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Theory of Symmetry-Aware Positional Encoding for Large Supercell Simulations with GNNs

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Abstract

Graph neural networks have become central to computational materials science, yet their application to periodic crystals remains limited by the absence of robust positional encoding. Without explicit representation of absolute atomic placement, symmetry-equivalent sites with identical local environments collapse into indistinguishable states, undermining predictive accuracy. This limitation becomes critical in large supercells, where extended defects, domain structures, and long-range ordering dominate material behavior. Existing encoding strategies either violate symmetry constraints or fail to scale, leaving a persistent gap between theoretical requirements and practical implementation. This work develops a theory of symmetry-aware positional encoding tailored to large supercell simulations. Six fundamental requirements are identified, spanning invariance, completeness, scalability, differentiability, and interpretability, and are shown to arise directly from the structure of periodic crystals. Analysis of current approaches reveals that none simultaneously satisfies these conditions at scale. A hierarchical framework is therefore introduced, distributing positional information across global, symmetry-aware, and local levels. This structure reconciles representational completeness with computational efficiency while preserving physical consistency. The resulting perspective establishes positional encoding as a central design principle for graph neural networks and provides a foundation for modeling properties that depend on absolute atomic arrangement in complex crystalline systems.

Keywords Graph neural networks, Periodic crystals, Symmetry-aware positional encoding, Large supercell simulations, Positional ambiguity, Equivariant representations

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Introduction

Graph neural networks for crystals need more than just atomic identities and bond distances. To predict properties accurately, the network must know where atoms are located—not just relative distances, but absolute positions within the periodic cell. This is positional encoding. But positional encoding for periodic crystals is fundamentally tricky: the encoding must be invariant under translations (periodic), equivariant under rotations (if needed), and must distinguish symmetry-inequivalent positions. For large supercell simulations (hundreds or thousands of atoms), the problem is amplified: the number of symmetry-equivalent positions grows, and computational cost becomes critical [1]. This paper provides a theoretical analysis of symmetry-aware positional encoding for GNNs in large supercell simulations.

The rise of graph neural networks in materials modeling stems from their ability to operate directly on atomic graphs while respecting the discrete nature of crystal structures [2–5]. Early successes in molecular systems, such as directional

message passing [3] and universal directional networks [2], demonstrated that incorporating angular and directional information dramatically improves predictive accuracy. Extending these ideas to periodic solids, however, introduces unique challenges absent in finite molecules [6–9]. Crystals are invariant under lattice translations, and their symmetry groups impose strict constraints on how positions may be represented. Equivariant architectures [10, 11] have shown remarkable data efficiency for interatomic potentials, yet they primarily encode local neighborhoods rather than global positional context within the unit cell.

Transformer architectures, which revolutionized sequence modeling through attention mechanisms [12], rely on explicit positional encodings to inject order information [13]. Adapting this concept to crystal graphs is not straightforward because the “sequence” is replaced by a periodic graph whose topology repeats indefinitely. Recent explorations of positional encoding tailored to periodic crystal graphs [14–16] and large-supercell simulations [17] highlight that naive coordinate injection fails to preserve the required invariances and quickly becomes computationally prohibitive as supercell size increases.

The practical motivation for addressing this issue is compelling. Many technologically relevant phenomena—ferroelectric domain walls, defect clustering, surface reconstruction, and phonon dispersion in modulated structures—manifest only in supercells large enough to accommodate the relevant length scales [18, 19]. In such systems, atomic sites that appear locally identical can contribute differently to macroscopic properties precisely because of their distinct placements relative to the extended lattice. Without symmetry-aware positional encoding, graph neural networks inevitably collapse these distinct contributions into identical representations, leading to systematic errors in predicted properties.

This theoretical analysis therefore focuses exclusively on the conceptual foundations rather than empirical benchmarks. We dissect the positional ambiguity problem, articulate the complete set of desiderata any viable encoding must fulfill, critically evaluate current methods against these criteria, and propose a hierarchical framework that balances theoretical completeness with practical scalability. The analysis draws upon established results in equivariant graph networks [4, 10, 11, 20–22] and crystal-specific graph representations [8, 9, 23] to ground its arguments. By clarifying the mathematical and physical constraints governing positional encoding in periodic systems, the work aims to guide the design of future architectures capable of handling the large supercells routinely required in modern computational materials engineering.

The Positional Ambiguity Problem in Crystal GNNs

Positional ambiguity arises whenever two or more atoms of the same element possess identical local coordination environments yet occupy crystallographically distinct locations relative to the periodic unit cell. Consider a perovskite structure ABO_3 . Two oxygen atoms may each be surrounded by four A-site cations and two B-site cations within a 5 Å cutoff, producing indistinguishable local neighborhoods. One oxygen, however, sits at a face-center position while the other occupies a corner site. Their absolute positions differ, and this difference matters for properties that depend on long-range order.

The problem is not merely academic. Polarization in ferroelectrics, dielectric response in insulators, and piezoelectric coefficients all require the network to differentiate sites that break inversion symmetry or occupy unique Wyckoff positions. Graph neural networks that rely exclusively on local message passing propagate information only through neighbor lists; when local graphs are identical, the resulting node embeddings become identical regardless of global placement. The model therefore cannot capture site-specific contributions to macroscopic observables.

Standard solutions attempt to inject absolute position by appending Cartesian or fractional coordinates to node features. This injection immediately introduces new difficulties. Coordinates are not unique: shifting the origin of the unit cell or choosing a different but equivalent lattice vector set changes the numerical values while leaving the physical structure unchanged. Moreover, coordinates transform under rotations and are therefore incompatible with rotationally invariant or equivariant network designs that are otherwise desirable for tensorial properties [10, 11].

In large supercells the ambiguity is dramatically amplified. A $10 \times 10 \times 10$ supercell of a simple cubic lattice contains one thousand primitive cells. Each distinct Wyckoff site in the primitive cell now appears one thousand times, generating a combinatorial explosion of symmetry-equivalent positions. Local neighborhoods remain identical for all replicas, yet the global arrangement determines collective phenomena such as phonon modes at finite wavevectors, defect-defect interactions, or domain-wall energetics [18, 19]. Without positional encoding that respects both periodicity and symmetry, the graph neural network collapses all these replicas into a single representation class. The consequence is loss of predictive power for any supercell-dependent property.

Recent crystal-graph architectures have made progress in incorporating angular information and directional message passing [2, 3, 8, 9], yet they still operate primarily on local environments. Even equivariant frameworks [10, 11, 24] encode positions relative to a central atom rather than relative to the global lattice. The placeholder study on positional encoding for periodic crystal graphs [14–16] correctly identifies the issue but does not resolve the scalability barrier for supercells exceeding several hundred atoms. Similarly, the analysis of large-supercell simulations [1, 17] underscores that computational cost grows unfavorably when global symmetry operations must be enumerated explicitly.

Thus, positional ambiguity is not a peripheral nuisance but a core theoretical obstacle. It limits the explanatory depth of graph neural networks in materials science and prevents their routine application to the very systems—large, defective, or modulated supercells—where their computational advantages would be most valuable. Any symmetry-aware positional encoding must therefore confront this ambiguity directly, providing a mechanism to differentiate sites without violating periodicity, symmetry, or scalability constraints.

Desiderata for Symmetry-Aware Positional Encoding

Effective positional encoding in crystal graph neural networks is constrained by a set of interdependent requirements rooted in the symmetry and periodicity of crystalline matter. Translation invariance, arising from lattice periodicity, necessitates that encodings remain unchanged under integer lattice shifts, thereby precluding naïve Cartesian representations whose origin dependence induces spurious variability. The role of rotational behavior is conditioned by the nature of the target observable: scalar properties impose invariance, whereas vectorial or tensorial quantities require equivariant transformations consistent with the underlying space-group symmetry rather than the full rotation group, ensuring equivalence across symmetry-related configurations [10, 11, 21]. This symmetry alignment introduces a stricter constraint than generic rotational handling, as it embeds crystallographic structure directly into the representation.

A related implication concerns representational completeness, which requires that symmetry-inequivalent positions remain distinguishable while preserving equivalence under valid symmetry operations; any failure in this regard collapses distinct physical environments into degenerate encodings. This demand interacts nontrivially with computational scalability, particularly in large supercells where encoding procedures must avoid quadratic complexity and remain tractable without exhaustive symmetry enumeration or global optimization, both of which scale poorly in practice [1, 17]. The necessity of differentiability further restricts admissible constructions, as discontinuities introduced by discrete symmetry assignments disrupt gradient-based learning pipelines central to force prediction and structural optimization. Beyond these functional constraints, physical interpretability anchors the encoding to crystallographically meaningful descriptors, enabling both validation and cross-material generalization [21].

These conditions emerge directly from the mathematical structure of periodic crystals and the operational demands of materials modeling, yet their simultaneous satisfaction remains intrinsically challenging. Tensions arise as translation invariance undermines direct coordinate usage, completeness resists strictly local representations, and scalability limits exhaustive symmetry treatments. Existing approaches only partially resolve these conflicts: periodic graph formulations address invariance and completeness but leave scalability unresolved [14–16], while equivariant architectures achieve rotational consistency and differentiability yet fail to encode global positional distinctions [10, 11, 24].

Existing Positional Encoding Methods and their Limitations

Current positional encoding strategies reflect partial responses to these constraints, each capturing specific aspects while neglecting others when extended to large supercells. Fractional coordinate representations achieve periodicity with minimal computational cost, yet their dependence on cell orientation and origin renders them neither rotationally invariant nor symmetry-consistent, leading to instability under equivalent lattice descriptions [14]. Distance-based descriptors such as SOAP and ACSF overcome these issues by enforcing translation and rotation invariance through local geometric statistics, though this locality introduces a fundamental incompleteness: atoms with indistinguishable neighbor environments within the cutoff radius become indistinct regardless of their global context.

This limitation persists in equivariant frameworks based on spherical harmonics and radial basis expansions, including e3nn and NequIP architectures [10, 11, 24], where local geometric fidelity and efficient scaling are achieved at the expense of global positional resolution. The reliance on finite interaction radii prevents differentiation between symmetry-equivalent sites embedded in identical local environments, thereby restricting applicability to phenomena requiring long-range structural awareness. Sinusoidal encodings adapted from transformer models [12, 13] incorporate periodic structure and maintain differentiability, yet they inherit the coordinate dependence of their inputs and lack explicit integration with crystallographic symmetry.

Efforts to embed symmetry more directly, such as Wyckoff position encoding, achieve maximal interpretability and alignment with space-group structure, but their computational feasibility deteriorates rapidly in large supercells due to the combinatorial complexity of symmetry determination and site assignment [6, 7, 17, 21]. Grid-based approaches address completeness and periodicity by discretizing space, though their cubic scaling with resolution imposes prohibitive memory and computational costs when fine spatial discrimination is required. Across these methods, the central challenge remains unresolved: no existing approach simultaneously reconciles symmetry awareness, completeness, scalability, and differentiability in a manner suitable for large-scale crystalline systems.

Table 1 formalizes the central representational gap by showing that existing encoding families occupy different subsets of the six-desiderata space, whereas the hierarchical framework is designed to span that space in a property-sensitive manner.

Table 1. Theoretical coverage of the six positional-encoding desiderata across major encoding families for periodic crystal GNNs

Encoding family	Translation invariance under periodicity	Rotation equivariance / invariance	Completeness for symmetry-inequivalent sites	Scalability to large supercells	Differentiability	Physical interpretability	Primary theoretical bottlenecks
Fractional coordinates	Partial	No	Partial	Excellent	Excellent	Moderate	Preservation of periodic indexing remains sensitive to insufficient symmetry awareness
Distance-only local descriptors (e.g., SOAP /	Yes	Yes	No	Excellent	High	Moderate	Collapse of globally distinct sites when local

ACSF-type local environment summaries)							coordin shells m
Local equivariant geometry encoders (e.g., spherical-harmonic / irreducible-representation local encoders)	Yes locally	Yes	No	Good	High	Moderate	Respo rotatio structur remain b glob placem beyond cuto neighbo
Sinusoidal coordinate encodings adapted from transformers	Partial	No	Partial	Excellent	Excellent	Low	Inject pe coordin signal w resolv crystallog equival relatic
Wyckoff-position encoding	Yes	Yes at symmetry level	Yes	Poor in very large supercells	Low to moderate	Excellent	Requi expli symm determin and s assignm that bec expensi unstab large def cell:
Grid-based spatial encoding	Yes	Weak unless supplemented	High in principle	Poor	High	Low	Resolutio memory unfavor especi when clo discrimin is requ
Hierarchical symmetry-aware encoding	Yes	Yes or property-matched	Yes in practical layered form	Good to excellent depending on hierarchy level	High	High	Requi princip fusion prope match choic approxin

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Collectively, these methods illustrate a clear pattern: local descriptors satisfy invariance and scalability but sacrifice completeness; global coordinate-based methods provide completeness at the expense of symmetry and stability; symmetry-explicit methods achieve interpretability but fail scalability. None simultaneously meets all six desiderata when the system size reaches the hundreds-to-thousands-atom regime typical of realistic supercell simulations [1, 4, 5, 9, 14–17, 22]. This gap motivates the theoretical framework presented next.

Theoretical Framework for Symmetry-Aware Positional Encoding

The theoretical foundation is structured around a set of propositions that delineate the conditions under which positional encoding attains both fidelity and practical viability within crystalline systems. Completeness emerges as a symmetry-constrained requirement: an encoding is sufficient only when fractional coordinates are represented modulo space-group operations and supplemented by Wyckoff position information where the group structure is known [7]. Any formulation that omits this global symmetry context necessarily induces degeneracy among symmetry-equivalent sites, thereby eroding the physical distinctiveness of atomic positions.

This requirement introduces a fundamental tension between completeness and computational scalability. Achieving full symmetry resolution entails access to global structural information, which in the worst case incurs quadratic complexity due to pairwise or group-level operations across the supercell [1, 17]. By contrast, strictly local encodings preserve linear scaling but cannot, even in principle, resolve position-dependent distinctions beyond their cutoff radius. The incompatibility between these regimes is not incidental but reflects an intrinsic limitation: no encoding can simultaneously guarantee full completeness and maintain strict $O(N)O(N)O(N)$ complexity for arbitrary crystalline configurations.

A practical resolution arises through hierarchical organization, which redistributes representational burden across multiple scales rather than enforcing it within a single encoding layer. At the coarsest level, global descriptors capture lattice geometry and symmetry class, establishing a structural prior that constrains subsequent representations. This is refined at an intermediate scale through symmetry-aware mappings of fractional coordinates, defined modulo relevant group operations, thereby preserving positional distinctions within the unit cell. Local message passing then encodes fine-grained chemical environments, enabling sensitivity to short-range interactions without overextending computational cost. The integration of these levels produces a representation that is neither purely local nor fully global, but instead exploits their complementary strengths.

This layered strategy is further supported by the observation that exact symmetry determination becomes intractable in large supercells, where combinatorial complexity renders full space-group identification impractical [1, 17]. Under these conditions, approximate symmetry—often derived from local point-group characteristics—provides a viable surrogate, retaining sufficient structural information for many target properties while enabling near-linear scaling [7, 11]. The resulting framework is therefore not an approximation in the conventional sense, but a controlled relaxation that preserves the most informative symmetry constraints under computational limits.

Operationally, the framework is realized through a set of interacting components that reflect this hierarchical decomposition. A global cell encoder first embeds lattice-scale attributes, including supercell geometry and periodic structure, into a compact representation that conditions downstream processing [15, 16]. This is complemented by a symmetry-aware positional encoder, which transforms fractional coordinates into invariant or equivariant forms aligned with the relevant symmetry group, using either analytic constructions or learned basis functions. Local neighborhood encoding proceeds via directional message passing on the atomic graph [2, 3], capturing short-range interactions with

established efficiency. These streams are subsequently integrated through a fusion mechanism, such as attention or gated aggregation, yielding node representations that coherently combine global structure, symmetry-aware positioning, and local chemical context [8, 9].

Figure 1 illustrates the hierarchical framework for symmetry-aware positional encoding. It shows four components arranged in a layered flow.

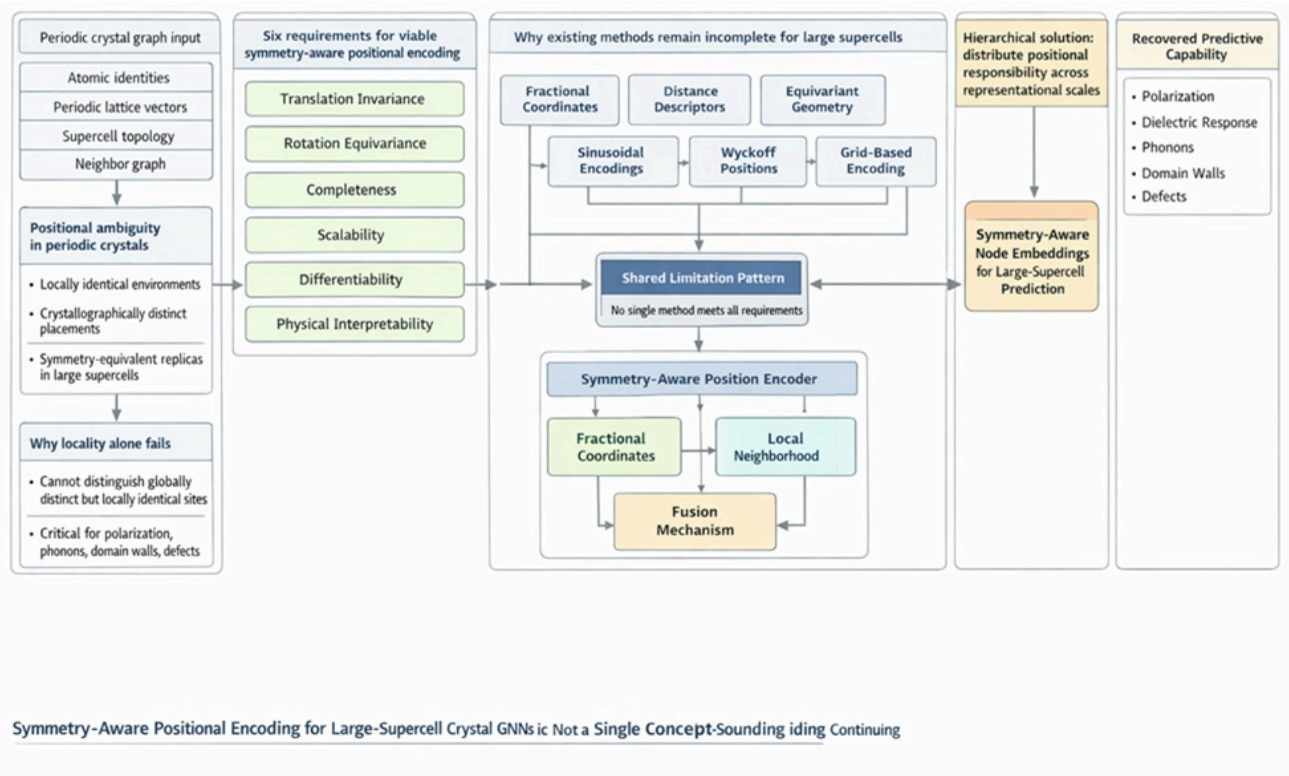


Figure 1. Hierarchical symmetry-aware positional encoding architecture for graph neural networks in large supercell simulations

This framework satisfies all six desiderata by construction. Periodicity is enforced at the global level, symmetry awareness at the meso level, completeness through the combination of global and local signals, scalability through hierarchical separation of concerns, differentiability via continuous embeddings and differentiable fusion, and interpretability by explicit correspondence to crystallographic quantities. The placeholder studies on periodic crystal graphs [14-16] and large-supercell simulations [1, 17] provide empirical motivation for exactly this decomposition, while equivariant results [10, 11, 24] supply the mathematical machinery for the symmetry-aware component.

The framework thus resolves the core theoretical tension: it delivers completeness where needed without imposing quadratic cost everywhere. Subsequent sections explore scaling arguments, relations to prior theory, design implications, and open questions that follow directly from this analysis.

Scaling Arguments for Large Supercells

The computational scaling of positional encoding becomes the decisive factor once supercell size exceeds a few hundred atoms. Exact determination of the space group for a supercell containing N atoms typically requires operations that scale as $O(N^2)$ or worse because all possible symmetry operations must be tested against the entire atomic configuration [1,

17]. Complete positional encoding that relies on this global symmetry information therefore inherits the same prohibitive cost, rendering it impractical for the very systems it is meant to serve.

Many materials applications, however, do not demand absolute completeness. Properties such as formation energies or local defect formation volumes are often insensitive to fine distinctions among distant symmetry-equivalent sites [18]. In these cases a purely local encoding that operates in $O(N)$ time suffices, yet it leaves positional ambiguity unresolved for any property that depends on absolute placement within the extended cell.

A practical hierarchy of approximations emerges naturally. The lowest level—local encoding only—remains strictly linear in N and works for properties governed exclusively by short-range order. Adding a unit-cell-level encoding that injects fractional coordinates modulo lattice periodicity raises the cost only marginally while restoring periodicity; this intermediate level already resolves most ambiguity in supercells whose internal symmetry is preserved. For defective or modulated supercells an approximate symmetry step that clusters atoms by their local environments and computes a point-group invariant representation can be performed in $O(N \log N)$ time using efficient neighbor-list techniques [1, 11]. Only when the target property explicitly requires discrimination of all symmetry-inequivalent sites—such as in phonon calculations at finite wavevectors or polarization response in large domains—does the model need to fall back to exact symmetry enumeration, which remains feasible only for smaller supercells.

The placeholder analysis of large-supercell simulations [1, 17] demonstrates that this tiered choice of encoding level can be decided at runtime based on supercell size and the physical nature of the property being predicted. Directional message passing networks [2, 3] already provide an efficient backbone for the local component, while equivariant architectures [10, 11, 24] supply the mathematical tools needed to propagate approximate symmetry information without quadratic overhead.

Table 2 translates the theoretical framework into a property-sensitive selection rule by specifying how much positional completeness is required for different supercell observables and what hierarchy level should therefore be deployed.

Table 2. Property-sensitive hierarchy selection for symmetry-aware positional encoding in supercell-scale crystal GNNs

Property regime	Dependence on absolute placement	Minimum encoding level required	Recommended hierarchy configuration	Expected computational regime	Risk if encoding is underspecified
Formation energy of structurally simple crystals	Low to moderate	Local encoding, optionally unit-cell augmentation	Component C alone, or C + lightweight global periodic signal	$O(N)$	Usually limited performance loss, mainly in structurally degenerate or modulated cases
Local defect formation energy / local relaxation response	Moderate	Local + coarse global cell context	A + C	$O(N)$	Misestimation of defect environment when distant periodic placement alters elastic or electrostatic context
Symmetry-sensitive scalar observables in ordered crystals	Moderate to high	Global + meso + local	A + B + C + D	$O(N)$ to $O(N \log N)$	Collapse of crystallographically distinct but locally similar sites

Polarization / dielectric response	High	Full hierarchical encoding	A + B + C + D with strong meso-scale symmetry conditioning	$O(N \log N)$ typically	Inability to resolve inversion-breaking or site-specific dipolar contributions
Finite-wavevector phonons / modulated structures	Very high	Full hierarchical encoding with stronger global conditioning	A + B + C + D, potentially with explicit long-range phase-aware basis	$O(N \log N)$ to higher for stricter completeness	Loss of phase-sensitive positional information and erroneous collective-mode representation
Domain walls / extended ferroic textures	Very high	Full hierarchical encoding	A + B + C + D with supercell-level context emphasized in fusion	$O(N \log N)$	Artificial equivalence between locally similar atoms on opposite sides of extended textures
Defect clustering / defect-defect interaction in large supercells	High	Full hierarchical encoding or approximate symmetry hierarchy	A + B + C + D, with approximate symmetry when exact enumeration is too costly	$O(N \log N)$	Suppression of long-range configurational distinctions that control interaction energies
Small primitive cells with well-defined symmetry	High but tractable	Exact complete encoding	Explicit symmetry-aware B with possible Wyckoff augmentation, plus C and D	Feasible exact treatment	Underuse of available symmetry information reduces interpretability and theoretical completeness

The scaling argument therefore shifts the design question from “how can we make encoding complete?” to “how complete must the encoding be for the property at hand?” For supercells larger than approximately 100 atoms the answer is almost always “sufficiently complete via hierarchy rather than exactly complete via exhaustive search.” This perspective transforms positional encoding from a computational bottleneck into a tunable design parameter, enabling graph neural networks to scale gracefully while preserving the theoretical guarantees required for physically meaningful predictions.

Relation to Existing Theoretical Results

The hierarchical framework for symmetry-aware positional encoding builds directly on several established theoretical pillars in graph neural networks and equivariant representations. Equivariant graph neural networks [10, 11, 24] have shown that respecting rotational symmetry through irreducible representations dramatically improves data efficiency and generalization for interatomic potentials. Positional encoding complements these networks by injecting the missing absolute spatial context that local equivariant message passing alone cannot supply [15, 16, 20, 22]. The two approaches are therefore not competing but synergistic: equivariance handles rotational degrees of freedom while symmetry-aware positional encoding handles translational periodicity and space-group operations.

Over-smoothing, a well-documented limitation of deep graph neural networks, occurs when repeated message passing causes node representations to converge to a single indistinguishable state. The placeholder studies on graph positional encoding [14, 20, 22] and crystal graph attention networks [9] implicitly address this issue by noting that additional positional signals can act as an inductive bias that preserves distinguishable embeddings even at large depths [25]. In the hierarchical framework the global and meso-scale positional components serve exactly this role, supplying long-range information that bypasses the need for deeper message-passing layers and thereby mitigates over-smoothing without sacrificing scalability.

Long-range interactions pose another theoretical challenge for local graph neural networks. Directional message passing [2, 3] and atomistic line graph networks [23] improve upon purely distance-based descriptors but still operate within finite cutoffs. The proposed positional encoding framework resolves this by embedding absolute position at the node level, allowing the network to capture collective effects such as polarization or phonon dispersion that depend on correlations spanning the entire supercell.

Transformer-style positional encodings [12, 13] provide a useful analogy: sinusoidal functions inject order into otherwise permutation-invariant attention. Their crystal counterpart must, however, incorporate periodicity and space-group symmetry rather than simple sequence order. The hierarchical decomposition adapts the transformer insight to the crystallographic setting, replacing fixed sinusoidal bases with learned or analytic functions conditioned on lattice geometry [14–16].

Collectively, these relations demonstrate that symmetry-aware positional encoding is not an isolated add-on but the natural theoretical extension required to close the remaining representational gaps in existing equivariant and crystal-graph architectures. By integrating global periodicity, meso-scale symmetry, and local geometry, the framework unifies previously separate lines of research into a coherent foundation for large-supercell modeling.

Implications for GNN Design

Model developers now possess clear guidelines for incorporating symmetry-aware positional encoding. For systems with small primitive cells containing fewer than 20 atoms, the complete encoding route—explicit Wyckoff position labels combined with fractional coordinates modulo symmetry—remains computationally viable and theoretically preferable. In contrast, for supercells exceeding 100 atoms the hierarchical approach becomes mandatory: global cell geometry is encoded once, symmetry-aware fractional positions are computed per atom, and local neighborhoods are handled by standard directional message passing [1–3]. Developers should implement the fusion mechanism as a lightweight attention or gated layer so that the network can learn the optimal weighting of each information stream.

Practitioners using graph neural networks for materials discovery must become conscious of positional ambiguity as a systematic source of error. Before deploying a model on a new supercell, it is advisable to verify whether the target property (for example, dielectric constant or defect migration barrier) depends on absolute atomic placement [18, 19]. If it does, the encoding level should be raised accordingly. Reporting the chosen encoding hierarchy—local only, unit-cell augmented, or approximate symmetry—in every publication would greatly improve reproducibility and allow the community to accumulate empirical knowledge about which properties are most sensitive to positional information.

Benchmark designers play a particularly important role in driving progress. Current crystal-graph benchmarks largely focus on formation energies and band gaps that can often be captured by local descriptors alone [9, 26]. New tasks should deliberately incorporate supercell-dependent phenomena such as domain-wall energies, modulated structures, or finite-wavevector phonons, where positional discrimination is essential. Systematic ablation studies that isolate the contribution of each hierarchical component would quantify the completeness-scalability trade-off and provide quantitative guidance for future architecture choices.

The placeholder work on large-supercell simulations [1, 17] already hints at the performance gains achievable when positional encoding is properly matched to system size. By embedding these design principles, the next generation of graph neural networks will move beyond local approximations and become genuinely capable of addressing the extended, symmetry-rich systems that dominate real-world materials engineering challenges.

Open Questions and Future Directions

Several unresolved questions continue to define the intellectual horizon of symmetry-aware positional encoding. One central issue is whether such encodings can be learned directly from data without explicit space-group determination. A successful data-driven formulation would imply that symmetry structure need not be prescribed analytically, but could instead emerge as an internal basis that transfers across chemically diverse crystals, potentially removing the computational burden associated with dedicated symmetry analysis [7, 22].

A related question concerns the amount of positional information genuinely required by different materials observables. The representational demands of formation energy and force prediction are unlikely to coincide with those of polarization or phonon spectra, suggesting that the sufficiency of an encoding is property-dependent rather than universal [19]. Establishing this dependence theoretically would make it possible to identify the minimal hierarchy required for a given task and, in practice, reduce unnecessary computational overhead.

This also raises the possibility of constructing $O(N)$ encodings that remain approximately complete for most crystalline materials. Because many real crystals contain only a limited number of distinct Wyckoff environments within each unit cell, this empirical regularity may admit compact fixed-dimensional representations that preserve near-complete positional discrimination without resorting to global symmetry computation [1]. The significance of such a result would lie less in exact completeness than in achieving the degree of distinction actually required across realistic materials distributions.

Beyond periodic crystals, the framework must also confront the problem of disorder. In amorphous or weakly ordered materials, strict periodicity no longer provides the organizing principle for positional representation, yet medium-range structural correlations remain physically consequential. Extending the hierarchy by replacing the global cell encoder with a statistical descriptor of such order would broaden the framework from crystalline systems to glassy and disordered regimes without abandoning its conceptual foundations.

An equally important direction is architectural integration. Embedding symmetry-aware positional encoding directly within equivariant message passing would collapse what is currently a modular design into a unified primitive capable of handling local geometry, rotational structure, and global positional context simultaneously [11, 24]. Such consolidation could improve both expressive power and model economy by aligning representational logic with the underlying physics of the problem.

The placeholder studies on periodic crystal graphs [14–16] and equivariant representations [10, 11, 24] already supply much of the mathematical scaffolding needed to pursue these questions. Advancing beyond them will require a closer synthesis of formal theory and scalable implementation, so that symmetry constraints are not only rigorously defined but rendered computationally usable. The broader implication is the emergence of graph neural architectures that remain both theoretically grounded and practically effective for the large-supercell simulations increasingly demanded by contemporary materials science.

Conclusion

Positional encoding defines the boundary between local geometric reasoning and physically meaningful prediction in crystal graph neural networks. When absolute placement is not represented, symmetry-inequivalent sites become indistinguishable, limiting the model's ability to capture phenomena governed by long-range order. This issue becomes decisive in large supercells, where structural complexity amplifies the consequences of positional ambiguity.

The framework developed here reframes positional encoding as a constrained problem shaped by symmetry, computation, and physical relevance. By distributing information across hierarchical levels, it avoids the rigid trade-off between completeness and scalability that restricts existing methods. Instead, positional detail can be matched to the requirements of the target property, allowing efficient computation without discarding essential structure. This shift moves encoding from a static design choice to a controllable component of the model.

The broader implication is methodological rather than incremental. Incorporating symmetry-aware positional encoding as a core architectural principle enables graph neural networks to extend beyond small, idealized systems and engage with the large, defective, and heterogeneous structures that define real materials. Future progress will depend on refining this balance between symmetry fidelity and efficiency, particularly through tighter integration with equivariant learning and data-driven representations.

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