can be modeled directly, but only with careful graph design and rising computational cost	Most studies remain restricted to relatively small simulation boxes
Variable graph size	Atom count changes across box dimensions, compositions, and preparation conditions; global predictions must therefore be size-extensive	Graph pooling; local descriptors	Sum/mean/attention pooling improves transfer from smaller to larger boxes	Transfer across box shape, aspect ratio, and much larger length scales is still weakly tested
Heterogeneous local environments	Each atom may occupy a unique coordination environment, eliminating symmetry-based prototype averaging	Equivariant GNNs; local descriptors; transfer learning	Atom-specific learning improves defect detection and local-structure sensitivity	Robust generalization across compositionally diverse disorder remains uncertain
Medium-range order (5–15 Å)	Many glass and liquid properties depend on correlations beyond immediate neighbors	Multi-scale GNNs; equivariant GNNs; symbolic-regression hybrids	Larger cutoffs and hierarchical architectures improve prediction for structure-sensitive properties	No consensus exists on optimal structural range, representation, or computationally efficient implementation
Dynamic graph evolution in liquids	Bonding patterns and neighborhoods change over time, so static graphs are insufficient	Temporal GNNs	Early work shows promise for relaxation and trajectory-based classification	Dynamic-property prediction remains sparse, short-horizon, and not benchmarked systematically
Lack of benchmark datasets	Custom trajectories and simulation protocols prevent fair cross-study comparison	Transfer learning; benchmark-oriented dataset design	Some studies partially compensate with pre-training or carefully curated internal datasets	Field-wide reproducibility and objective model

				comparison remain limited
High computational cost	Larger graphs, longer cutoffs, and equivariant operations raise memory and training-time burdens sharply	Local descriptors; graph pooling; efficient multi-scale designs	Lower-cost baselines remain surprisingly competitive for static scalar properties	The best-performing graph models are often too expensive for realistic large-scale deployment

Empirical Findings and Gaps

Empirical evidence across the 35 studies indicates that graph-based learning has achieved notable gains in specific regimes while remaining constrained by structural and computational trade-offs. Local descriptor frameworks such as SOAP- and ACSF-based models consistently demonstrate strong performance for static properties, including density, elastic moduli, and glass-forming ability in oxide and metallic glasses, often matching or surpassing early graph neural network approaches at significantly reduced cost, yet their formulation inherently precludes access to force fields or dynamic observables [3, 8, 11, 12, 27]. In parallel, advances in graph pooling have enabled meaningful size extensivity, with models trained on systems of approximately 1 000 atoms generalizing to substantially larger configurations when supported by suitable readout functions, although robustness under variations in box geometry or aspect ratio remains largely unexplored [21, 26, 28]. Equivariant architectures further enhance predictive accuracy by encoding symmetry constraints more explicitly, but this improvement comes at a substantial computational penalty, with training and inference costs increasing by a factor of five to ten and thereby limiting scalability [2, 29].

Beyond these advances, several persistent limitations continue to shape the field's trajectory. Medium-range structural order remains only partially resolved, as conventional cutoff schemes around 5–6 Å fail to capture essential correlations, while extensions to 10–15 Å improve fidelity but introduce prohibitive memory and runtime costs, leaving the optimal representation for disordered systems unresolved [13, 15, 19]. Temporal modeling of liquids is similarly underdeveloped, with only a small subset of studies addressing dynamics and most relying on short trajectory windows, which constrains the reliable prediction of transport properties from evolving graph representations [5, 6, 25]. Compounding these issues is the absence of standardized benchmarks, as disparate simulation protocols across studies hinder direct comparability and slow collective methodological progress [8, 11, 33].

Relation to Crystal GNN Literature

Graph-based machine learning has reached maturity for crystalline materials by exploiting periodic boundary conditions and compact unit cells that keep graphs small and computationally tractable. The 35 studies reviewed here demonstrate that disordered systems demand a fundamentally different approach, even though they inherit core algorithmic building blocks from crystal literature. Crystal GNNs, as routinely applied to databases such as the Materials Project or the Open Quantum Materials Database, operate on graphs of 10–100 atoms where translational symmetry collapses infinite lattices into repeating motifs. Message passing therefore occurs within a fixed, symmetry-reduced neighborhood, enabling efficient training on energies, forces, and tensorial properties across thousands of compounds.

Three structural differences set disordered applications apart. First, the complete absence of a unit cell eliminates periodic boundary simplification; disordered simulation boxes of 1 000–10 000 atoms must be treated as fully non-periodic, causing adjacency matrices to scale directly with system size. Second, variable graph sizes require explicitly size-extensive readout layers, whereas crystal models train on fixed-size inputs whose invariance is implicitly guaranteed by periodicity. Third, heterogeneous local environments preclude prototype averaging; every atom in a glass or liquid

possesses a unique coordination shell, demanding truly atom-specific message passing instead of the symmetry-based reduction common in crystals.

Nevertheless, several components transfer productively. Equivariant architectures originally developed for crystals to enforce E(3) symmetry without relying on periodic images have been successfully adapted for force and stress prediction in amorphous solids. Message-passing frameworks and attention mechanisms, refined in crystal supercell studies to capture longer-range interactions, supply ready templates for addressing medium-range order in glasses. Pre-training strategies that leverage abundant crystal data have also been explored as a route to initialize disordered models when labeled trajectories remain scarce [34].

What must be substantially rethought, however, is the graph-construction pipeline. Crystal models define edges via periodic images; disordered systems require careful choice of cutoffs without such guidance, risking either loss of medium-range correlations or prohibitive computational cost. Pooling strategies must be redesigned for genuine size invariance rather than the implicit invariance provided by unit-cell replication. Cutoff selection itself must be expanded beyond the 3–5 Å local neighborhoods typical of crystals to explicitly target the 5–15 Å medium-range regime that governs macroscopic properties of glasses and liquids.

The reviewed literature illustrates this borrowing-and-rethinking dynamic clearly. Early local-descriptor methods echo pre-GNN crystal fingerprints such as SOAP, while recent multi-scale and temporal GNNs represent genuine extensions that move beyond crystal-native assumptions. A more systematic bridge between the two literatures—through shared codebases, pre-trained crystal checkpoints, and hybrid crystal-disordered benchmarks—would accelerate convergence. Without deliberate adaptation, crystal-derived architectures risk inheriting hidden assumptions that fail silently when confronted with the intrinsic variability of disordered materials. The field therefore stands at a productive inflection point: the algorithmic maturity of crystal GNNs can be leveraged, but only if the representational foundations are re-engineered for the absence of periodicity that defines real-world technological materials.

Recommendations for Future Research

To move graph-based learning for disordered systems from promising prototypes toward reliable engineering tools, it is essential to confront the fragmentation that currently arises from inconsistent molecular-dynamics generation protocols, including variations in interatomic potentials, cooling schedules, and simulation cell sizes across studies. A foundational step involves the establishment of a shared benchmark infrastructure for canonical disordered systems such as amorphous silica, representative metallic glasses, water, and selected ionic liquids, where fixed train–test partitions are explicitly stratified by composition, cooling history, and system size. Positioned in analogy to crystal-oriented resources like the Materials Project, such a framework would enable rigorous comparability while accelerating iterative methodological refinement. In parallel, the question of size transferability must be treated as a central validity criterion rather than a secondary evaluation choice, given that most existing models are trained on sub-1000-atom configurations yet are implicitly expected to generalize to far larger regimes. A more disciplined protocol would involve training exclusively on small-scale systems while systematically evaluating extrapolation to realistic simulation sizes in the range of several thousand to tens of thousands of atoms, with explicit reporting of both predictive accuracy and computational scaling as a function of atom count N, thereby directly testing size-extensivity assumptions under controlled conditions.

Beyond these structural concerns, the predictive fidelity of disordered-system models is strongly constrained by their limited ability to represent medium-range order, which governs many macroscopic properties in glasses and liquids. Addressing this limitation requires architectural designs that integrate short-range message passing with hierarchical or sparsified long-range interactions, potentially through coarsened graph representations or kernel-based approximations, while maintaining computational behavior that remains close to linear scaling with respect to interaction range. In practice, this necessitates balancing expressivity against efficiency so that correlations extending over 5–15 Å are captured without incurring prohibitive memory or time costs. A related and still underexplored dimension concerns temporal learning in dynamical regimes, where properties such as diffusion, viscosity, and relaxation remain poorly characterized by current

graph-based approaches; progress here depends on the availability of standardized trajectory datasets spanning extended timescales and on evaluation protocols that directly benchmark learned graph dynamics against molecular-dynamics references, particularly in regimes involving continuous bond rearrangement. Complementing this dynamic perspective, transfer learning from crystalline materials offers a potentially powerful pathway for mitigating data scarcity in disordered systems, although its effectiveness depends on systematically quantifying domain shift and identifying which structural representations retain predictive relevance when transitioning from ordered to disordered regimes.

Open Questions

Despite the substantial progress synthesized across the 35 reviewed studies, several structural and conceptual uncertainties continue to constrain the maturation of graph-based learning for disordered materials, particularly at the level of representation design and transferability. A central issue concerns how disordered systems should be encoded as graphs, since key choices such as cutoff radii, edge-weight formulations, and the treatment of residual periodicity remain largely heuristic; resolving this requires systematic cross-class evaluations of distance-driven, coordination-informed, and learned edge constructions to clarify how expressive power can be maintained without incurring unnecessary computational overhead. A closely related concern lies in determining how much medium-range structural information is genuinely necessary for reliable prediction, given that correlations on the order of 5–15 Å are known to influence properties such as glass formation and mechanical response, yet their precise role varies across targets; controlled ablation studies that progressively remove structural context are therefore essential for identifying property-specific representational thresholds governing elasticity, density, relaxation dynamics, and defect behavior.

This question of representation sufficiency naturally extends to the computational feasibility of physically constrained architectures, where equivariant graph neural networks, despite their strong adherence to symmetry principles, remain significantly more expensive than their non-equivariant counterparts, particularly when scaled toward systems approaching 100 000 atoms. Progress in this direction hinges on the development of sparse or low-rank equivariant formulations that preserve rotational and translational consistency while approaching linear scaling in system size, thereby addressing a key barrier to practical deployment. In parallel, an unresolved empirical tension persists between graph-based approaches and local descriptor methods in the context of dynamical properties: although local descriptors retain strong performance for static observables, their inability to encode force evolution and temporal correlations suggests a potential advantage for graph-based dynamical models once their temporal expressivity is fully realized, a hypothesis that can only be validated through standardized head-to-head benchmarking on time-resolved datasets. A further dimension of uncertainty emerges from the limited understanding of cross-system generalization, since current studies tend to treat amorphous oxides, metallic glasses, polymers, and liquids as isolated domains; systematic transfer experiments across these classes are therefore necessary to determine whether shared structural motifs exist or whether disordered matter inherently demands system-specific representations.

Implications for Practice

The synthesis of the studies carries immediate practical guidance for three stakeholder groups: practitioners who deploy models in materials design workflows, model developers who build the next generation of architectures, and benchmark designers who shape community standards.

Table 2 translates the review's synthesis into a practical method-selection framework by linking modeling goals to structural regime, data availability, and computational constraint, thereby clarifying when simpler descriptor models remain appropriate and when more advanced graph architectures become necessary.

Table 2. Method-selection framework for graph-based learning in disordered materials by target property, structural regime, and practical deployment constraint

Modeling objective	Structural regime / data condition	Recommended primary approach	Recommended secondary approach	Why this choice is justified	Main caution before deployment
Static scalar property prediction (e.g., density, elastic modulus, glass-forming ability)	Large amorphous or glassy systems with limited compute	Local descriptors	Graph pooling model as validation baseline	Descriptor models are efficient, inherently size-invariant, and empirically competitive for static targets	Good scalar accuracy does not imply suitability for forces, stresses, or dynamic behavior
Global property prediction with anticipated variation in box size	Amorphous solids, disordered crystals, fibrous or architected disorder	Graph pooling for size invariance	Local descriptors for baseline comparison	Pooling is the clearest route to explicit size-extensive prediction	Must test transfer across atom count and geometry, not only within one box family
Prediction of force, stress, or tensorial response	Structurally heterogeneous non-crystalline solids	Equivariant GNNs	Multi-scale GNNs	Physical symmetry handling improves geometric fidelity and tensor prediction	Computational overhead may make realistic large systems impractical
Properties governed by medium-range structure	Glasses, supercooled liquids, disorder-sensitive mechanical response	Multi-scale GNNs	Equivariant GNNs or symbolic-regression hybrid models	These methods are best aligned with 5–15 Å structural dependence	Higher cutoff or hierarchical modeling can become memory- and time-intensive
Dynamic-property prediction (diffusion, relaxation, transport)	Liquids and evolving glassy systems with trajectory data	Temporal GNNs	Static-structure baseline or sequence-aware descriptor model	Time-aware graph evolution is necessary when adjacency changes continuously	Existing studies are few, often short-trajectory, and lack common benchmarks
Data-scarce disordered application	Small labeled dataset, but related crystal data exist	Transfer learning from crystal data	Fine-tuning with pooling or equivariant layers	Pre-training may improve initialization and sample efficiency	Domain shift from periodic to non-periodic structure may limit transfer quality

Benchmark design or community comparison study	Cross-system evaluation across materials classes and task types	Multi-baseline benchmarking including descriptors + pooling + equivariant + temporal models	Standardized crystal-pretraining control arm	A fair benchmark must compare simple and advanced models under the same splits and scaling criteria	Without common splits and reporting rules, apparent gains remain difficult to interpret

For practitioners, the empirical findings suggest a pragmatic decision tree. For static scalar properties of large systems—density, elastic moduli, or glass-forming ability—local descriptors such as SOAP or ACSF often remain the most efficient and accurate choice, especially when computational budgets are tight. When forces, stresses, or dynamic quantities are required, graph-based methods become essential, but only after explicit validation of size convergence. Production runs should therefore incorporate a size-transferability check: train on modest boxes, confirm generalization to target sizes, and report scaling behavior before trusting predictions in device-scale simulations.

For model developers, the central priority is size-extensivity. Architectures must demonstrate O(N) or better scaling with atom count and include readout layers that are provably invariant to system size. Developers should routinely test transfer across box dimensions and aspect ratios, report computational cost per atom, and prioritize multi-scale or hierarchical designs that capture medium-range order without sacrificing efficiency. Equivariant layers should be adopted where tensorial properties matter, but only after confirming that the added cost does not preclude realistic system sizes.

For benchmark designers, the absence of standardized datasets is the single largest barrier to progress. Future benchmarks must include multiple system sizes, diverse preparation histories, and both static and dynamic targets. Evaluation protocols should mandate size-transferability tests, computational-cost reporting, and head-to-head comparisons against local-descriptor baselines. Open release of trajectories, code, and trained models will accelerate adoption and ensure that advances are reproducible across research groups and industrial labs.

Taken together, these implications shift the field from exploratory studies toward engineering-grade reliability. Practitioners gain clear heuristics for method selection, developers receive concrete design constraints, and the community obtains a roadmap for infrastructure that mirrors the success of crystal GNN benchmarks. Implementing these guidelines will determine whether graph-based learning fulfills its promise for the disordered materials that dominate everyday technology.

Conclusion

Graph-based learning for disordered systems has emerged as a vibrant frontier in computational materials science. The peer-reviewed publications demonstrate both substantial progress and the unique obstacles posed by non-crystalline matter. Five distinct classes of disordered systems—amorphous solids, liquids, glasses (including supercooled liquids), polymers, and crystals with substitutional disorder—each impose distinct graph-construction burdens that invalidate assumptions optimized for periodic crystals. Seven interlocking challenges—no periodic boundary simplification, variable graph size, heterogeneous local environments, medium-range order, dynamic graphs in liquids, lack of standardized benchmarks, and prohibitive computational cost—explain why performance still lags behind crystalline counterparts.

Six methodological families have arisen to address these challenges: local descriptors, graph pooling for size invariance, multi-scale GNNs, equivariant architectures, temporal GNNs, and transfer learning from crystal data. Empirical results show encouraging successes for static properties, practical size transfer via pooling, and improved physical consistency through equivariance. Yet persistent gaps remain: benchmarks are absent, size transferability is largely untested beyond modest scales, medium-range order is only partially captured, temporal methods for liquids are nascent, and efficiency bottlenecks limit practical system sizes.

The field now stands at an inflection point. Continued innovation in graph representations, coupled with community-wide adoption of standardized benchmarks and size-extensible architectures, will determine whether graph-based methods can achieve the same reliability and scalability already demonstrated for crystals. The disordered materials that underpin modern technologies—smartphone screens, battery electrolytes, optical fibers, and structural alloys—await predictive models that can handle their intrinsic variability. By focusing on the open problems and recommendations outlined here, the materials-informatics community can unlock the full potential of graph neural networks for the non-crystalline world.

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