ORIGINAL RESEARCH **Open access**

The "Applicability Domain" Problem in Materials AI: A Theoretical Treatment of When Models Should Stay Silent

Lucas Meyer[1*], Anna Schmid[2], Stefan Braun[1]

Abstract

The applicability domain in materials artificial intelligence (AI) represents a fundamental epistemic boundary, beyond which predictive claims lose their scientific legitimacy. Rather than viewing it as a mere technical metric of model performance, this perspective frames the applicability domain as a decision boundary that demarcates regions where AI outputs are conditionally meaningful from those that demand principled silence. In materials science, where heterogeneous chemistries, structures, and processing protocols create complex epistemic landscapes, AI accelerates discovery, but risks overreach through unjustified extrapolation. We introduce a novel theory of scientific silence in materials AI, emphasizing restraint as an active epistemic virtue. This boundary-based framework maps claim types to required warrants, identifying interior regions for warranted predictions, boundary zones for conditional application, and exterior spaces where silence prevents hazard. By posing questions about the limits of generalization and the costs of misplaced confidence, the framework highlights how ignoring boundaries can turn AI from an accelerator into a source of epistemic risk. Ultimately, embracing silence fosters more robust materials innovation, ensuring AI serves as a tool for knowledge rather than illusion.

Keywords Materials AI, Applicability domain, Epistemic boundary, Scientific silence, Extrapolation risk, Decision framework

*Correspondence:
Lucas Meyer
lucas.meyer@gmail.com
[1] Department of Materials Modeling and Artificial Intelligence, Faculty of Engineering, ETH Zurich, Zurich, Switzerland
[2] Department of Data-Driven Materials Science, Faculty of Engineering, University of Bern, Bern, Switzerland

Introduction

Materials design stands at the forefront of scientific and technological progress, confronting the grand challenge of creating substances with tailored properties to address pressing global issues, from energy storage to sustainable manufacturing. The vast parameter space of possible materials—encompassing chemical compositions, crystal structures, microstructures, and processing conditions—renders traditional trial-and-error approaches inefficient and resource-intensive [1, 2]. The complexity arises not only from the sheer number of variables but also from their interdependent interactions, where small changes in one aspect can lead to emergent behaviors in others. This intricacy demands decision-making under incomplete knowledge, where designers must navigate uncertainties inherent in experimental outcomes and theoretical approximations [3, 4].

Artificial intelligence has emerged as a powerful tool to expand the reach of materials science, enabling the exploration of this expansive space at unprecedented speeds. By leveraging machine learning algorithms, AI can discern patterns in large datasets, predict properties of unseen materials, and suggest novel candidates for synthesis. For instance, AI has facilitated the identification of potential superconductors and catalysts, compressing timelines that once spanned decades

into months [5, 6]. However, this acceleration introduces epistemic risks, as AI models often operate as black boxes, blurring the lines between reliable inference and speculative guesswork. The temptation to extend models beyond their trained regimes can lead to predictions that appear confident but lack foundational justification, potentially misguiding experimental efforts and wasting resources.

The applicability domain problem is particularly acute in materials science due to the field's unique characteristics. Unlike domains with more homogeneous data, materials datasets exhibit high heterogeneity: chemical elements vary in their bonding behaviors, structures range from crystalline to amorphous, processing protocols differ across laboratories, and measurement conditions introduce protocol-specific biases [7, 8]. These factors create fragmented knowledge landscapes, where AI models trained on one subset may fail to capture the nuances of another. For example, a model optimized for organic polymers might not account for the quantum effects dominant in inorganic semiconductors, leading to distorted generalizations [9]. Moreover, the multiscale nature of materials—from atomic to macroscopic—amplifies this issue, as models at one scale may ignore emergent phenomena at another [10].

This perspective poses several guiding questions to illuminate the epistemic stakes: Where do AI predictions stop being scientific claims and become mere conjectures? When does extrapolation cross the line into epistemic overreach, eroding the field's credibility? Why is silence—abstaining from output—preferable to unjustified confidence in boundary cases? These questions underscore the need for a conceptual shift, viewing AI not as an infallible oracle but as a bounded instrument requiring vigilant oversight [11, 12].

To address these concerns, we introduce the decision-boundary metaphor as a unifying conceptual framework. In this view, the applicability domain is an epistemic decision boundary, analogous to a frontier in a multidimensional materials space. Within this boundary, AI outputs are conditionally meaningful, supported by sufficient warrants from training data and domain knowledge. Near the boundary, outputs require heightened restraint, perhaps through qualified interpretations. Beyond the boundary, models should enforce silence, refusing to extrapolate without a basis, to avoid propagating errors [13, 14]. This metaphor draws from philosophical traditions in science, where boundaries delineate valid knowledge claims from speculation [15].

The contribution of this paper is a novel theory of when materials AI should abstain, framed through this boundary lens. By developing a progressive argument—from conceptual distinctions to framework application—we argue that silence is not a failure but a principled action that safeguards scientific integrity. This theory has consequences for how we conceptualize AI's role in materials innovation, shifting emphasis from maximizing output to ensuring epistemic soundness [16, 17]. In the following sections, we build this case, beginning with the conceptual background and culminating in a silence framework tailored to materials AI.

Conceptual Background: Applicability, Boundaries, and Risk

Applicability domain vs. out-of-distribution vs. generalization

The concepts of applicability domain, out-of-distribution (OOD) detection, and generalization are closely related in materials AI, yet they encode fundamentally different epistemic commitments. Treating them as interchangeable obscures where model-based claims remain justified and where they become speculative. Framing these concepts in terms of epistemic boundaries helps clarify their distinct roles and associated risks.

The applicability domain refers to the region of feature or representation space within which a model's predictions are considered reliable, given the coverage, diversity, and structure of the training data [18]. Operationally, this domain is often approximated using convex hulls, distance-to-training metrics, or density thresholds. Still, its deeper function is epistemic: it marks where empirical warrants derived from observed material instances remain intact. Within this region, predictions are supported by precedent—either direct or interpolative—and thus retain justificatory grounding.

In contrast, out-of-distribution (OOD) inputs correspond to cases that deviate from the statistical or structural distribution encountered during training [19]. While OOD is frequently defined in statistical terms, in materials science it often reflects more profound discontinuities, such as new bonding motifs, unrepresented phase regimes, or unfamiliar processing conditions. OOD therefore signals potential boundary crossings, in which learned correlations may no longer track the governing physical mechanisms. Importantly, OOD detection does not define where the boundary lies; it merely attempts to flag when an input may have crossed it.

Generalization, meanwhile, concerns a model's ability to extend learned relationships to unseen data drawn from related distributions [20]. Generalization implicitly assumes continuity in the underlying structure–property relationships—a premise that is frequently fragile in materials systems due to heterogeneity, multiscale coupling, and regime-dependent physics. A model may generalize effectively across incremental compositional changes, but fail abruptly at phase boundaries or stability limits. **Table 1** formalizes these distinctions, clarifying their different epistemic functions and failure modes in materials contexts.

Table 1. Conceptual distinctions between applicability domain, out-of-distribution detection, and generalization in materials AI

Concept	What it defines	Epistemic role	Typical failure if misused	Why it matters in materials AI
Applicability domain	Region of warranted inference	Defines epistemic boundary	Overconfident extrapolation	Materials heterogeneity breaks continuity
OOD detection	Statistical deviation signal	Boundary warning, not boundary	False alarms or missed violations	Novel chemistries mimic known features
Generalization	Extension within related regimes	Tests the boundary permeability	Regime collapse at phase limits	Physics changes discontinuously

Using boundary language, the applicability domain constitutes the core epistemic enclosure, OOD marks potential exterior incursions, and generalization probes the permeability of the boundary itself. These distinctions matter because conflating them can lead to misplaced trust. A model may demonstrate strong generalization within a known materials family yet fail catastrophically at OOD boundaries due to unseen shifts in thermodynamic stability, defect behavior, or kinetic constraints [21, 22]. Such failures are not merely predictive errors but epistemic violations arising from boundary misinterpretation.

Why uncertainty does not define the boundary

Uncertainty quantification is frequently invoked as a proxy for epistemic boundaries in materials AI, yet uncertainty alone cannot define where justified inference ends. This limitation arises from a fundamental mismatch between uncertainty as a statistical signal and warrants as epistemic justification.

Aleatoric uncertainty captures irreducible variability in data, such as experimental noise, measurement error, or intrinsic materials heterogeneity [23]. Epistemic uncertainty reflects limitations in the model's knowledge, arising from finite data, incomplete representations, or underspecified physics. While both are informative, neither uniquely encodes whether a prediction lies within or beyond the applicability domain.

Crucially, high uncertainty does not necessarily indicate boundary violation. Predictions well inside the applicability domain may exhibit substantial uncertainty due to sparse sampling or noisy measurements, yet still be epistemically admissible when properly qualified. Conversely, low uncertainty can be dangerously misleading outside the boundary.

Models may express unwarranted confidence in regions where their assumptions silently fail, leading to predictions that lack physical validity [24].

In materials AI, uncertainty estimates often derive from ensemble variance, Bayesian approximations, or stochastic inference techniques. While useful, these methods typically remain agnostic to deeper epistemic assumptions embedded in representations, such as symmetry constraints, conservation laws, or scale-specific validity [25]. As a result, a model may report low uncertainty for a novel alloy that appears feature-wise similar to known systems, while ignoring fundamental differences in phase stability or metastability [26].

Thus, uncertainty should be viewed as contextual information rather than a boundary-defining criterion. It informs decision-making but does not delineate where epistemic warrants hold. Defining the boundary requires integrating uncertainty with broader assessments of representation validity, physical plausibility, and domain relevance [27].

Boundary distortions in materials AI

Epistemic boundaries in materials AI are particularly susceptible to distortion due to the heterogeneous, multiscale, and evolving nature of materials data. Unlike many benchmark ML domains, the boundary is neither static nor uniform, but continuously reshaped by domain-specific factors.

Protocol shifts represent a major source of boundary deformation. Models trained on data generated under one synthesis route, characterization technique, or environmental condition may encounter incompatible regimes when applied elsewhere. Even modest changes in processing history can alter microstructure–property relationships, effectively warping the boundary and creating *leakage zones* where predictions appear admissible but lack causal support [28].

Scale transitions further strain boundary coherence. Atomistic or electronic-scale models often fail to capture mesoscale phenomena such as defect networks, grain boundaries, or phase coexistence. When predictions are extrapolated across scales without explicit invariance preservation, epistemic gaps emerge that are invisible to purely statistical diagnostics [29].

Label drift—the gradual evolution of property definitions, measurement protocols, or performance metrics—also erodes boundary integrity. What counts as “stability,” “durability,” or “efficiency” may shift over time or across subfields, rendering historical training labels epistemically misaligned with contemporary interpretations.

Finally, hidden assumptions embedded in feature engineering or model design can introduce systematic distortions. Ignoring environmental exposure, degradation pathways, or long-term kinetics may not trigger OOD detection, yet such omissions subtly reshape the boundary and bias downstream decisions [30].

Collectively, these effects underscore the epistemic fragility of materials AI. Boundaries are dynamic constructs, shaped by data provenance, representational choices, and evolving scientific understanding, rather than fixed geometric regions [31, 32].

Decision risk across the boundary

The practical significance of epistemic boundaries lies in decision-making under asymmetric risk. In materials discovery and deployment, the consequences of crossing the boundary often far outweigh the potential gains.

Within the applicability domain, decisions are supported by strong warrants and typically entail manageable risk. Near the boundary, decisions enter a conditional regime, where actions may be justified only with explicit caveats, additional validation, or constrained deployment strategies [33]. Beyond the boundary, however, decisions risk cascading failures—such as pursuing infeasible materials candidates, misallocating experimental resources, or overlooking safety and sustainability constraints [14].

In this context, model silence emerges as a rational and scientifically responsible response. Silence is not predictive failure but an acknowledgment of insufficient warrant. By declining to recommend actions beyond the epistemic boundary, AI systems preserve epistemic capital and redirect effort toward boundary-strengthening activities, such as targeted data acquisition, representation refinement, or domain expansion [1, 15]. **Figure 1** maps epistemic regions to concrete decision trajectories, emphasizing silence as a legitimate and constructive outcome rather than predictive failure.

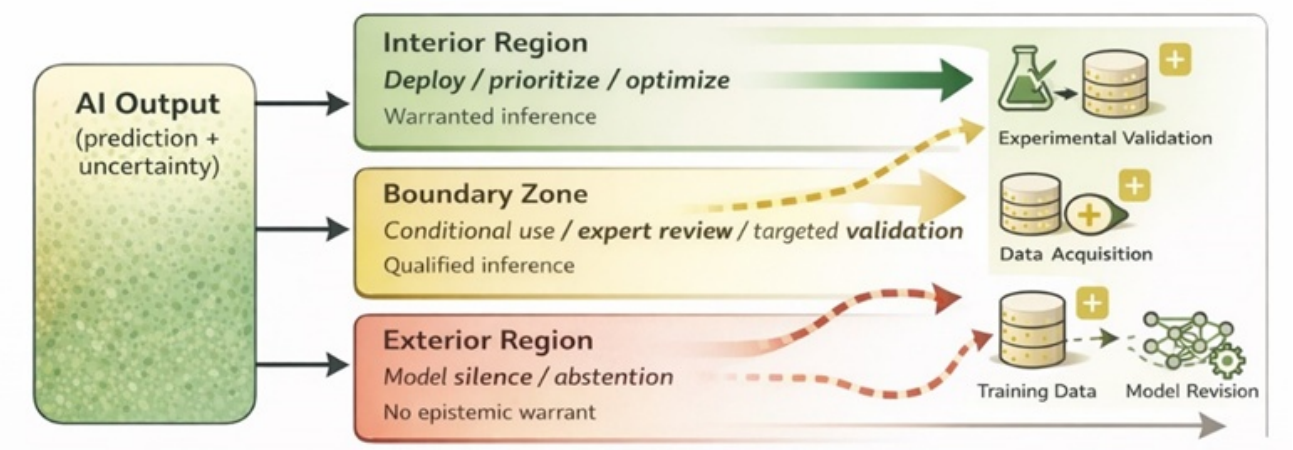

Figure 1. Decision trajectories across the applicability boundary

Silence thus functions as a risk-mitigating strategy aligned with scientific accountability. Rather than maximizing coverage, trustworthy materials AI prioritizes justified action, recognizing that knowing when not to speak is as critical as knowing what to predict.

Consequences

Ignoring boundaries converts AI from a tool to a hazard in materials science. Unchecked extrapolation can propagate flawed claims, undermining trust in AI-driven discoveries and slowing genuine progress [2, 3]. Conversely, embracing boundary-aware practices enhances reliability, positioning AI as a collaborator in epistemic advancement [4, 5].

A boundary-based silence framework for materials AI

The proposed framework conceptualizes a boundary map linking claim types in materials AI to the required epistemic warrants and corresponding silence conditions. Claim types range from property predictions (e.g., bandgap estimation) to design suggestions (e.g., alloy compositions), each requiring specific warrants, such as data coverage or physical consistency [6, 7].

Regions are delineated as follows: the interior, where warrants are robust and claims are fully warranted; the boundary zone, where partial warrants allow conditional use with explicit qualifications; and the exterior, mandating silence to avoid unsubstantiated assertions [8, 9].

At least five boundary checks are essential: (1) semantic alignment, ensuring input features match training semantics (e.g., consistent chemical descriptors); (2) domain coverage, assessing if the input falls within the training distribution's hull; (3) invariance preservation, verifying adherence to physical symmetries like rotational invariance in crystal structures; (4) consequence sensitivity, evaluating if errors could lead to high-stakes failures (e.g., in structural materials); and (5) conflict with known physics, flagging violations of established laws like thermodynamics [10-12]. **Table 2** operationalizes these checks by linking each to explicit silence conditions.

Table 2. Boundary checks linking epistemic warrants to silence conditions in materials AI

Boundary check	What is evaluated	Example failure mode	Silence condition
Semantic alignment	Feature meaning consistency	Descriptor mismatch across datasets	Abstain from prediction
Domain coverage	Training data support	Extrapolation beyond the hull	Require new data
Invariance preservation	Physical symmetries	Scale or symmetry violation	Conditional silence
Consequence sensitivity	Risk of error	Safety-critical materials	Enforce abstention
Physics conflict	Law consistency	Thermodynamic violation	Hard silence

Failure modes include: (1) boundary erosion, where repeated extrapolations normalize overreach; (2) false confidence, arising from miscalibrated uncertainty near boundaries; (3) silent collapse, where excessive caution stifles innovation; and (4) protocol-induced leakage, allowing distorted data to infiltrate interior regions [13-16]. **Figure 2** illustrates an epistemic region in materials space, highlighting warranted claims, conditional uncertainty, and silence zones along with characteristic failure modes.

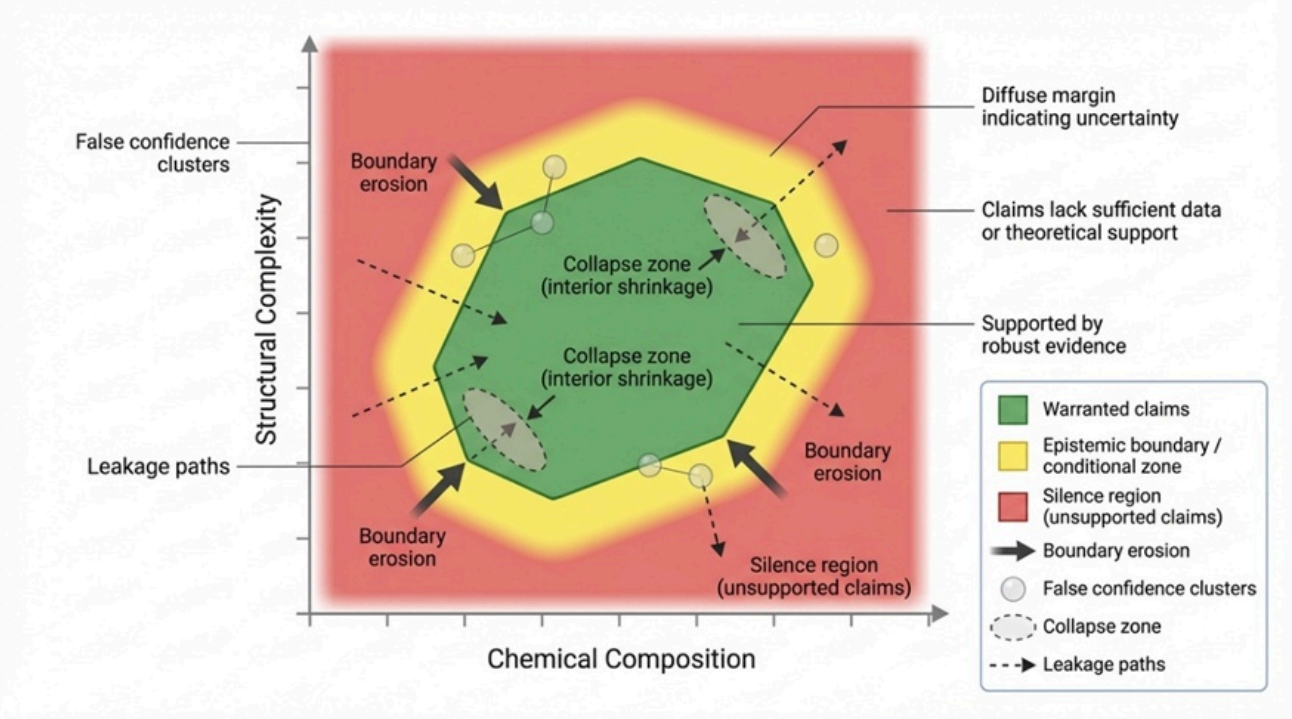

Figure 2. Schematic epistemic region in materials space, with green warranted interior, yellow uncertain boundary, red silence exterior, and annotated failure modes

Implications

The boundary-based silence framework proposed herein carries significant implications for materials discovery pipelines, AI ethics in science, and the integration of human expertise. In materials discovery, where AI is increasingly embedded in workflows for high-throughput screening and inverse design, recognizing epistemic boundaries can restructure how

models are deployed. Traditional pipelines often prioritize volume of predictions, assuming that more outputs equate to faster innovation [18, 19]. However, by incorporating silence conditions, pipelines can shift toward quality over quantity, allocating resources to warranted claims while flagging exterior regions for experimental validation or data augmentation. This could reduce false positives in candidate selection, such as in battery materials, where overly confident predictions of stability can lead to costly synthesis failures [20, 21]. Consequently, discovery cycles become more efficient, with AI serving as a gatekeeper that directs human effort to boundary zones, fostering a hybrid approach in which models abstain, highlighting opportunities for targeted experimentation [22].

On the ethical front, the framework addresses AI's role in scientific practice by promoting transparency and accountability. In science, epistemic overreach can erode public trust, particularly when AI outputs influence policy or industry decisions, such as those on sustainable materials for climate mitigation [23, 24]. By framing silence as a virtue, the theory counters the "hype" surrounding AI, encouraging developers to disclose boundaries rather than conceal limitations through inflated confidence scores [25]. This has consequences for AI ethics, as ignoring boundaries risks perpetuating biases embedded in training data, such as underrepresentation of rare-earth-free materials, leading to skewed innovation toward privileged chemistries [26]. Mandating silence in exterior regions enforces a precautionary principle, akin to "do no harm" in medicine, preventing the dissemination of unreliable knowledge that could mislead downstream users [27]. Moreover, it aligns with broader discussions on responsible AI, where epistemic humility—acknowledging when to stay silent—mitigates risks of misinformation in scientific literature [28, 29].

Integration with human expertise emerges as a key implication, transforming AI from an autonomous agent to a collaborative tool. Materials scientists bring domain knowledge that AI lacks, such as an intuitive understanding of physical constraints and the historical context of protocol shifts [30]. The boundary map facilitates this synergy by identifying interior regions for automated processing, boundary zones for expert review, and exterior areas for human-led exploration [31]. For instance, in structure-property mapping, AI might predict within warrants, but near boundaries, scientists can apply qualitative judgments to assess invariance preservation [32]. This hybrid model enhances robustness by prompting interdisciplinary dialogue, blending computational efficiency with human insight [33]. Consequences include elevated scientific standards, where AI augments rather than supplants expertise, potentially accelerating breakthroughs in complex domains such as nanomaterials and perovskites [14, 15]. Overall, these implications underscore how boundary-aware AI can elevate materials science, balancing acceleration with epistemic integrity.

Limitations

While the boundary-based silence framework offers a conceptual lens for addressing applicability domains in materials AI, it is inherently limited by its abstract nature. As a purely theoretical construct, it does not provide prescriptive algorithms or operational tools for implementation, relying instead on philosophical reasoning to guide interpretation [1, 2]. This conceptual focus means it cannot directly resolve practical challenges, such as computational overhead in real-time boundary checks, nor does it account for the variability in how different AI architectures manifest distortions [3]. For example, in deep neural networks versus Gaussian processes, boundary definitions may differ, yet the framework treats them agnostically, potentially oversimplifying domain-specific nuances [4, 5].

Defining epistemic boundaries philosophically presents another limitation, as boundaries are not objective but contingent on warrants such as semantic alignment or physical consistency, which are subject to interpretation [6, 7]. In materials science, where heterogeneity abounds, consensus on "known physics" might vary across subfields, leading to ambiguous silence conditions [8]. Moreover, the metaphor assumes a static map, but material spaces evolve with new data, risking outdated boundaries that either overly restrict or insufficiently caution [9, 10]. Failure modes like boundary erosion could be exacerbated if users adapt the framework inconsistently, highlighting the need for community standards that the theory does not specify [11].

Finally, the framework's emphasis on silence might inadvertently discourage risk-taking in exploratory research, where speculative extrapolation has historically sparked innovation [12, 13]. Without empirical grounding, its applicability to

emerging AI paradigms, such as foundation models, remains speculative [14, 15].

Future Directions

The boundary-based silence framework opens avenues for conceptual extensions that could deepen its utility in materials AI. One direction involves dynamic boundaries, where the epistemic map adapts in real time to incoming data or domain shifts, transforming static frontiers into evolving landscapes [16]. This could incorporate feedback loops, allowing silence conditions to relax as warrants accumulate, such as through active learning strategies that prioritize boundary-zone sampling [18]. In materials contexts, this might enable adaptive modeling of time-dependent phenomena, such as degradation in functional materials.

Another extension lies in multidimensional boundary representations that integrate scales from atomic to macroscopic to address transitions that distort current maps. Philosophical inquiries represent a fertile ground, drawing from epistemology to refine silence as a normative principle—questioning, for instance, how cultural or institutional factors influence warrant thresholds. This could foster interdisciplinary collaborations, merging AI theory with science studies to explore overreach in historical case studies.

Future work might also examine integration with emerging technologies, such as quantum computing, where boundaries encompass both computational and epistemic limits. Additionally, conceptualizing collective boundaries across model ensembles could mitigate individual distortions, promoting silence only when consensus fails [28, 29]. Ultimately, these directions call for broader discourse on AI's epistemic role, ensuring materials innovation advances with restraint and rigor.

Acknowledgements

None

Conflict of interest

None

Financial support

None

Ethics statement

None

Received: 28 Jul 2023 Revised: 16 Oct 2023 Accepted: 13 Nov 2023
Published online: 18 January 2024

References

Sutton Ch, Boley M, Ghiringhelli LM, Rupp M, Vreeken J, Scheffler M. Identifying domains of applicability of machine learning models for materials science. Nat Commun. 2020;11(1):4428.
https://doi.org/10.1038/s41467-020-17112-9.

Morgan D, Jacobs R. Opportunities and Challenges for Machine Learning in Materials Science. Annu Rev Mater Res. 2020;50:71-103.
https://doi.org/10.1146/annurev-matsci-070218-010015.

Pilania G. Machine learning in materials science: From explainable predictions to interpretable models. Comput Mater Sci. 2021;193:110360.
https://doi.org/10.1016/j.commatsci.2021.110360.

Liu Y, Zhao T, Yang G, Ju W, Shi S. Small data machine learning in materials science. npj Comput Mater. 2023;9(1):42.
https://doi.org/10.1038/s41524-023-01000-z.

Karande P, Gallagher B, Yong-Jin Han T. A Strategic Approach to Machine Learning for Material Science: How to Tackle Real Problems in a New Field. Chem Mater. 2022;34(17):7723-30.
https://doi.org/10.1021/acs.chemmater.2c01333.

Chong SS, Ng YS, Wang HQ, Zheng JC. Advances of machine learning in materials science: Ideas and techniques. Front Phys. 2023;19(1):43305.
https://doi.org/10.1007/s11467-023-1325-z.

Fung V, Hu J, Ganesh P, Sumpter BG. Interpretable and Explainable Machine Learning for Materials Science and Chemistry. Acc Mater Res. 2022;3(7):669-79.
https://doi.org/10.1021/accountsmr.1c00244.

Vasudevan RK, Choudhary K, Mehta A, et al. Materials science in the artificial intelligence age: high-throughput library generation, machine learning, and a pathway to autonomy. Appl Phys Rev. 2020;7(2):021406.
https://doi.org/10.1063/1.5132373.

Oliynyk AO, Meredig B. Big data and machine learning for materials science. Discov Mater. 2021;1(1):3.
https://doi.org/10.1007/s43939-021-00012-0.

Kuntz K, Lane JE, Gardner WP, Johnson NB. Applicability domains of neural networks for toxicity prediction. AIMS Math. 2023;8(11):27274-301.
https://doi.org/10.3934/math.20231393.

Lim H, Jung J, Kim K. The utility of composition-based machine learning models for band gap prediction. Comput Mater Sci. 2021;198:110692.
https://doi.org/10.1016/j.commatsci.2021.110692.

Takamoto S, Izumi M. Effects of data bias on machine-learning-based material discovery. Mater Inform. 2022;2(1):12.
https://doi.org/10.1080/27660400.2022.2109447.

Li J, Song Z, Wang Y. Predicting and investigating cytotoxicity of nanoparticles by translucent plate method and artificial neural network method. Chemosphere. 2021;276:130183.

https://doi.org/10.1016/j.chemosphere.2021.130183.

Mrosek M, Tchatchoua U, Isaeva A, Greif C, Nürnberger F, Maier A. Uncertainty Prediction for Machine Learning Models of Material Properties. ACS Omega. 2021;6(48):32431-440.
https://doi.org/10.1021/acsomega.1c03752.

Psaros AF, Meng X, Zou Z, Guo L, Karniadakis GE. Uncertainty quantification in scientific machine learning: Methods, metrics, and comparisons. J Comput Phys. 2023;477:111902.
https://doi.org/10.1016/j.jcp.2022.111902.

Fung V. Explainable machine learning in materials science. npj Comput Mater. 2022;8(1):204.
https://doi.org/10.1038/s41524-022-00896-2.

Damewood JR, Karaguesian J, Lunger JR, Tan AR, Xie M, Peng J, et al. Representations of Materials for Machine Learning. Annu Rev Mater Res. 2023;53:565-89.
https://doi.org/10.1146/annurev-matsci-080921-085947.

Liu Y, Yang Z, Zou X, Ma S, Liu D, Avdeev M, et al. Data quantity governance for machine learning in materials science. Natl Sci Rev. 2023;10(7):nwad125.

Juan Y, Dai Y, Yang Y, Zhang J. Accelerating Materials Discovery Using Artificial Intelligence, High Performance Computing and Robotics. npj Comput Mater. 2021;7(1):135.
https://doi.org/10.1038/s41524-021-00589-7.

Schmidt J, Marques MRG, Botti S, Marques MAL. Recent advances and applications of machine learning in solid-state materials science. npj Comput Mater. 2020;5(1):83.
https://doi.org/10.1038/s41524-019-0221-0.

Dan Y, Zhao Y, Li X, Li S, Hu M, Hu J. Generative adversarial networks (GAN) based efficient sampling of chemical composition space for inverse design of inorganic materials. npj Comput Mater. 2020;6(1):84.
https://doi.org/10.1038/s41524-020-00352-0.

Chen C, Ye W, Zuo Y, Zheng C, Ong SP. Graph Networks as a Universal Machine Learning Framework for Molecules and Crystals. Chem Mater. 2020;31(9):3564-72.
https://doi.org/10.1021/acs.chemmater.9b01294.

Butler KT, Davies DW, Cartwright H, Isayev O, Walsh A. Machine learning for molecular and materials science. Nature. 2020;559(7715):547-55.
https://doi.org/10.1038/s41586-018-0337-2.

Ramakrishnan R, Dral PO, Rupp M, von Lilienfeld OA. Big Data Meets Quantum Chemistry Approximations: The Δ-Machine Learning Approach. J Chem Theory Comput. 2020;11(5):2087-96.
https://doi.org/10.1021/acs.jctc.5b00099.

Janet JP, Duan C, Yang T, Nandy A, Kulik HJ. A quantitative uncertainty metric controls error in neural network-driven chemical discovery. Chem Sci. 2021;10(32):7913-22.
https://doi.org/10.1039/C9SC02298H.

Janet JP, Kulik HJ. Resolving Transition Metal Chemical Space: Feature Selection for Machine Learning and Structure-Property Relationships. J Phys Chem A. 2020;121(46):8939-52.
https://doi.org/10.1021/acs.jpca.7b08750.

Kim E, Huang K, Saunders A, McCallum A, Olivetti E. Materials synthesis insights from scientific literature via text extraction and machine learning. Chem Mater. 2020;29(21):9436-44.
https://doi.org/10.1021/acs.chemmater.7b03570.

Haghighatlari M, Vishwakarma G, Altarawy D, Subramanian R, Kota BU, Sonpal A, et al. ChemML: A machine learning and informatics program package for the analysis, mining, and modeling of chemical and materials data. Wiley Interdiscip Rev Comput Mol Sci. 2020;10(4):e1458.
https://doi.org/10.1002/wcms.1458.

Saidi WA, Shadid W, Vesely EJ. Cross-Domain transfer learning in materials science. npj Comput Mater. 2020;6(1):164.
https://doi.org/10.1038/s41524-020-00448-5.

Chen L, Tran H, Batra R. Graph neural network predictions of solute segregation in iron. Acta Mater. 2021;215:117058.

Zhang L, Lin DY, Wang H, Car R, E W. Active learning of Gaussian processes for composite functions. npj Comput Mater. 2021;7(1):1-12.
https://doi.org/10.1038/s41524-021-00521-z.

Batra R, Pilania G, Uberuaga BP, Ramprasad R. Identifying point defects in multicomponent oxides with graph neural networks. npj Comput Mater. 2021;7(1):75.
https://doi.org/10.1038/s41524-021-00545-5.

Damewood J, Hall DM, Chen L, Ramprasad R. Machine learning for new materials discovery. MRS Commun. 2023;13:1-12.
https://doi.org/10.1557/s43579-023-00340-1.