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Theoretical Foundations of Geometric Deep Learning for Amorphous Structures: Beyond the Periodicity Assumption

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Abstract

Geometric deep learning has advanced computational materials science, yet most existing approaches remain constrained by the periodicity assumption inherent to crystalline systems. While crystal-based graph neural networks exploit translational symmetry and periodic boundary conditions, amorphous materials—such as glasses, liquids, polymers, and disordered alloys—lack long-range order, exhibit non-repetitive atomic arrangements, and span widely varying system sizes. This mismatch renders periodicity-dependent methods both theoretically inadequate and practically unreliable for disordered structures. This work identifies three key distinctions—non-periodic graph construction, symmetry limited to $E(3)$ equivariance, and non-physical boundary conditions—which collectively give rise to fundamental challenges, including scaling limitations, loss of transferability, and structural representation imbalances. Through theoretical analysis, the limitations of crystal-oriented graph neural networks in amorphous settings are clarified. To address these issues, a new framework is proposed based on size-extensive, $E(3)$ -equivariant architectures that eliminate periodic assumptions and integrate multi-scale encoding of local, intermediate, and global structure with size-normalized aggregation. This formulation provides a principled foundation for geometric deep learning models tailored to amorphous materials and their applications in energy, optics, and structural systems.

Keywords Graph neural networks, $E(3)$ equivariance, Geometric deep learning, Amorphous materials, Periodicity assumption, Disordered systems

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Introduction

Geometric deep learning for materials has focused almost exclusively on crystals [1–4]. This is not surprising: crystals have periodicity, which provides symmetry, finite unit cells, and well-defined graphs. But many important materials are amorphous: glasses, liquids, polymers, disordered alloys. For these, the periodicity assumption fails completely. There is no unit cell. No translational symmetry. Graph size varies. This paper provides a theoretical analysis of geometric deep learning for amorphous structures, identifying where periodicity-based methods break and proposing foundations for amorphous-specific architectures.

The success of crystal-oriented graph neural networks stems from their ability to encode the lattice as an intrinsic part of the graph representation [1, 4, 5]. Periodic boundary conditions allow every atom to be treated as having an identical local environment up to lattice translation, enabling efficient message passing and exact symmetry enforcement. In contrast, amorphous systems are generated from large simulation boxes whose boundaries are artificial constructs rather than physical realities [6, 7]. The resulting graphs are large, irregular, and lack any repeating motif. Recent applications of

graph neural networks to glassy states and metallic glasses have already begun to expose these limitations in practice [8–15], yet a systematic theoretical treatment remains absent.

Theoretically, the periodicity assumption is not merely a computational convenience; it is a foundational axiom that collapses without a repeating lattice. Removing it forces a re-examination of every stage of the geometric deep learning pipeline: how graphs are constructed, how symmetries are enforced, how information propagates, and how predictions remain consistent as system size changes. This paper conducts that re-examination. It begins by formalizing the periodicity assumption and cataloguing its enabling consequences for crystal GNNs. It then contrasts crystalline and amorphous structures across five fundamental differences. Next, it articulates six theoretical challenges that arise when periodicity is absent. Finally, it proposes a cohesive theoretical framework built on size-extensivity and $E(3)$ equivariance alone.

Throughout the analysis, the discussion remains strictly conceptual—no datasets, no performance metrics, no simulation results. The goal is to supply the missing theoretical scaffolding for future amorphous geometric deep learning models that are provably robust to the absence of periodicity. By grounding the discussion in the existing literature on both crystal and disordered systems [1, 3, 5, 6, 11, 12, 14, 16, 17], the paper demonstrates that the transition from periodic to non-periodic domains is not incremental but requires entirely new design principles. The framework introduced here offers those principles, positioning amorphous materials as a distinct theoretical domain within geometric deep learning rather than a marginal extension of crystal methods.

The Periodicity Assumption in Crystal GNNs

Periodicity assumption — The assumption that the material has a repeating unit cell, enabling finite graph representation with periodic boundary conditions.

What periodicity enables in crystal GNNs is a compact, symmetric, and computationally tractable graph structure. First, it guarantees finite graph size. Because the unit cell typically contains fewer than 100 atoms, the entire periodic crystal can be represented by replicating that small motif indefinitely [1, 3, 4]. Message passing therefore operates on a bounded neighborhood whose size is independent of the macroscopic sample. Second, translational symmetry emerges automatically: translating any atom by a lattice vector maps it onto an equivalent environment, allowing the model to enforce exact equivariance under the crystal's space group [5]. This symmetry supports data augmentation strategies that rotate or reflect the unit cell while preserving physical equivalence.

Third, neighbor lists become well-defined and reproducible. Periodic images of atoms outside the unit cell are folded back in, ensuring every atom possesses the same coordination shell regardless of its position within the cell [1]. Fourth, the graph structure itself is consistent across chemically identical materials, enabling transfer learning and batching of multiple crystals in a single training pass. Crystal GNNs therefore rely on space group symmetries for data augmentation, small unit cells for computational efficiency, fixed graph size for stable batching, and periodic boundary conditions for neighbor finding [3, 5].

Collectively, these features rest on the hidden assumption that all materials are periodic. For amorphous structures, this assumption is false. The literature already documents attempts to apply crystal-trained models directly to glasses, where the lack of a repeatable motif leads to inconsistent neighbor definitions and unstable message-passing dynamics [6, 7, 11–14]. Theoretically, once periodicity is removed, every benefit listed above collapses: graph size becomes variable and large, translational symmetry disappears, neighbor lists acquire artificial cutoffs at box boundaries, and batching must contend with heterogeneous graph dimensions. The periodicity assumption is therefore not a minor implementation detail but the theoretical cornerstone that permits crystal GNNs to achieve both efficiency and formal guarantees. Its absence demands a complete reformulation of the geometric deep learning paradigm.

Why Amorphous Structures are Different

Amorphous structures diverge from crystalline order in ways that each erode a foundational assumption of periodicity-based geometric deep learning. The absence of a unit cell means that, unlike crystals—which are compactly encoded by 10–100 atoms within a repeating lattice—amorphous materials demand simulation boxes of 1000–100 000 atoms to capture statistically representative disorder [6-8, 10-12, 14], rendering graph sizes both variable and prohibitively large while nullifying the unit-cell reduction that sustains tractable crystal representations. This structural openness further dissolves translational symmetry: where lattice translations in crystals guarantee identical local environments, arbitrary shifts in amorphous systems yield distinct neighborhoods [9, 15, 19], invalidating symmetry-driven augmentations and preventing models from equating translated subgraphs with equivalent physics.

A related implication arises with periodic boundary conditions, which in crystals faithfully reflect an infinite lattice yet serve merely as an artificial device in amorphous simulations to suppress surface artifacts [13, 18]; consequently, boundary atoms suffer truncated neighbor shells that inject non-physical artifacts absent in genuine disordered matter. This local heterogeneity compounds when each atom of a given species can exhibit a unique coordination environment, unconstrained by the symmetry-enforced uniformity typical of crystals and requiring models to accommodate high diversity without defaulting to overly generic embeddings [6, 7, 20].

Ultimately, the lack of any primitive repeating unit—whose properties would replicate across the system—forces macroscopic behavior in amorphous materials to emerge only at the full-box scale [19, 21], demanding architectures that are strictly size-extensive and scale correctly with system size N rather than presupposing a fixed or minimal N .

Table 1 systematically decomposes the periodicity assumption into its functional components and shows how each collapses into distinct theoretical failure modes in amorphous systems.

Table 1. Structural Breakdown of Periodicity-Dependent Assumptions and Their Theoretical Failure Modes in Amorphous Systems

Periodicity-Dependent Assumption	Functional Role in Crystal GNNs	Structural Violation in Amorphous Systems	Resulting Theoretical Failure Mode	Implication for Model Design
Finite unit cell representation	Enables compact graphs and bounded computation	No repeating motif; graphs scale to 10^3 – 10^5 atoms	Loss of computational tractability assumptions	Architectures must scale $O(N)$ with explicit size-extensivity
Translational symmetry (lattice equivariance)	Guarantees identical local environments under translation	Translation alters local structure arbitrarily	Invalid symmetry-based generalization	Restrict symmetry to $E(3)$ equivariance only
Periodic boundary conditions	Ensures complete neighbor shells and consistent coordination	Boundaries are artificial truncations	Incomplete neighborhoods near edges	Introduce boundary-aware graph construction (padding/mirroring)
Fixed graph size	Enables batching and transfer learning across crystals	Graph size varies across samples	Instability in training and inference scaling	Use size-normalized representations and flexible batching
Symmetry-based data augmentation	Expands dataset via rotations/translations	No symmetry equivalence across	Data augmentation invalid or	Replace with stochastic or physics-informed

		configurations	misleading	augmentation
Primitive representation (unit cell)	Provides minimal sufficient representation	No minimal representation exists	Property emergence depends on full system	Require global encoding and aggregation mechanism

These five differences are not merely quantitative; they are qualitative shifts in the mathematical structure of the data. Graph size, symmetry group, boundary semantics, local variability, and scaling behavior all change simultaneously. Literature on glass-forming liquids and metallic glasses consistently reports that crystal-derived GNNs encounter precisely these obstacles when forced to operate outside their native periodic domain [8-10, 13, 15, 17, 23]. The theoretical task is therefore not to patch existing architectures but to rebuild the geometric deep learning pipeline from axioms that do not presuppose periodicity.

Theoretical Challenges for Amorphous Geometric Deep Learning

The absence of periodicity generates six interlocking theoretical challenges.

Graph construction in amorphous systems immediately exposes a critical limitation of periodicity-dependent pipelines. While crystal graphs exploit cutoff radii augmented by periodic images to ensure complete neighborhoods, amorphous graphs rely on cutoff radii alone; yet the finite simulation box inevitably truncates neighbor shells for edge atoms [13, 18, 20], violating the core premise that every node carries a fully realized local descriptor.

This local incompleteness reverberates into symmetry considerations. Crystal GNNs routinely harness both E(3) equivariance and periodic translational equivariance, yet amorphous configurations retain only E(3) symmetry [3, 16, 24]. Whether pure E(3) equivariance proves theoretically sufficient, or whether supplementary global invariances—such as invariance under arbitrary rotations of the entire disordered box—must be explicitly imposed, remains an open question for maintaining consistency with the underlying physics.

Beyond symmetry, scalability emerges as a pressing mechanistic concern. Message-passing on crystal unit cells operates at $O(N)$ cost with small fixed N , whereas amorphous systems impose $O(N)$ scaling where N now spans 10^3 – 10^5 atoms [6, 7, 11, 12, 14]; without deliberate redesign toward strictly linear or near-linear complexity on large irregular graphs, standard layers quickly become computationally prohibitive.

A related theoretical demand surfaces in transferability across system sizes. Models trained on 1000-atom boxes frequently fail when applied to 10 000-atom configurations, as finite-size effects reshape the statistics of medium-range correlations [19, 21]; establishing explicit conditions for convergence in the thermodynamic limit thus becomes essential for reliable size transferability.

Finally, the absence of long-range crystalline order shifts the balance between local and global information. In crystals, local descriptors often suffice precisely because periodicity propagates order; in amorphous matter, however, properties such as connectivity or percolation hinge on global topology [8, 15, 17, 23, 25], compelling architectures whose receptive fields remain tunable rather than rigidly dictated by periodic structure. This same distinction renders periodic boundaries themselves problematic: physical in crystals yet merely computational in amorphous simulations, they necessitate models capable of distinguishing genuine physical boundaries—particularly at free surfaces or interfaces—from artificial ones, without recourse to periodic folding [18, 20].

Table 2 establishes a direct correspondence between the six theoretical challenges of amorphous geometric deep learning and the architectural mechanisms required to resolve them.

Table 2. Mapping Between Theoretical Challenges and Required Architectural Mechanisms in Amorphous Geometric Deep Learning

Theoretical Challenge	Underlying Cause	Failure Risk if Unaddressed	Required Architectural Mechanism	Associated Framework Component
Graph construction artifacts	Boundary truncation without periodic images	Incomplete local descriptors and inconsistent neighborhoods	Smooth cutoff functions + boundary mitigation (padding/mirroring)	Input Graph Design
Reduced symmetry (loss of lattice equivariance)	Absence of translational invariance	Incorrect invariance assumptions and poor generalization	Strict E(3)-equivariant message passing	Local Encoder (A)
Scalability with large N	Graph size grows to 10 ³ –10 ⁵ atoms	Computational infeasibility	Linear or near-linear scaling message passing and pooling	Local + Medium Encoder (A+B)
Size transferability	Finite-size effects alter distributions	Model predictions diverge across system sizes	Size-extensive normalization and invariant aggregation	Aggregator (D)
Local–global information imbalance	Lack of long-range order	Missing global topology or over-localized predictions	Multi-scale decomposition with hierarchical propagation	Medium Encoder (B)
Global property dependence	Emergent system-wide behavior	Failure to capture connectivity/percolation	Attention-based full-graph readout	Global Encoder (C)
Boundary condition ambiguity	Artificial vs physical boundaries indistinguishable	Non-physical predictions at edges	Explicit boundary encoding or masking	Input + Global Components

Each challenge is interdependent. For example, poor graph construction exacerbates symmetry violations, which in turn undermine scalability guarantees. Solving any single challenge in isolation is insufficient; the framework must address all six simultaneously while preserving formal properties of invariance and extensivity. Existing literature on disordered systems already illustrates these failures in practice [6-9, 11-14, 19], confirming that theoretical reformulation is both necessary and urgent.

A Theoretical Framework for Amorphous Geometric Deep Learning

Graph construction for amorphous systems begins with a cutoff radius applied without periodic images, accompanied by deliberate boundary handling—through mirroring or smooth padding—and edge weights that decay continuously to zero at the cutoff, thereby eliminating spurious discontinuities in the local descriptor [18, 20]. This foundation directly informs the symmetry requirements: the minimal invariance is E(3) equivariance under rotations, translations, and reflections, augmented by permutation invariance over identical atomic species, while periodic translational invariance loses all relevance in the absence of long-range order [3, 16, 24].

A related theoretical necessity is size extensivity. A model satisfies this condition when computational cost scales as $O(N)$ or $O(N \log N)$, finite-size effects decay such that predictions converge with increasing system size, and representations learned on smaller configurations transfer reliably to larger ones [21, 26].

Beyond these constraints lies the challenge of local-global decomposition. Amorphous properties naturally separate into short-range contributions governed by the cutoff radius, medium-range effects extending to 5–15 Å, and global topological features—such as connectivity or percolation—that span the entire system; different properties thus demand distinct interaction ranges, necessitating architectures with tunable receptive fields rather than periodicity-imposed fixed horizons [8, 15, 17, 23].

The proposed framework integrates four interlocking components to address these intertwined demands. A local encoder performs conventional message passing within the short-range cutoff, yielding $E(3)$ -equivariant node embeddings. This feeds into a medium-range encoder that leverages hierarchical graph coarsening or multi-scale pooling to propagate information efficiently up to 15 Å without quadratic cost explosion. A global encoder then applies attention-based readout across the full graph to extract system-wide topological signatures. Finally, a size-extensive aggregator normalizes each contribution independently of N , guaranteeing consistent predictions across varying box sizes and thereby closing the loop on theoretical consistency for disordered matter.

Figure 1 illustrates the hierarchical architectural reformulation required for geometric deep learning in amorphous systems, showing how the removal of periodicity propagates into theoretical challenges that are resolved through a size-extensive, multi-scale encoder–aggregator framework.

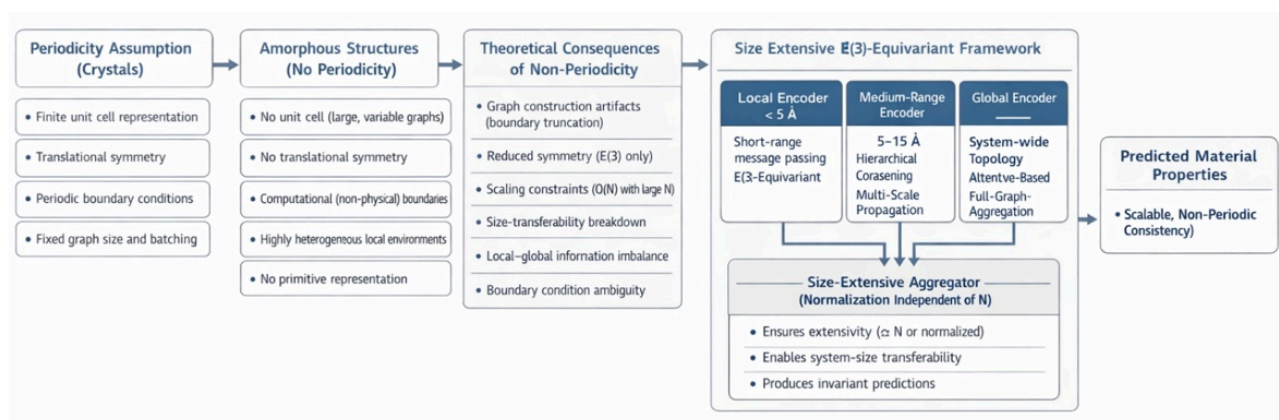


Figure 1. Hierarchical Size-Extensive Architecture for Amorphous Geometric Deep Learning Without Periodicity Assumptions

This framework removes every periodicity-dependent element while retaining the core strengths of geometric deep learning. It is therefore both theoretically sound and practically realizable using only the tools already present in the literature on equivariant networks and disordered materials [3, 5–7, 11, 12, 14–16, 24]. Future architectures built on these propositions will be provably robust to the absence of periodicity and will open the door to reliable geometric deep learning for the vast class of amorphous structures.

Implications for Model Architecture

The theoretical framework developed in Section 5 carries direct implications for how amorphous-specific geometric deep learning architectures should be designed. The key is to match the receptive field of the model to the physical range over which the target property is determined, while preserving size extensivity and $E(3)$ equivariance at every stage [3, 16, 24].

For local property prediction such as atomic forces or local stress tensors, only the local encoder (Component A) is required. Message passing is confined to a short-range cutoff that exceeds the correlation length characteristic of the particular amorphous material [6, 7, 13, 26]. Because the prediction at each node depends solely on its immediate neighborhood, size-extensivity is satisfied automatically: the per-atom contribution remains independent of total system size, and the overall property scales linearly with N . No medium-range or global components are necessary, keeping computational cost strictly $O(N)$.

For medium-range properties such as medium-range order parameters or ring statistics in glasses, the architecture must incorporate Component B, the medium-range encoder. Hierarchical graph coarsening or multi-scale message passing propagates information outward in successive layers, each operating on a coarsened graph whose nodes represent clusters of 5–15 Å [8, 10, 15, 17, 23, 25]. This controlled expansion of the receptive field captures the longer but still finite correlations typical of disordered systems without requiring full-graph operations. The coarsening step also maintains linear scaling because the number of super-nodes decreases geometrically with each level.

For global properties such as glass transition temperature, ionic conductivity, or percolation thresholds, the global encoder (Component C) becomes essential. An attention-based readout aggregates information across the entire graph, allowing the model to detect system-wide topological features that cannot be inferred from local neighborhoods alone [9, 19, 21]. To preserve size extensivity, Component D normalizes the global contribution by system size (or by a size-independent structural descriptor such as average coordination number), ensuring that predictions converge rather than diverge as N grows [6, 7].

The recommended design workflow is therefore incremental: begin with a local-only model and validate its adequacy for the target property; introduce the medium-range encoder only when local information proves insufficient; add the global encoder solely when system-wide statistics are demonstrably required. This staged approach avoids unnecessary complexity while guaranteeing that every added component respects the propositions of $E(3)$ equivariance and size extensivity [2, 3, 5]. Architectures built this way remain theoretically robust precisely because they contain no hidden periodicity assumptions.

Relation to Existing Work

The framework stands in clear relation to prior geometric deep learning literature while exposing the limitations imposed by the periodicity assumption. Crystal GNNs such as those reviewed by Reiser *et al.* and Duval *et al.* achieve elegance and efficiency precisely because they embed periodic boundary conditions and lattice translations into the graph construction and symmetry group [1–4]. The present framework removes those elements entirely, demonstrating that crystal methods cannot be transplanted unchanged to amorphous graphs without violating size extensivity and introducing boundary artifacts [6, 7, 13].

Molecular GNNs, including equivariant architectures such as those underlying Musaelian *et al.* and the broader class of message-passing networks, provide a closer starting point [2, 3, 16, 24]. Molecules are finite and non-periodic, much like amorphous simulation boxes. However, molecular systems are small (tens of atoms), whereas amorphous systems routinely exceed 10 000 atoms. The framework therefore extends molecular ideas by adding explicit medium-range coarsening and size-normalizing aggregation, components unnecessary for small molecules but indispensable for large disordered structures [5].

Equivariance theory remains central: $E(3)$ equivariance is retained as the minimal symmetry requirement, exactly as in state-of-the-art crystal and molecular models, yet periodic translation equivariance is discarded because it has no physical meaning in aperiodic systems [3, 16, 24]. The over-smoothing problem, well documented in large graphs, becomes more acute in amorphous settings where graph diameter is larger and long-range order is absent [1, 8, 15]. The hierarchical coarsening in Component B and the skip connections implicit in the local-global decomposition supply a theoretical countermeasure that keeps the architecture shallow while still reaching global scales.

Collectively, the proposed framework is not a rejection of existing work but a principled generalization. It preserves the theoretical guarantees of invariance and locality that have driven progress in crystalline and molecular domains, while replacing periodicity-dependent machinery with constructs that are provably valid for disordered materials [6, 7, 17, 19, 21]. This positions amorphous geometric deep learning as a distinct subfield that builds directly on, yet substantially extends, the foundations laid in the cited literature.

Open Questions and Future Directions

Although the framework provides a coherent theoretical foundation for geometric deep learning on amorphous materials, several foundational questions must be resolved before this emerging paradigm attains the maturity of its crystalline counterpart. Central among them is the optimal construction of amorphous graphs: the principled selection of cutoff radius, the functional form of edge-weight decay, and the rigorous treatment of box-boundary atoms—whether through mirroring or padding—remain to be derived from first principles rather than heuristic tuning [13, 18, 20].

This uncertainty in local representation directly compounds the challenge of designing provably size-extensive GNNs. While the framework articulates necessary conditions encompassing $O(N)$ or $O(N \log N)$ scaling, the decay of finite-size effects, and cross-scale transferability, rigorous mathematical guarantees of convergence in the thermodynamic limit for irregular graphs are still absent and will demand novel analytical tools tailored to disordered topologies [21, 26].

A related implication concerns the role of medium-range order. Determining how much information beyond the short-range cutoff is required for different properties—whether a universal length scale exists or whether the necessary range is material- and observable-specific—would enable systematic pruning of model components and ensure minimal yet sufficient complexity [8, 10, 15, 17, 23].

Beyond these scaling considerations lies the practical question of transferability: whether models trained on small amorphous boxes of approximately 1000 atoms can reliably generalize to configurations nearing 100 000 atoms, a capability that the framework positions as definitional for true size extensivity yet whose enabling training regimes and regularization strategies remain unknown [6, 7, 9, 11, 12, 14].

Finally, when simulation boxes incorporate genuinely non-periodic boundaries, as in the modeling of free surfaces and interfaces, the boundary itself acquires physical significance; new theoretical mechanisms are therefore required to allow models to distinguish meaningful physical surfaces from purely computational artifacts without reverting to periodic folding [18, 20].

Addressing these interlocking challenges will necessitate sustained theoretical effort that weaves together scaling arguments, symmetry analysis, and fresh concepts drawn from the statistical mechanics of disordered systems. Progress on any single front promises to accelerate resolution of the others, ultimately yielding architectures that are not only conceptually robust but practically dominant across the vast landscape of amorphous materials [1-3, 5, 15].

Implications for Practice

The theoretical analysis translates into concrete guidance for three stakeholder groups.

For model developers the message is unambiguous: never assume periodicity when targeting amorphous structures. Replace periodic image handling with explicit boundary mitigation, enforce $E(3)$ equivariance without lattice augmentations, and embed size-extensivity constraints into every layer and readout [2, 3, 16, 24]. Validation must include explicit tests of transferability across system sizes; any model that diverges with increasing N fails the foundational requirements of the framework [19, 21, 26].

For practitioners applying geometric deep learning to glasses, liquids, or polymers the workflow is staged. Local properties can be addressed with lightweight local encoders alone, provided the cutoff exceeds the relevant correlation length [6, 7, 10–14]. Medium-range structural descriptors require the addition of hierarchical pooling, while global material characteristics demand the full local-medium-global cascade with size-normalized aggregation [8, 15, 17, 23]. In all cases, convergence with system size must be verified before the model is trusted for production use.

For benchmark designers the responsibility is to create amorphous-specific evaluation suites that expose periodicity-induced failures. Benchmarks must vary simulation-box size systematically, include both periodic and non-periodic boundary conditions, and report scaling behavior with N rather than single-point accuracy [9, 18, 20]. Only such rigorous testing will drive the community toward architectures that are genuinely robust to the absence of long-range order.

Adopting these practices will accelerate the shift from crystal-centric tools to a new generation of amorphous-capable models, ensuring that geometric deep learning can address the disordered materials that constitute the majority of functional substances in energy, optics, and structural applications [4, 27–29].

Conclusion

The periodicity assumption in crystal GNNs fails for amorphous structures. Three fundamental differences—no unit cell, no translational symmetry, variable graph size—render periodicity-based methods theoretically inadequate. Six theoretical challenges—graph construction, symmetry, scalability, transferability, local-global balance, boundary conditions—arise directly from the removal of periodicity and must be confronted simultaneously. The proposed framework supplies the necessary foundations through four components: local encoder, medium-range encoder, global encoder, and size-extensive aggregator. These components satisfy $E(3)$ equivariance, size extensivity, and local-global decomposition without relying on any lattice-dependent constructs.

The resulting theoretical scaffold enables the design of amorphous-specific geometric deep learning architectures that are provably robust to the absence of periodicity and validated on system-size transferability. By grounding future work in these principles rather than in extensions of crystal methods, the community can unlock reliable, scalable, and conceptually sound modeling of glasses, liquids, polymers, and disordered alloys—the very materials that dominate real-world applications yet have remained outside the reach of mainstream geometric deep learning. The transition from periodic to non-periodic domains is therefore not an incremental adjustment but the opening of a distinct theoretical chapter in materials informatics.

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