

ORIGINAL RESEARCH

Open access

When Long-Range Interactions Break ML Potentials: A Failure Mode Study of Charge-Transfer Sensitivity

Peter Novak^{1*}, Jana Svoboda¹

Abstract

Machine learning interatomic potentials achieve high accuracy at molecular-dynamics scales but rely on local descriptors that truncate long-range interactions. In charge-transfer-sensitive materials, where electrostatics decay as $1/r$, this assumption fails. The resulting mismatch produces systematic errors, including non-convergent energies, force discontinuities, unstable charge distributions, oxidation-state ambiguity, suppressed ionic transport, and collapsed dielectric response. These effects are not incidental but arise directly from the absence of global electrostatic coupling. This work presents a failure-mode analysis that links these breakdowns to their physical origin and introduces practical diagnostics based on standard simulation outputs. It further outlines mitigation strategies that restore long-range physics through electrostatic solvers, charge equilibration, multipole representations, and hybrid architectures. By establishing when and why locality fails, the study defines the minimal requirements for charge-transfer-aware machine learning potentials and provides a pathway toward reliable simulation of ionic and polar materials.

Keywords Failure mode analysis, Machine learning potentials, Long-range electrostatics, Charge transfer, Ionic conductors, Solid electrolytes

*Correspondence:

Peter Novak
peter.novak@gmail.com

¹ Department of Data-Driven Materials Systems, Faculty of Engineering, Charles University, Prague, Czech Republic

Introduction

Machine learning potentials have transformed atomistic simulation for covalent and metallic systems [1–5]. But for materials where charge transfer matters—ionic conductors, solid electrolytes, polar oxides, battery materials—local ML potentials fail systematically. The reason: charge transfer creates long-range electrostatic interactions that decay as $1/r$, not exponentially. A finite cutoff of 6 Å captures only a fraction of this interaction. This paper analyzes failure modes of local ML potentials for charge-transfer-sensitive systems, explains why cutoffs break, and proposes detection and mitigation strategies.

The rapid adoption of ML potentials stems from their ability to reproduce density-functional-theory potential-energy surfaces at a fraction of the computational cost [6, 7]. Equivariant graph neural networks [1], deep potential models [3], and Gaussian-process-based approaches [2, 6] now routinely enable nanosecond-scale simulations of thousands of atoms. Their success, however, rests on an implicit locality assumption: the energy and forces on any atom depend only on its immediate chemical environment inside a spherical cutoff [8, 9]. This approximation is benign when bonding is short-ranged and directional, as in silicon or copper. In ionic and polar compounds, however, electrons are not localized; they redistribute over distances far beyond nearest-neighbor shells. The resulting partial charges generate Coulomb fields

whose magnitude decreases slowly with separation. Because the $1/r$ form lacks an intrinsic decay length, any finite cutoff necessarily discards a non-negligible tail of the electrostatic energy.

Early ML potentials were deliberately designed for materials with localized electrons [2, 3, 10]. Their descriptors—symmetry functions, bispectrum components, or message-passing graphs—encode geometry within a few angstroms. When these models are applied to systems with significant ionicity, the missing long-range contributions manifest as qualitative errors rather than mere quantitative noise. Energy no longer converges with supercell size, forces acquire artificial discontinuities, and predicted transport properties deviate dramatically from experiment. These failures are not random; they are the predictable consequence of truncating a long-range interaction.

The present failure-mode study deliberately avoids performance tables or dataset comparisons. Instead it dissects the physical mechanisms that cause local ML potentials to break in charge-transfer environments. Five principal mechanisms are identified and linked to six observable failure modes. Detection principles are offered that rely on standard simulation workflows rather than specialized diagnostics. The analysis is grounded in the conceptual architecture of existing ML frameworks [1, 10–12] while remaining agnostic to specific numerical implementations.

Understanding these failure modes is urgent. Ionic conductors and solid electrolytes are central to solid-state batteries, fuel cells, and electrochemical sensors. Polar oxides underpin dielectrics, ferroelectrics, and memristors. Battery electrode materials exhibit mixed valence and dynamic charge redistribution during cycling. If ML potentials are to accelerate discovery in these domains, their architectures must incorporate the long-range physics that local descriptors omit [8, 13, 14]. This paper therefore serves both as a cautionary guide for current users and as a blueprint for developers who wish to extend the reach of ML potentials into the ionic realm. By clarifying where and why local approximations collapse, it paves the way for the next generation of charge-transfer-aware models that treat electrostatics explicitly rather than hoping that a larger cutoff or deeper network will suffice.

Figure 1 maps the full analytical progression from the physical non-locality of charge transfer to the architectural truncation imposed by local ML potentials, the resulting breakdown mechanisms, the observable failure modes, and the corresponding detection and mitigation pathways.

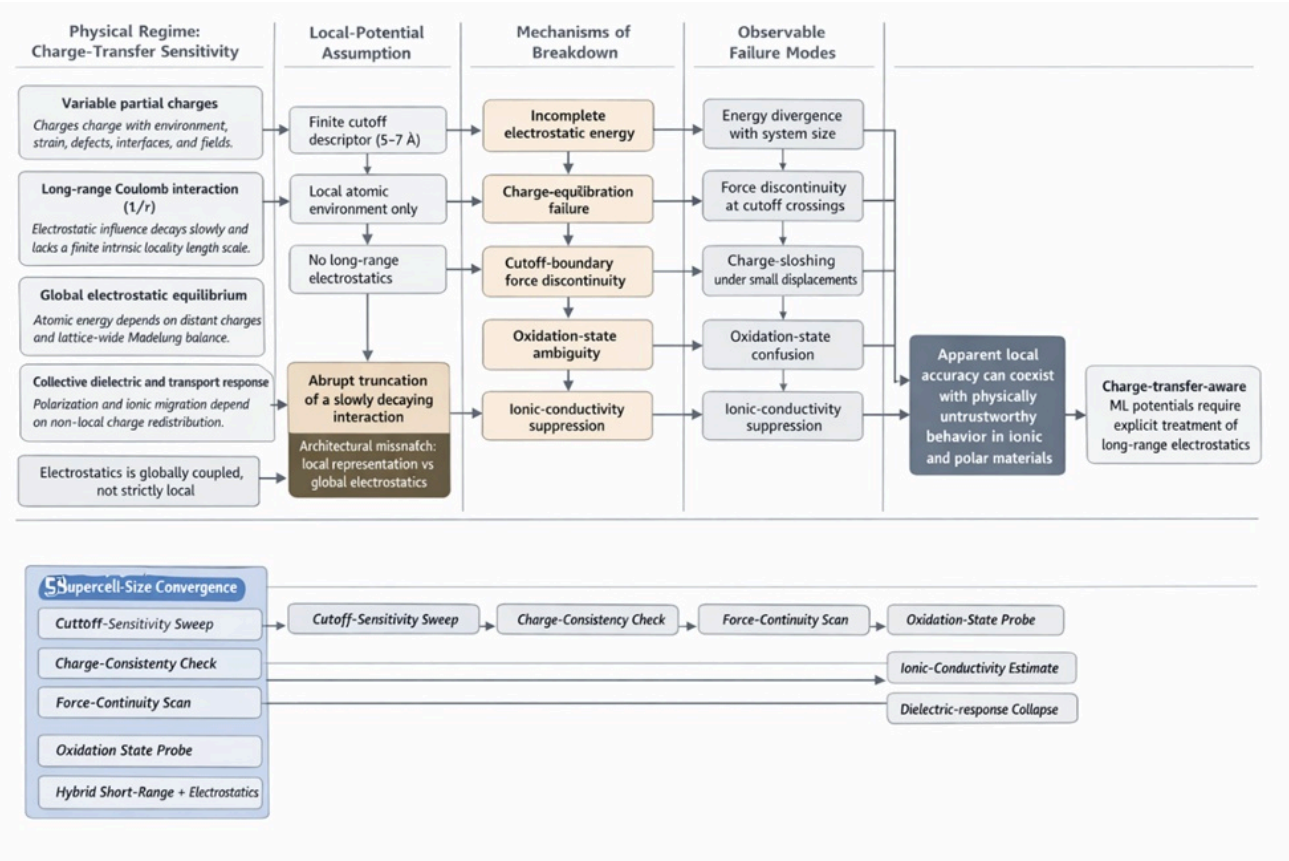


Figure 1. Structural Architecture of Electrostatic Truncation Failure in Charge-Transfer-Sensitive Machine Learning Potentials

What are Charge-Transfer Sensitive Systems?

A charge-transfer-sensitive system is any material in which atomic charges vary significantly with local environment and electrostatic interactions dominate the total energy. In such materials the formal oxidation state is only a starting point; actual partial charges respond to strain, temperature, defects, interfaces, and applied fields. The electrostatic contribution therefore cannot be treated as a small perturbation. It constitutes a major fraction of the cohesive energy and dictates structural, dynamic, and transport behavior.

Classic examples include solid electrolytes such as Li_3PS_4 and $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$, where lithium ions move through a framework of partially charged metal anions [15–18]. Ionic oxides— MgO , Al_2O_3 , TiO_2 —exhibit strong ionicity even in the bulk crystal [5, 19]. Polar intermetallics and battery electrode materials such as LiCoO_2 and LiFePO_4 display mixed valence and rapid charge redistribution during lithium insertion or extraction [20, 21]. Even seemingly simple compounds like Fe_3O_4 contain iron atoms in different oxidation states whose balance is maintained by long-range electrostatic equilibrium.

Charge transfer matters for three reasons. First, ions carry partial charges that are not fixed integers; the magnitude and sign of these charges adjust continuously to minimize the global electrostatic energy. Second, any perturbation—lattice expansion, vacancy formation, or surface creation—triggers charge redistribution that propagates beyond nearest neighbors. Third, the electrostatic energy itself scales as $1/r$. At a typical cutoff of 6 Å the interaction retains roughly 17 % of its contact strength; at 10 Å it is still 10 %. No cutoff small enough for efficient computation can make this tail negligible.

Consequently, local descriptors that ignore atoms beyond 6–7 Å inherently miss a substantial and structurally decisive piece of the physics.

Local cutoffs therefore fail at a fundamental level. The environment of an atom is defined only by its immediate neighbors, yet its energy depends on the positions and charges of atoms many coordination shells away. A lithium ion in a solid electrolyte “feels” the Madelung field of the entire crystal, not just the four or six nearest anions. When an ML potential truncates this field, the predicted energy landscape distorts. Diffusion barriers are altered, defect formation energies become size-dependent, and collective phenomena such as polarization or ionic conduction are suppressed. The failure is not a question of insufficient training data or poor hyper-parameters; it is an architectural mismatch between the model’s locality and the long-range character of the underlying physics.

Mechanisms of Failure

The breakdown of local machine learning potentials in charge-transfer systems arises from interdependent failure modes rooted in the truncation of long-range $1/r$ electrostatics. Limiting descriptors to a finite cutoff excludes a non-negligible Coulombic tail, so electrostatic energy does not converge with system size as in a true Madelung sum, introducing a spurious dependence of energy per atom on supercell volume [8, 22]. This truncation also constrains charge assignment to local environments, preventing the self-consistent redistribution required to minimize global electrostatic energy; charges remain effectively frozen with respect to distant fields, even when explicitly predicted, and thus cannot satisfy Coulombic equilibrium conditions [23–25]. As a related consequence, interactions that should vary smoothly instead undergo abrupt changes when atoms cross the cutoff boundary, producing discontinuities in force evaluations that destabilize molecular dynamics, particularly in highly ionic systems [4, 9].

Beyond these immediate effects, the same locality undermines the resolution of electronically distinct states whose stability depends on lattice-wide electrostatic balance. Oxidation states that are separable only through long-range compensation become indistinguishable within a truncated representation, collapsing multiple configurations onto a single energy surface and distorting derived properties. This limitation extends to polarization phenomena, where the inherently collective response to fields or strain cannot be captured without long-range coupling, leading to suppressed or unphysical dielectric behavior [8, 19, 26]. Under these conditions, the individual failure modes reinforce one another, forming a coherent structural limitation that cannot be remedied through additional local data alone.

A Typology of Failure Modes

The five mechanisms manifest as six observable failure modes that appear consistently across charge-transfer-sensitive materials.

Table 1 consolidates the causal structure of charge-transfer failure by linking each truncation mechanism to its lost physical dependency, its immediate modeling distortion, its dominant observable manifestation, and its most discriminating diagnostic readout.

Table 1. Mechanism-to-Manifestation Matrix for Electrostatic Truncation Failure in Charge-Transfer-Sensitive ML Potentials

Failure-generating mechanism	Lost physical dependency	Immediate modeling distortion	Observable manifestation	Most discriminating diagnostic readout	Why this matters scientifically

Incomplete electrostatic energy	Lattice-wide Coulomb stabilization and destabilization	Energy landscape omits non-negligible long-range tail	Energy per atom drifts with supercell size	Supercell convergence test	Reveals that the model is not representing the thermodynamic limit correctly
Charge-equilibration failure	Global redistribution of electron density under electrostatic balance	Charges remain locally assigned rather than self-consistently adjusted	Charge sloshing; inconsistent charge patterns across equivalent environments	Charge-consistency check	Shows that the model cannot recover the correct global electronic response even when local geometry is similar
Cutoff-boundary force discontinuity	Smooth spatial evolution of electrostatic forces	Force components jump as neighbors cross the cutoff	Spikes in forces, energy drift, unstable molecular dynamics	Force-continuity scan	Demonstrates that the potential is dynamically unreliable even if static energies appear acceptable
Oxidation-state ambiguity	Non-local valence stabilization across the lattice	Distinct redox states collapse into one locally defined representation	Incorrect site preference, magnetic state, or redox assignment	Oxidation-state probe	Indicates that local coordination alone is insufficient to represent mixed-valence chemistry
Polarization-response failure	Collective dielectric coupling and long-range dipolar response	Polar response becomes artificially localized or suppressed	Dielectric-response collapse	Field-response or dielectric test	Shows that macroscopic electromechanical behavior cannot emerge from the architecture
Combined transport-path distortion	Long-range electrostatic barrier shaping along diffusion pathways	Migration landscape becomes flattened, shifted, or discontinuous	Ionic-conductivity suppression	Elevated-temperature conductivity estimate	Exposes failure in the very property class most relevant to solid electrolytes and battery materials

Failure modes in charge-transfer systems

Energy divergence becomes evident when the predicted energy per atom varies systematically with supercell size rather than approaching a stable limit. Whereas a true ionic crystal rapidly converges to the Madelung value, truncation of long-range interactions yields a persistent drift as distant charges are incrementally included, producing a non-plateauing dependence on inverse system size. This sensitivity to truncation extends to dynamical behavior, where atoms crossing the cutoff boundary trigger abrupt changes in interaction terms, leading to discontinuities in forces and corresponding spikes in total energy that disrupt energy conservation and induce artificial thermostat responses. A related instability emerges in charge assignment: small atomic displacements can induce disproportionate oscillations in predicted charges, including abrupt sign changes, reflecting the model's inability to maintain a globally consistent electrostatic equilibrium. Under these conditions, the absence of long-range coupling also obscures distinctions between oxidation states that depend on lattice-wide charge compensation, collapsing electronically distinct configurations and distorting derived magnetic or structural properties. The same limitation propagates to transport predictions, where missing electrostatic barriers flatten migration landscapes and suppress ionic conductivity relative to reference behavior, and to dielectric response, where the inability to sustain collective polarization reduces the predicted permittivity toward unity, precluding meaningful representation of polar phenomena [18, 19, 26]. Taken together, these signatures provide direct empirical manifestations of the underlying architectural constraint imposed by local approximations.

Detection principles

Detection of such failures can be achieved through computationally inexpensive diagnostics that exploit these characteristic responses without recourse to new reference data. Systematic variation of supercell size reveals whether energy per atom converges within a physically reasonable tolerance, while controlled expansion of the cutoff radius exposes undue sensitivity of energies and forces to truncation [8, 9]. Consistency of predicted charges across equivalent local environments embedded in different global configurations probes whether charge assignment remains invariant under changes beyond the cutoff, and gradual displacement of an ion across a cutoff boundary tests the continuity of force predictions. Application to mixed-valence systems further interrogates the model's capacity to resolve oxidation states through correct magnetic or site-specific behavior, while finite-temperature molecular dynamics combined with transport analysis exposes deficiencies in ionic conductivity arising from missing long-range barriers [17, 18]. When multiple diagnostics indicate anomalies, the presence of charge-transfer failure becomes unambiguous, providing a practical criterion for excluding unsuitable models and, conversely, a stringent benchmark for validating approaches that claim to incorporate long-range electrostatics.

Mitigation Principles

Several practical strategies can restore the missing long-range physics without sacrificing the efficiency of local ML potentials. These mitigation principles integrate explicit electrostatic treatments while preserving the strengths of short-range descriptors.

Table 2 converts the manuscript's diagnostic principles into a decision framework by showing which failure signatures indicate merely local behavior and what minimum architectural response is required before a model can be considered charge-transfer-aware.

Table 2. Diagnostic-to-Mitigation Alignment Framework for Determining Whether a Potential Is Merely Local or Truly Charge-Transfer-Aware

Diagnostic principle	Failure signature if a model is only local	Interpretive implication	Minimum acceptable response from an improved architecture	Most relevant mitigation family	Acceptance criterion for charge-transfer-aware status
Supercell convergence test	Energy per atom continues drifting as cell size grows	Missing electrostatic tail is still structurally important	Energy approaches a stable plateau with size	Ewald summation with predicted charges; hybrid local-plus-long-range architecture	No meaningful drift once the supercell exceeds the electrostatic interaction span relevant to the material
Cutoff-sensitivity sweep	Large changes in total energy or forces when the cutoff is enlarged	The model remains strongly dependent on arbitrary truncation radius	Predictions become weakly sensitive to cutoff extension	Larger damped cutoffs for moderate cases; explicit long-range solver for strongly ionic systems	Cutoff enlargement changes results only marginally
Charge-consistency	Equivalent local motifs receive	Local representation	Charges adjust consistently with	Self-consistent charge	Charge assignment remains physically

check	different effective charges across different global contexts	cannot enforce global charge equilibrium	full electrostatic environment	equilibration; electrostatic-aware loss	coherent across equivalent environments embedded in different cells
Force-continuity scan	Force jumps appear at neighbor entry or exit from cutoff shell	Dynamics are numerically and physically unstable	Forces vary smoothly along displacement trajectory	Smooth damping; explicit long-range Coulomb treatment	No discontinuous force jump along controlled crossing
Oxidation-state probe	Mixed-valence sites collapse into indistinguishable representations	Redox-sensitive chemistry is not encoded correctly	Distinct valence environments remain distinguishable under global charge balance	Charge equilibration; multipole or polarization-aware models	Correct site differentiation and chemically plausible valence-sensitive energetics
Ionic-conductivity estimate	Conductivity is near zero or severely underestimated	Migration barriers and collective ionic interactions are misrepresented	Diffusive motion and barrier topology remain physically realistic	Hybrid electrostatic architectures; charge-response models	Conductivity and migration behavior fall within physically credible range
Dielectric or field-response test	Response is vacuum-like or unrealistically local	Collective polarization is absent	Macroscopic response emerges from coupled charge redistribution	Multipole models; polarizable long-range terms	Dielectric behavior is qualitatively and quantitatively non-collapsed

Incorporating long-range electrostatics into machine learning potentials can be achieved by coupling locally predicted quantities with globally consistent interaction schemes [8, 13, 22]. One effective strategy augments locally inferred atomic charges with an Ewald summation, allowing the total energy to recover the full Coulomb contribution under periodic boundary conditions. Because the electrostatic term converges efficiently and can be evaluated with near-linear scaling after standard optimizations, this correction introduces minimal overhead while restoring physically meaningful energetics; its stability in strongly ionic systems has been demonstrated by Rowe *et al.* [10] and Ko *et al.* [13]. A related development embeds charge equilibration directly within the model, replacing fixed charge assignment with parameters that define a self-consistent minimization of global electrostatic energy at each molecular-dynamics step. This formulation enables charges to respond dynamically to the evolving environment, and quasi-linear scaling implementations have been shown by Gubler *et al.* and Khajepasha *et al.* to recover accurate ionic transport behavior despite the added computational layer [11, 25].

Beyond explicit electrostatic solvers, extensions of the local representation itself can partially mitigate truncation effects. Increasing the cutoff radius while enforcing smooth damping at its boundary captures a larger fraction of the Coulomb tail and removes force discontinuities, improving convergence in moderately ionic regimes without incurring the full cost of long-range summation [9]. Greater fidelity can be achieved by enriching the representation with higher-order multipoles, allowing the model to encode anisotropic charge distributions and recover dielectric responses that monopole-only descriptions cannot reproduce, as demonstrated in polarizable frameworks by Mohri *et al.* and Zinovjev [12, 22]. These developments converge toward hybrid architectures in which short-range interactions are modeled by flexible neural networks while electrostatics are handled by dedicated physics modules, combined through carefully designed switching functions that preserve continuity and avoid double counting; such strategies have yielded system-size-consistent behavior in the work of Wang *et al.* and Zhou [7, 27]. Complementing architectural changes, the training objective itself

can be modified to include explicit electrostatic terms, constraining the learned representation to reproduce reference long-range contributions rather than compensating through local errors [22]. Through these interconnected adjustments, local potentials are transformed into charge-transfer-aware models, retaining computational efficiency while eliminating the systematic failures associated with truncated electrostatics.

Relation to Other Failure Modes

The charge-transfer failure mode is not isolated; it intersects with several previously identified limitations of ML potentials. It shares a common root with polar-crystal failures: the absence of long-range electrostatics prevents correct dielectric and ferroelectric behavior. Both issues arise because local descriptors cannot propagate polarization or charge response beyond the cutoff sphere. Where polar-crystal analyses emphasize macroscopic response, the present study highlights microscopic charge redistribution and its impact on ionic transport.

The problem also connects to over-smoothing in deep networks. Over-smoothing limits information flow through many layers, while long-range electrostatics demand explicit global coupling. Deeper networks alone cannot compensate for a missing $1/r$ term; the architecture must incorporate non-local physics rather than relying on additional message-passing hops.

Domain-adaptation techniques address distribution shifts between training and target data but cannot inject missing fundamental interactions. Training on more ionic examples may reduce quantitative errors, yet the underlying architectural locality remains. Domain adaptation therefore masks symptoms without curing the root cause.

Uncertainty quantification offers another perspective. Models often report high uncertainty precisely in charge-transfer regimes because local descriptors fail to generalize. While uncertainty estimates correctly flag unreliable predictions, they do not provide a corrected energy or force [4]. Explicit long-range corrections are still required to convert high-uncertainty regions into reliable ones [8, 13].

These relations underscore a broader pattern: many failure modes in ML potentials trace back to the tension between local descriptors and global physical effects. Charge-transfer sensitivity is simply the most pronounced case when electrostatics dominate. Recognizing the overlap helps developers prioritize architectural extensions that simultaneously resolve multiple weaknesses rather than patching each failure in isolation.

Implications for ML Potential Development

For model developers the central lesson is that local cutoffs are fundamentally insufficient for charge-transfer systems. Any new architecture intended for ionic conductors or polar oxides must incorporate at least one of the mitigation principles outlined above. Implementing Ewald summation or charge equilibration should become standard practice rather than an optional add-on [13, 22, 25]. Developers should routinely test on ionic-conductivity benchmarks and reject models that fail supercell-convergence checks [4, 18].

Practitioners must adopt stricter validation protocols before deploying ML potentials. Local models should not be used for solid electrolytes, battery electrodes, or ionic oxides without first confirming charge-transfer awareness. Hybrid models that embed long-range electrostatics are now the safer default [7, 8, 13, 22]. Routine application of supercell convergence and cutoff-sensitivity tests will quickly reveal hidden failures and prevent wasted simulation time.

Benchmark designers bear equal responsibility. Future community benchmarks must include charge-transfer systems and require reporting of energy convergence with supercell size, dielectric constants, and ionic conductivities [4, 18]. Accuracy tables that ignore these metrics create a false sense of generality. Requiring explicit disclosure of failure modes—rather than averaging them away—will accelerate progress toward truly transferable potentials.

The implications extend beyond technical choices. Funding agencies and journals should prioritize architectures that demonstrably handle long-range electrostatics when evaluating proposals or manuscripts on energy materials. Only by elevating charge-transfer performance to a core evaluation criterion will the field produce ML potentials that match the real-world demands of next-generation batteries and electrochemical devices.

Toward Charge-Transfer-Aware ML Potentials

Charge-transfer-aware ML potentials must satisfy four minimal requirements [8, 13]. First, they predict variable atomic charges rather than fixed or purely local values [25]. Second, they compute long-range electrostatic energy through an Ewald summation or equivalent method that converges with system size [22]. Third, they incorporate charge equilibration or a learned charge-response mechanism so that charges adjust self-consistently [13, 25]. Fourth, they capture polarizability by responding correctly to external fields or local strain.

Promising research directions include differentiable Ewald implementations inside ML frameworks, allowing end-to-end training of the full electrostatic contribution [22]. Graph networks that output charge-response tensors could enable fast prediction of polarization under arbitrary conditions. Multi-scale designs that delegate short-range bonding to local networks while reserving long-range physics for an explicit solver offer an attractive balance of accuracy and speed [7].

Success will be measured by concrete physical benchmarks. A charge-transfer-aware potential should reproduce density-functional-theory ionic conductivity within a factor of two, exhibit energy per atom that plateaus with supercell size, and predict dielectric constants in agreement with experiment [18]. When these criteria are met across diverse ionic and polar chemistries, ML potentials will finally become general-purpose tools for the materials that matter most to sustainable energy technologies.

Conclusion

Local machine learning potentials fail in charge-transfer systems because finite cutoffs cannot represent long-range electrostatics. This limitation leads to predictable breakdowns in energy convergence, force continuity, charge stability, redox behavior, transport, and dielectric response. These failures reflect a structural mismatch rather than insufficient data or model capacity.

Reliable use in ionic and polar materials therefore requires explicit validation and incorporation of long-range interactions. Diagnostic tests reveal when locality breaks, while established extensions—such as Ewald summation, charge equilibration, multipole models, and hybrid architectures—restore physical consistency with modest overhead. Progress in machine learning potentials thus depends on moving beyond local approximations toward models that encode global electrostatic behavior.

Acknowledgements

None

Conflict of interest

None

Financial support

None

Ethics statement

None

Received: 09 Nov 2023

Revised: 24 Feb 2024

Accepted: 02 Jun 2024

Published online: 18 July 2024

Rights and permissions

Open Access The author(s) retain copyright. This article is licensed under the Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License. It may be shared and adapted for non-commercial purposes with appropriate attribution, an indication of changes, and distribution of adaptations under the same license. Third-party material may be subject to separate terms identified in its credit line. View the license at <https://creativecommons.org/licenses/by-nc-sa/4.0/>.

References

- Batzner S, Musaelian A, Sun L, Geiger M, Mailoa JP, Kornbluth M, et al. E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials. *Nat Commun.* 2022;13(1):2453.
<https://doi.org/10.1038/s41467-022-29939-5>.
- Bartók AP, De S, Poelking C, Bernstein N, Kermode JR, Csányi G, et al. Machine learning unifies the modeling of materials and molecules. *Sci Adv.* 2017;3(12):e1701816.
<https://doi.org/10.1126/sciadv.1701816>.
- Zhang L, Han J, Wang H, Car R, E W. Deep potential molecular dynamics: A scalable model with the accuracy of quantum mechanics. *Phys Rev Lett.* 2018;120(14):143001.
<https://doi.org/10.1103/PhysRevLett.120.143001>.
- Zuo Y, Chen C, Li X, Deng Z, Chen Y, Behler J, et al. Performance and cost assessment of machine learning interatomic potentials. *J Phys Chem A.* 2020;124(4):731-45.
<https://doi.org/10.1021/acs.jpca.9b08723>.
- Chan H, Narayanan B, Cherukara MJ, Sen FG, Sasikumar K, Gray SK, et al. Machine learning classical interatomic potentials for molecular dynamics from first-principles training data. *J Phys Chem C.* 2019;123(12):6941-57.
<https://doi.org/10.1021/acs.jpcc.8b09917>.
- Deringer VL, Bartók AP, Bernstein N, Wilkins DM, Ceriotti M, Csányi G. Gaussian process regression for materials and molecules. *Chem Rev.* 2021;121(16):10073-141.
<https://doi.org/10.1021/acs.chemrev.1c00022>.
- Wang G, Wang C, Zhang X, Li Z, Zhou J, Sun Z. Machine learning interatomic potential: Bridge the gap between small-scale models and realistic device-scale simulations. *iScience.* 2024;27(5):109673.
<https://doi.org/10.1016/j.isci.2024.109673>.
- Anstine DM, Isayev O. Machine learning interatomic potentials and long-range physics. *J Phys Chem A.* 2023;127(11):2417-31.
<https://doi.org/10.1021/acs.jpca.2c06778>.
- Novikov IS, Shapeev AV. Improving accuracy of interatomic potentials: More physics or more data? A case study of silica. *Mater Today Commun.* 2019;18:74-80.
<https://doi.org/10.1016/j.mtcomm.2018.11.008>.

Rowe P, Csányi G, Alfè D, Michaelides A. Development of a machine learning potential for graphene. *Phys Rev B*. 2018;97(5):054303.
<https://doi.org/10.1103/PhysRevB.97.054303>.

Gubler M, Finkler JA, Schäfer MR, Behler J, Goedecker S. Accelerating fourth-generation machine learning potentials using quasi-linear scaling particle mesh charge equilibration. *J Chem Theory Comput*. 2024;20(16):7264-71.
<https://doi.org/10.1021/acs.jctc.4c00334>.

Mohri M, Rostamizadeh A, Talwalkar A. *Foundations of machine learning*. 2nd ed. Cambridge (MA): MIT Press; 2018. 504 p.

Ko TW, Finkler JA, Goedecker S, Behler J. General-purpose machine learning potentials capturing nonlocal charge transfer. *Acc Chem Res*. 2021;54(4):808-17.
<https://doi.org/10.1021/acs.accounts.0c00689>.

Eckhoff M, Reiher M. Lifelong machine learning potentials. *J Chem Theory Comput*. 2023;19(12):3509-25.
<https://doi.org/10.1021/acs.jctc.3c00279>.

Moriel A, Richard D, Lerner E, Bouchbinder E. Elementary processes in dilatational plasticity of glasses. *Phys Rev Res*. 2024;6(2):023167.
<https://doi.org/10.1103/PhysRevResearch.6.023167>.

Kim K, Dive A, Grieder A, Adelstein N, Kang S, Wan LF, et al. Flexible machine-learning interatomic potential for simulating structural disordering behavior of Li7La3Zr2O12 solid electrolytes. *J Chem Phys*. 2022;156(22):221101.
<https://doi.org/10.1063/5.0090341>.

Goedecker SA, Tahmasbi H, Khajepasha ER, Rostami S, Asnaashari H, Faraji S, et al. Structure prediction of ionic materials using the Minima Hopping method and the CENT machine learning potential. In: *APS March Meeting 2021; 2021 Mar 15-19; Virtual. College Park (MD): American Physical Society; 2021. Abstract M41.00008*.

Pan Y. *Predictive modeling of ionic conductivity in solid polymer electrolytes [master's thesis]*. Seattle (WA): University of Washington; 2024.

Mortazavi B, Zhuang X, Rabczuk T, Shapeev AV. Atomistic modeling of the mechanical properties: The rise of machine learning interatomic potentials. *Mater Horiz*. 2023;10(6):1956-68.
<https://doi.org/10.1039/d3mh00125c>.

Bjørheim TS, Hoedl MF, Merkle R, Kotomin EA, Maier J. Proton, hydroxide ion, and oxide ion affinities of closed-shell oxides: Importance for the hydration reaction and correlation to electronic structure. *J Phys Chem C*. 2020;124(2):1277-84.
<https://doi.org/10.1021/acs.jpcc.9b07570>.

Alpaydin E. *Machine learning*. Rev updated ed. Cambridge (MA): MIT Press; 2021. 280 p.

Zinovjev K. Electrostatic embedding of machine learning potentials. *J Chem Theory Comput*. 2023;19(6):1888-97.
<https://doi.org/10.1021/acs.jctc.2c00914>.

Staacke CG, Wengert S, Kunkel C, Csányi G, Reuter K, Margraf JT. Kernel charge equilibration: Efficient and accurate prediction of molecular dipole moments with a machine-learning enhanced electron density model. *Mach Learn Sci Technol*. 2022;3(1):015032.
<https://doi.org/10.1088/2632-2153/ac568d>.

Ongari D, Boyd PG, Kadioglu O, Mace AK, Keskin S, Smit B. Evaluating charge equilibration methods to generate electrostatic fields in nanoporous materials. *J Chem Theory Comput*. 2019;15(1):382-401.
<https://doi.org/10.1021/acs.jctc.8b00669>.

Khajepasha ER, Finkler JA, Kühne TD, Ghasemi SA. CENT2: Improved charge equilibration via neural network technique. *Phys Rev B*. 2022;105(14):144106.

<https://doi.org/10.1103/PhysRevB.105.144106>.

Friederich P, Häse F, Proppe J, Aspuru-Guzik A. Machine-learned potentials for next-generation matter simulations. *Nat Mater.* 2021;20(6):750-61.

<https://doi.org/10.1038/s41563-020-0777-6>.

Zhou ZH. Machine learning. Singapore: Springer Nature Singapore; 2021.

<https://doi.org/10.1007/978-981-15-1967-3>.