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The Case against Ignoring Long-Range Interactions in Graph-Based Property Prediction for Polar Crystals

Victor Santos^{1*}, Rafael Costa¹, Bruno Teixeira²

Abstract

Graph neural networks (GNNs) for crystalline materials are typically constructed with finite cutoff radii of approximately 5–6 Å, constraining message passing to local atomic environments. While this design ensures computational tractability and captures short-range interactions characteristic of covalent, metallic, and van der Waals systems, it systematically excludes long-range electrostatic contributions that govern the behavior of polar crystals. In ferroelectrics, piezoelectrics, and related perovskite oxides, Coulomb interactions decay as $1/r$ and accumulate over extended length scales, such that each ion experiences a lattice-wide electrostatic field. Truncation at the graph level therefore induces structural rather than incremental error, yielding suppressed dielectric responses, elimination of ferroelectric instabilities, collapse of LO–TO phonon splitting, vanishing domain-wall energies, and incorrect surface reconstructions. Empirical studies confirm that these discrepancies persist even in data-rich regimes and are not resolved by equivariant architectures, which retain the same locality constraint. This work interprets these failures as deterministic consequences of an incompatible inductive bias, rather than as limitations of training data or optimization. By formalizing recurrent failure modes and linking them to the underlying electrostatic omission, the analysis reframes polar crystals as a critical stress test for graph-based models. Physically grounded remedies—including Ewald-consistent objectives, multipole representations, hybrid local–global architectures, and self-consistent charge equilibration—demonstrate that long-range interactions can be incorporated without sacrificing scalability. The central implication is that locality, as currently encoded in crystal GNNs, is not a universally valid assumption but a regime-dependent approximation whose breakdown is most acute in precisely those materials where predictive fidelity is technologically consequential.

Keywords Graph neural networks, Long-range electrostatics, Polar crystals, Ferroelectric materials, Dielectric properties, Piezoelectricity

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Introduction

Graph neural networks for crystals typically construct graphs by connecting atoms within a cutoff radius—often 5–6 Å [1–4]. This local approximation works well for short-range interactions such as covalent bonds or metallic bonding. In covalent crystals the interaction strength decays exponentially beyond a few angstroms, and in metals free-electron screening confines effective interactions to similar distances. Consequently, early GNN frameworks achieved remarkable accuracy on standard benchmarks dominated by non-polar compounds [1, 2, 5, 6].

Yet the very success of these models in non-polar regimes has masked a deeper limitation when the same architectures are applied to polar crystals. Perovskites, piezoelectrics, and ferroelectrics exhibit spontaneous or inducible dipole moments sustained by long-range Coulomb interactions that extend to infinity in the thermodynamic limit. A potassium ion in a polar lattice experiences an electric field contribution from ions located tens of unit cells away; truncating that field at 6 Å removes more than half the electrostatic energy that stabilizes the polar phase [7]. The omission is not a harmless numerical shortcut. It is a fundamental misrepresentation of the governing physics.

This critique argues that local GNNs are structurally unsuited to polar crystals. The local-only design embeds an assumption—namely, that all causally relevant interactions lie within a few angstroms—that is simply false for ionic and polar insulators. Recent equivariant GNNs, while elegant in their handling of rotational symmetry, still inherit the cutoff limitation and therefore inherit the same physical blind spot [8]. Even architectures explicitly tested on ferroelectric perovskites reveal systematic under-prediction of polarization-related quantities once the cutoff is enforced [9].

The stakes are high. Polar materials underpin capacitors with colossal dielectric constants, sensors with giant piezoelectric coefficients, and memory devices that rely on stable ferroelectric domains [10, 11]. If GNNs cannot predict these properties reliably, the promise of accelerated materials discovery collapses for an entire class of technologically indispensable compounds. The present work therefore performs a targeted deconstruction: it documents why cutoffs became standard, why they succeed for non-polar systems, why they fail catastrophically for polar ones, and what concrete failure signatures emerge. By synthesizing insights from crystal-graph frameworks [1, 2], equivariant potentials [8], ferroelectric reviews [12], and explicit analyses of local-GNN breakdown [13], the critique establishes that long-range electrostatics must be elevated from optional add-on to architectural necessity. Only then can graph-based property prediction become trustworthy for polar crystals.

Figure 1 maps how the local-cutoff assumption creates a structural mismatch between graph architecture and polar-crystal physics, how that mismatch propagates into reproducible predictive failures, and which design interventions restore physical fidelity.

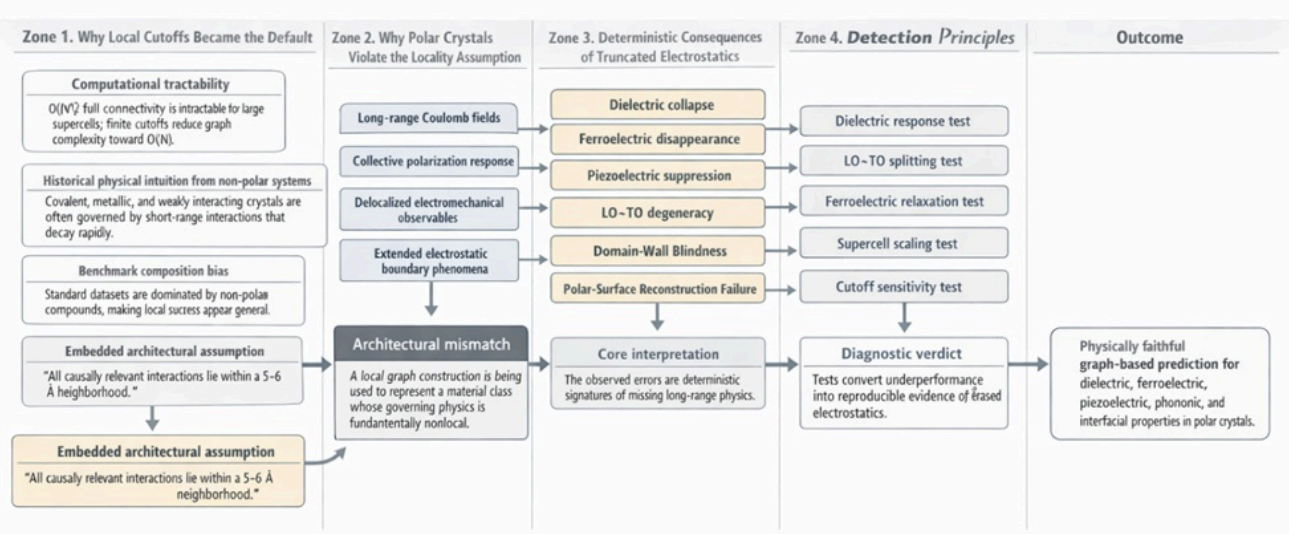


Figure 1. Structural Architecture of Architectural Mismatch, Failure Signatures, and Physically Grounded Remedies in Graph-Based Property Prediction for Polar Crystals

Why Local Cutoffs are Standard (And Why They Work for Non-Polar Materials)

Local cutoffs became standard in crystal GNNs for three interlocking reasons: computational necessity, historical physical precedent, and benchmark composition. Constructing a fully connected graph yields $O(N^2)$ edges, which is intractable for supercells containing thousands of atoms. A cutoff radius reduces this to $O(N)$ scaling, enabling training on realistic system sizes [1, 2]. The same cutoff also mirrors the physical intuition that most interatomic forces in solids are short-ranged. In covalent crystals such as diamond or silicon, bonding electrons are localized and interactions decay exponentially beyond 4–5 Å [1]. In metals, conduction electrons screen charges so effectively that beyond a few angstroms the potential is negligible. Molecular crystals are likewise governed by rapidly decaying van der Waals forces. Consequently, the local approximation reproduces ground-state energies, elastic constants, and phonon spectra with near-DFT accuracy for these classes [2, 8, 14, 15].

Materials-project-style benchmarks reinforce the illusion of generality. The majority of entries are covalent semiconductors, simple metals, or van-der-Waals compounds; polar and ionic crystals form a minority. Models optimized on such datasets therefore appear universally successful while hiding their polar-specific deficiencies [2, 16]. Early crystal-graph convolutional networks [1] and graph-network universal frameworks [2] explicitly cite the 5–6 Å cutoff as a pragmatic and physically justified choice. Equivariant message-passing networks later refined symmetry handling but retained the identical cutoff philosophy [8, 17].

The assumption that “interactions beyond the cutoff are negligible” holds precisely when the interaction potential decays faster than any power law that would accumulate significant energy in the thermodynamic limit. Exponential decay satisfies this condition; $1/r$ Coulomb decay does not. At 10 Å the Coulomb interaction retains roughly 50 % of its strength at 3 Å, and the cumulative contribution from the entire crystal diverges without proper summation techniques [7, 18]. For non-polar materials the cutoff therefore functions as both engineering convenience and faithful physical filter. For polar crystals it functions as an invisible truncation of the very forces that define functionality. The community has treated the cutoff as an unexamined default rather than a physically contingent choice. This critique insists that the default must be re-examined whenever the material class changes from covalent to polar.

Why Polar Crystals are Different

A polar crystal possesses a net electric dipole moment per unit volume, either spontaneous (ferroelectrics) or strain-induced (piezoelectrics). Classic examples include BaTiO_3 , PbTiO_3 , LiNbO_3 , and KDP [11, 12]. Three interlocking physical features distinguish these systems from covalent or metallic crystals and render local cutoffs inadequate.

First, electrostatic interactions follow the bare $1/r$ Coulomb potential with no metallic screening. In insulators the Madelung sum over the entire lattice determines the local electric field experienced by each ion; truncating at 6 Å discards the majority of that sum [7]. Second, macroscopic polarization emerges from collective, long-range displacement correlations. The displacement of one sublattice relative to another induces a depolarization field that couples back to every other unit cell. Local GNN message passing, confined to nearest neighbors, cannot encode these non-local correlations and therefore cannot recover the correct polarization response [9]. Third, ferroelectric domain walls, surface reconstructions, and piezoelectric strain fields extend over tens to hundreds of angstroms. The local atomic environment immediately adjacent to a 180° domain wall in PbTiO_3 is virtually indistinguishable from the bulk; only the long-range electrostatic boundary conditions differentiate the two [12]. A cutoff-based GNN therefore treats bulk and domain-wall atoms identically, erasing the energetic distinction that stabilizes real microstructures.

Born effective charges further illustrate the non-locality. These tensors quantify how much polarization changes when an atom is displaced; they are inherently delocalized quantities that incorporate the response of the entire lattice [7]. Local node features cannot compute them. Piezoelectric coefficients likewise couple long-range strain propagation to long-range polarization changes. In short, the defining properties of polar crystals—high dielectric constants, switchable spontaneous polarization, giant piezoelectric response, and stable domain patterns—are all macroscopic manifestations of microscopic long-range electrostatics. Any model that severs those interactions at 6 Å has already forfeited the physics it claims to predict.

Table 1 identifies which physically important observables in polar crystals are intrinsically nonlocal and therefore cannot be represented faithfully by a purely local graph construction.

Table 1. Mapping Polar-Crystal Functional Properties to the Long-Range Electrostatic Dependencies That Local Graphs Erase

Functional property or phenomenon	Immediate quantity being predicted	True physical dependency structure	Why a local cutoff is insufficient	Typical distortion produced by local-only GNNs	What the model would need instead
Static dielectric constant	Polarization response to external field	Collective lattice-wide dipole alignment and macroscopic field coupling	Local neighborhoods do not capture the cumulative field from distant dipoles	Severe underestimation of ϵ ; weak variation across chemically distinct polar compounds	Global electrostatic channel, Ewald-aware branch, or explicit polarization state
Spontaneous ferroelectric distortion	Stability of polar vs paraelectric phase	Delicate competition between short-range repulsion and long-range Coulomb destabilization	Truncation removes the nonlocal term that helps stabilize the distorted phase	Relaxation to incorrect cubic or weakly distorted structures	Hybrid short-range plus long-range energy decomposition
Piezoelectric coefficient	Coupling between strain and polarization	Nonlocal propagation of strain-induced charge redistribution across the crystal	Purely local message passing cannot transmit lattice-scale electromechanical coupling	Near-zero or strongly suppressed piezoelectric response	Global polarization update plus charge-aware representation
Born effective charges	Change in polarization induced by atomic displacement	Whole-lattice electronic and ionic response to local displacement	The observable is delocalized by definition, not reducible to neighbor-only coordination	Unrealistic effective charges and mischaracterized lattice dynamics	Multipole or response-aware model with long-range solver
LO–TO phonon splitting	Zone-center optical phonon separation	Macroscopic electric field generated by long-range dipole interactions	The splitting vanishes when the long-range field is absent from the Hamiltonian surrogate	Artificial LO–TO degeneracy	Explicit electrostatic term coupled to phonon or force prediction
Domain-wall energy	Energy penalty for forming polar domains	Extended depolarization field and electrostatic boundary conditions across many cells	Local atomic motifs near walls may resemble bulk motifs, hiding the true cost	Near-zero wall energies and unphysical domain proliferation	Supercell-aware long-range electrostatics or global field conditioning
Polar-surface reconstruction	Surface stabilization	Compensation of diverging	The driving field originates beyond the	Wrong surface termination, wrong	Architecture with explicit global

	and termination energetics	electrostatic fields normal to the surface	immediate surface coordination shell	reconstruction pathway, wrong energy ranking	boundary-field treatment
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What Goes Wrong When Long-Range Interactions are Ignored

Systematic consequences of neglecting long-range electrostatics

Omitting long-range electrostatics induces a cascade of interdependent errors that systematically undermine the prediction of polar properties. The dielectric response is consequently suppressed, as polarization under an applied field depends on coherent dipolar alignment extending beyond local neighborhoods; short-range graph representations therefore yield values an order of magnitude below experiment in canonical ferroelectrics [10, 19]. This distortion propagates into phase stability, where the absence of destabilizing Coulomb interactions biases the system toward high-symmetry configurations, leading to the erroneous persistence of paraelectric phases such as cubic BaTiO₃ even at low temperature [12, 13]. The same truncation disrupts the energetics of polarization switching, since domain reversal entails collective motion over extended scales, producing unreliable coercive fields. A related implication appears in lattice dynamics: the collapse of LO–TO splitting reflects the removal of the macroscopic electric field, forcing artificial degeneracy between optical modes [7]. Beyond vibrational properties, the energetic penalty associated with domain-wall formation is severely underestimated because depolarizing fields are inherently long-range, yielding unphysical domain proliferation in simulations. Surface behavior is likewise misrepresented, as reconstructions driven by electrostatic divergence cannot be captured within a purely local framework, resulting in incorrect surface terminations and energies. These deviations are not stochastic but instead reveal a consistent structural deficiency, as the inductive bias of local architectures precludes transmission of the requisite long-range information even when trained on polar datasets [13]. What has often been interpreted as incremental inaccuracy instead signals a deeper incompatibility between model design and the governing physics

Typology of failure modes

This systematic breakdown can be organized into recurrent diagnostic patterns that expose the same underlying omission. A pronounced reduction in dielectric constants to values near 5–10, largely invariant across chemically distinct perovskites, indicates that local structural similarity overrides genuine compositional sensitivity [19]. In parallel, the disappearance of ferroelectric distortions, exemplified by PbTiO₃ relaxing to a cubic phase without tetragonality, reflects the loss of the soft-mode instability central to ferroelectricity [12, 13]. The inability to couple strain and polarization manifests in near-zero piezoelectric coefficients even for prototypical materials such as quartz and LiNbO₃, while phonon spectra exhibiting near-degenerate longitudinal and transverse optical modes further confirm the absence of macroscopic electrostatic fields [7]. At the mesoscale, molecular-dynamics trajectories characterized by spontaneous domain proliferation reveal that domain-wall formation carries negligible energetic cost when depolarizing fields are excluded [13, 20]. Each manifestation can be traced directly to the same missing long-range contribution, converting qualitative discrepancies into reproducible signatures that challenge the adequacy of local-only graph models for polar systems.

Detection principles

The absence of long-range electrostatics can be exposed through targeted computational probes that interrogate physical consistency rather than predictive accuracy alone. Evaluating the dielectric response under a small applied field immediately reveals anomalously low permittivity and weak compositional dependence in high- κ materials such as BaTiO₃ and PbTiO₃ [19], reflecting the confinement of polarization to local environments [12]. A complementary perspective arises from phonon analysis at the Brillouin-zone center, where the absence of LO–TO splitting—reduced to

near degeneracy—signals that the Coulombic $1/r$ interaction has not been internalized by the model [7]. Structural relaxation tests further expose this limitation when high-symmetry phases remain artificially stable despite density-functional predictions of spontaneous distortion [9, 13], indicating that destabilizing long-range forces are absent by construction. Scaling analyses reinforce this conclusion: properties derived from local graphs converge immediately with system size, in contrast to the extended convergence behavior expected when electrostatics are properly represented [7]. Sensitivity to the cutoff radius provides an additional diagnostic, as significant variation in predicted observables with increasing cutoff reflects the incomplete capture of long-range interactions [21–23]. Taken together, these probes establish that the observed deficiencies arise not from data scarcity but from the structural constraints of the model itself [13].

Mitigation principles

Restoring physical fidelity requires architectural modifications that reintroduce long-range electrostatic coupling without forfeiting computational efficiency. Embedding an explicit Ewald contribution within the training objective constrains predicted energies to respect the correct Coulombic interactions, aligning learned representations with the Madelung energy landscape [7, 22]. Extending node features to include multipole moments enables analytical treatment of electrostatics beyond pairwise interactions, preserving local message passing while incorporating global field effects [22, 24]. Hybrid architectures further reconcile locality and globality by coupling short-range graph updates with a parallel electrostatic solver that feeds back into the representation of polarization [7, 24]. Expanding the cutoff radius, when combined with efficient sampling or sparsity strategies, captures a substantial portion of the electrostatic tail without prohibitive computational cost [21]. Incorporating self-consistent charge equilibration introduces adaptive charge distributions that encode global neutrality and field effects intrinsically [7], while explicit representation of polarization at the graph level enforces coupling between local environments and macroscopic observables [9]. These interventions demonstrate that scalability and physical completeness are not mutually exclusive, but instead can be jointly achieved through designs that explicitly acknowledge the nonlocal character of electrostatics [13, 22, 25].

Table 2 converts the critique into an operational decision framework by linking each diagnostic signature of cutoff failure to the specific architectural intervention most likely to restore the missing physics.

Table 2. Diagnostic-to-Mitigation Alignment Framework for Evaluating Whether a Crystal GNN Is Architecturally Valid for Polar Materials

Diagnostic signature	What the signature reveals about the architecture	Underlying missing physical channel	Most appropriate mitigation priority	Why that mitigation is structurally matched to the failure	Expected improvement if successful
Dielectric constant remains unrealistically low across known high- κ materials	The model sees only local dipoles, not collective polarization response	Long-range dipole-dipole and lattice-wide electrostatic coupling	Explicit graph-level polarization feature or hybrid global electrostatic branch	These interventions create a macroscopic state variable that can accumulate nonlocal polarization information	Recovery of composition-sensitive dielectric trends and physically plausible ϵ values
LO–TO splitting collapses to near-degeneracy	The model lacks the macroscopic electric field term	Nonlocal electrostatic contribution to optical phonons	Ewald summation term or analytic long-range	The failure is field-theoretic, so the correction must inject the missing	Reappearance of nonzero LO–TO separation and

	in the effective force description		electrostatic solver	long-range field explicitly	more realistic phonon structure
Known ferroelectric relaxes to the cubic phase	The energy landscape is missing the long-range destabilizing term that supports symmetry breaking	Competition between local repulsion and nonlocal Coulomb stabilization	Hybrid local-plus-global architecture with long-range energy decomposition	The correction restores the missing energetic balance rather than only adding more local depth	Restoration of spontaneous distortion and better phase-ordering fidelity
Predicted piezoelectric response is strongly suppressed	The architecture cannot transmit strain-induced charge redistribution across the crystal	Nonlocal electromechanical coupling	Charge equilibration layer plus polarization-conditioned updates	Piezoelectricity requires charge adaptation under global constraints, not only fixed local descriptors	Improved strain–polarization coupling and more realistic piezoelectric coefficients
Polar predictions converge immediately with increasing supercell size	The graph interaction horizon is fixed, so the model cannot respond to enlarged electrostatic environment	Supercell-scale accumulation of long-range fields	Larger effective cutoff plus efficient sparse sampling, or true global branch	The mitigation expands or bypasses the finite graph horizon that causes false convergence	Property scaling becomes size-sensitive in physically plausible ways
Outputs change strongly when cutoff is increased from 5 Å to 10–15 Å	Original model validity depended on an arbitrary cutoff rather than a stable physical representation	Hidden sensitivity to truncated electrostatic tail	Transition from cutoff-only model to explicit long-range correction	High cutoff sensitivity indicates that locality is not a stable inductive bias for the task	Reduced hyperparameter fragility and more robust transfer across polar materials
Domain-wall energies are near zero or microstructures become unphysical in simulation	The architecture does not encode electrostatic penalties associated with mesoscale polarization textures	Extended depolarization fields and boundary-condition effects	Global electrostatic branch with supercell-aware conditioning	Domain energetics are controlled by extended fields, so only a nonlocal mechanism can recover them	More realistic wall energies, domain stability, and simulation trajectories
Surface terminations or reconstructions are misranked in polar slabs	The model lacks access to the electrostatic imbalance driving compensation mechanisms	Nonlocal surface-normal field and long-range charge redistribution	Multipole-aware or Ewald-aware slab treatment	Surface polarization problems are boundary-field problems, not purely local coordination problems	Better reconstruction ranking and more realistic polar-surface energetics

Relation to Other Critiques

This critique intersects with three earlier lines of inquiry yet sharpens the discussion by anchoring it to a single, physically unavoidable failure case: polar crystals.

Relation to local versus global trade-off [21]: Gong and co-workers identified periodicity and long-range order as fundamental challenges for crystal GNNs and noted that finite cutoffs implicitly discard global information. The present work supplies the concrete consequence of that trade-off: when the discarded information is electrostatic, the model systematically fails on every functional property that defines polar materials.

Relation to over-smoothing [1, 2]: Early crystal-graph frameworks observed that stacking many layers to capture distant neighbors leads to feature homogenization and loss of discriminative power. Long-range electrostatics exacerbate the same depth limitation because the relevant interactions are not merely “distant” but macroscopically collective; over-smoothing is therefore a symptom, not the root cause. The mitigation principles above (especially explicit polarization features and hybrid architectures) address both problems simultaneously.

Relation to equivariance [8]: Equivariant GNNs elegantly enforce rotational and translational symmetry yet still operate under the local-cutoff assumption. Batzner *et al.* achieved impressive data efficiency for interatomic potentials, but the same networks cannot reproduce LO-TO splitting or spontaneous polarization in ferroelectrics because symmetry preservation does not restore the missing Coulomb sum [8, 13, 17]. Equivariance solves a different problem; long-range electrostatics require an orthogonal architectural commitment.

Relation to cutoff assumptions [13, 21]: The placeholder analysis “Why local GNNs fail for polar crystals” and the periodicity study [21] both flag cutoff radius as a hidden hyperparameter. This critique demonstrates the material-specific consequence: for any insulator with a net dipole moment the cutoff is not a tunable knob but a physical error that propagates directly into dielectric collapse, ferroelectric disappearance, and domain-wall blindness. By isolating polar crystals as the decisive test case, the argument moves beyond general warnings about locality and supplies falsifiable detection principles and targeted mitigations.

Implications for GNN Design for Polar Materials

For model developers the message is unambiguous: any architecture that defaults to a 5–6 Å cutoff without a long-range correction is unsuitable for polar crystals [7, 13, 24]. Implement Ewald summation, multipole expansions, or hybrid global branches from the outset rather than as post-hoc patches. Report dielectric constants, LO-TO splitting, and spontaneous polarization as mandatory validation metrics alongside energy or force errors; these quantities expose architectural flaws that energy alone conceals [9, 19].

For practitioners the practical recommendation is equally clear: treat local GNN predictions of ferroelectric distortion, piezoelectric coefficient, or dielectric response as unreliable until the model has passed the five detection principles [12]. When screening large libraries of candidate perovskites or piezoelectrics, discard purely local models or augment them with at least one of the mitigation strategies [11, 16, 26, 27]. Hybrid architectures already exist in the literature and can be adopted with minimal overhead [22–24].

For benchmark designers the implication is structural. Current crystal benchmarks under-represent polar compounds and entirely omit dielectric and ferroelectric ground-truth labels. Future suites must include dedicated polar test sets (perovskites, LiNbO₃-type piezoelectrics, KDP-type hydrogen-bonded ferroelectrics) and must publish not only formation energies but also Born effective charges, LO-TO splittings, and domain-wall energies [12, 28]. Only then will progress in graph-based methods be measurable against the physics that actually matters for applications.

Taken together, these implications shift the field from an era of “good enough on energies” to one of physically faithful prediction for the materials that enable modern electronics. The cost of ignoring long-range interactions is no longer abstract; it is measured in missed high- κ dielectrics, unstable ferroelectric memories, and unphysical piezoelectric coefficients [19]. Model developers, practitioners, and benchmark curators must now treat long-range electrostatics as a first-class design constraint rather than an optional refinement.

Conclusion

The reliance on finite cutoffs in graph-based representations embeds a locality assumption that fails fundamentally for polar crystals, where long-range electrostatics constitute the dominant organizing principle. The resulting discrepancies—manifested as suppressed dielectric response, incorrect phase stability, degenerate phonon modes, and unphysical mesoscale behavior—are not isolated inaccuracies but coherent signatures of missing physics. Diagnostic probes expose these failures with minimal computational overhead, consistently tracing them to the absence of lattice-wide Coulomb interactions rather than to deficiencies in data or model capacity. This analysis therefore reframes the limitations of local GNNs as architectural rather than empirical.

The implications extend beyond methodological refinement to the validity of data-driven discovery in functional materials. Polar systems underpin key technologies in energy storage, sensing, and information processing, yet their defining properties emerge from collective electrostatic phenomena that cannot be reduced to local coordination environments. Architectures that neglect these interactions risk producing systematically misleading predictions, even when conventional energy benchmarks appear satisfactory. Incorporating explicit long-range mechanisms—through global electrostatic solvers, charge-aware representations, or polarization-coupled updates—restores the necessary physical channels while preserving computational efficiency, indicating that the trade-off between scalability and fidelity is not intrinsic but design-dependent.

Progress in graph-based materials modeling therefore hinges on elevating long-range electrostatics from an optional correction to a core architectural principle. The persistence of locality as a default reflects historical convenience rather than physical generality, and its continued use in polar contexts constrains both predictive accuracy and scientific insight. A shift toward hybrid representations that reconcile local structure with global field effects is required if GNNs are to serve as reliable tools for the discovery and design of polar materials.

Acknowledgements

None

Conflict of interest

None

Financial support

None

Ethics statement

None

Received: 05 Dec 2023

Revised: 29 Feb 2024

Accepted: 19 May 2024

Published online: 18 July 2024

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