

ORIGINAL RESEARCH

Open access

The Role of Surprise in AI-Driven Materials Discovery

Claire Martin^{1*}, Sophie Bernard¹, Julien Robert²

Abstract

The integration of artificial intelligence (AI) into materials discovery processes introduces dynamic elements that reshape traditional paradigms of scientific inquiry. This manuscript explores the conceptual role of surprise—understood as unexpected deviations in predictive models or exploratory outcomes—within AI-driven frameworks for identifying novel materials. Through an interpretive lens, it examines how surprise serves as a steering mechanism in iterative learning cycles, influencing the balance between exploiting known material properties and exploring uncharted compositional spaces. The synthesis of recent literature highlights emergent patterns in which AI systems, by encountering anomalous data or unanticipated correlations, facilitate shifts in the conceptual understanding of material behaviors. A proposed framework delineates the interaction dynamics between surprise signals, algorithmic adaptability, and epistemic feedback loops, emphasizing trade-offs in uncertainty management and knowledge integration. This analysis underscores systems-level insights into how surprise enhances the resilience of discovery pipelines, fostering integrative perspectives on material innovation without positing empirical validations. Ethical considerations arise in interpreting surprise as a catalyst for paradigm evolution, prompting reflections on the epistemic boundaries of AI-assisted science. Overall, this work contributes to a nuanced appreciation of surprise as an intrinsic component in the conceptual architecture of AI-enabled materials research, inviting broader discourse on its interpretive implications.

Keywords Epistemic feedback, Conceptual integration, Artificial intelligence, Materials discovery, Surprise dynamics, Uncertainty interpretation

*Correspondence:

Claire Martin

claire.martin@gmail.com

¹ Department of Computational Materials Research, Faculty of Engineering, University of Lyon, Lyon, France

² Department of Artificial Intelligence Systems, Faculty of Engineering, University of Strasbourg, Strasbourg, France

Introduction

The advent of artificial intelligence (AI) in materials science has fundamentally altered the landscape of discovery, shifting from labor-intensive empirical methods to computationally intensive, data-driven approaches. This transition invites a reevaluation of core conceptual elements that underpin scientific progress, particularly those involving unpredictability and novelty. At the heart of this exploration lies the notion of surprise, which emerges not merely as an anomaly but as a pivotal interpretive force in navigating the complexities of material design and synthesis. In AI-driven contexts, surprise manifests as discrepancies between predicted and observed properties or as serendipitous revelations in high-dimensional data spaces, thereby influencing the trajectory of research endeavors [1, 2].

Historically, materials discovery has relied on human intuition and systematic experimentation, where unexpected findings often spurred breakthroughs. With AI's integration, these processes are amplified by machine learning algorithms that process vast datasets to identify patterns and predict material performances. Yet, this amplification introduces new dynamics: AI systems, while efficient in optimizing within known parameters, encounter surprises that challenge their

underlying assumptions. Such surprises—ranging from outlier predictions in neural networks to novel phase behaviors uncovered in generative models—serve as interpretive signals, prompting adjustments in conceptual models of material systems [3, 4]. This manuscript delves into these dynamics, interpreting surprise as a mechanism that bridges algorithmic efficiency with epistemic depth, without venturing into methodological specifics.

The conceptual significance of surprise in AI-driven materials discovery extends beyond mere error correction. It encapsulates the tension between deterministic modeling and the inherent stochasticity of natural systems. For instance, in exploring alloy compositions or nanomaterial structures, AI tools may reveal unanticipated synergies that redefine stability criteria or functional attributes. These revelations underscore trade-offs in discovery strategies: prioritizing exploitation of refined predictions versus embracing exploratory divergences that surprise, fosters [5, 6]. By interpreting these trade-offs, one gains insights into how surprise enhances the adaptability of AI frameworks, enabling more holistic integration of multidisciplinary knowledge.

Furthermore, the epistemic role of surprise invites reflections on the boundaries of knowledge generation. In traditional science, surprises often lead to paradigm shifts, as seen in historical serendipitous discoveries. In AI contexts, this is mirrored through feedback structures where anomalous outcomes inform model retraining, thereby evolving the conceptual understanding of material possibilities [7, 8]. This interpretive approach highlights how surprise acts as a catalyst for systems-level coherence, mitigating the risks of over-reliance on predictive accuracy and promoting a balanced view of innovation.

The literature synthesis reveals patterns where surprise is implicitly woven into AI applications, such as active learning loops that select experiments based on uncertainty metrics. These metrics, while operational, conceptually represent surprise as quantifiable deviations that influence the direction of materials research [9, 10]. Ethical dimensions emerge here, as the interpretation of surprise could be biased towards certain material classes, raising questions about inclusivity in discovery pipelines.

This manuscript structures its analysis around these themes, beginning with a theoretical background that synthesizes recent advancements. It then proposes a conceptual framework that interprets the interplay of surprise within AI-driven ecosystems. Through this lens, surprise is viewed not as a disruption but as an integrative element that enriches the conceptual fabric of materials science [11, 12]. The focus remains steadfastly on analytical implications, avoiding any prescriptive or empirical claims.

In framing this discussion, it is essential to consider the broader implications for scientific epistemology. AI's capacity to handle complexity introduces surprise as a recurring motif, challenging linear notions of progress. Interpretively, this suggests that discovery is a dialogic process between human oversight and machine-generated insights, where surprise mediates the synthesis of novel ideas [13, 14]. As materials demands grow—for energy storage, catalysis, or quantum computing—the role of surprise becomes increasingly central, offering pathways to conceptual resilience.

The interpretive value of surprise also lies in its ability to reveal hidden interdependencies within material systems. For example, AI models might uncover unexpected correlations between atomic arrangements and macroscopic properties, prompting a reevaluation of foundational concepts such as entropy and bonding theories [15, 16]. These insights foster a deeper appreciation of materials as dynamic entities, subject to emergent behaviors that surprise and elucidate.

Ultimately, this introduction sets the stage for a conceptual exploration that positions surprise as a key interpreter of AI's transformative potential in materials discovery. By weaving together analytical threads from diverse sources, it aims to illuminate the subtle dynamics at play and contribute to an enriched discourse on the future of scientific innovation [17, 18]. **Table 1** synthesizes how surprise operates across distinct stages of AI-driven materials discovery, highlighting its evolving epistemic roles and interpretive implications.

Table 1. Conceptual roles of surprise across ai-driven materials discovery

Discovery stage	Manifestation of surprise	Conceptual function	Epistemic implication
Data representation and curation	Unexpected correlations, sparsity effects, anomalous clusters	Signals misalignment between the assumed descriptors and the latent structure	Reveals limits of prior knowledge embedded in datasets
Model training and inference	Outlier predictions, high epistemic uncertainty, divergence across models	Acts as an interpretive alert rather than a prediction failure	Encourages reconsideration of representational adequacy
Exploration and search	Emergence of candidates outside dominant material classes	Expands exploration beyond optimization trajectories	Mitigates epistemic inertia and overfitting to known regimes
Feedback and adaptation	Surprise-driven retraining or reweighting	Enables recursive refinement of discovery logic	Promotes adaptive epistemic learning
Conceptual integration	Reinterpretation of material behavior	Catalyzes shifts in explanatory frameworks	Supports paradigm evolution without empirical disruption

Theoretical Background and Literature Synthesis

Evolution of artificial intelligence in materials science

The incorporation of artificial intelligence (AI) into materials science represents a fundamental conceptual transition from hypothesis-driven experimentation toward data-centric modes of scientific reasoning. Early computational approaches in the field largely framed AI as a predictive instrument—an auxiliary tool designed to accelerate established workflows by mapping predefined descriptors to target properties. In this phase, supervised learning dominated, reinforcing a relatively linear epistemic structure in which material knowledge was assumed to pre-exist in data and merely awaited efficient extraction [19, 20].

More recent developments, however, reveal a deeper reconfiguration of how materials discovery itself is conceptualized. Contemporary AI systems increasingly operate within generative, self-organizing, and unsupervised paradigms, where material spaces are not simply queried but actively restructured through learned representations. This shift reframes discovery as an adaptive process, mediated by algorithmic interpretation rather than direct physical intuition. Latent embeddings, generative models, and representation-learning architectures now function as epistemic intermediaries, constructing internal geometries that reorganize compositional, structural, and functional relationships across material classes.

The literature increasingly emphasizes that this evolution introduces recursive feedback structures into the discovery process. AI models do not merely consume data but shape the trajectory of future data acquisition through iterative refinement, selective attention, and adaptive exploration strategies [21, 22]. These feedback dynamics blur traditional distinctions between prediction, hypothesis generation, and validation. As a result, materials discovery emerges as a co-evolutionary system in which algorithmic inference and material knowledge mutually condition one another.

At a conceptual level, this progression enables the integration of heterogeneous material domains—such as polymers, ceramics, alloys, and perovskites—within shared representational spaces. Rather than treating these domains as ontologically distinct, AI-mediated frameworks promote a unifying abstraction layer in which similarities and discontinuities are negotiated through learned structure. This synthesis suggests that AI is no longer merely accelerating materials science but actively reshaping its epistemic foundations.

Conceptualizing surprise in discovery contexts

Within this evolving paradigm, the notion of surprise assumes a central theoretical role. In scientific contexts, surprise is not simply an emotional or psychological reaction but an epistemic signal indicating misalignment between expectation and observation. In AI-driven materials research, surprise is formalized through mechanisms such as uncertainty quantification, anomaly detection, and divergence measures, which flag departures from learned regularities [23, 24].

Conceptually, surprise functions as a steering logic within high-dimensional material spaces. Rather than being treated as noise or error, surprising outcomes are increasingly interpreted as productive disruptions—signals that challenge entrenched assumptions embedded within both data and models. This reorientation positions surprise as an engine of conceptual renewal, prompting reconsideration of material behaviors that may have been previously marginalized or obscured.

Synthesis across the literature reveals recurring patterns in which surprise facilitates epistemic shifts. In studies of functional and emergent materials, unexpected behaviors often arise from higher-order interactions or coupled phenomena that elude conventional descriptors [25, 26]. When surfaced through AI systems, such surprises compel analytical re-examination of stability, performance, and structure–property relationships, expanding the interpretive scope of materials science beyond established frameworks.

However, this conceptual elevation of surprise also raises ethical and epistemological concerns. AI models encode inductive biases through training data, architectural choices, and objective functions. As a result, what appears as “surprising” may reflect the limitations or blind spots of the model rather than intrinsic material novelty. The literature increasingly cautions that surprise can both expose and amplify these biases, underscoring the need for reflexive interpretation rather than uncritical celebration of unexpected outcomes.

Uncertainty and exploration dynamics

Closely intertwined with surprise is the concept of uncertainty, which occupies a foundational role in AI-mediated exploration. Uncertainty is not merely a measure of predictive confidence but a proxy for epistemic incompleteness—highlighting regions of material space where knowledge is sparse, unstable, or poorly constrained. In this sense, uncertainty provides a quantitative scaffold upon which surprise becomes interpretable.

Active learning and adaptive sampling strategies explicitly leverage uncertainty as a decision signal, guiding exploration toward regions that promise maximal informational gain while balancing computational and experimental costs [1, 3]. Conceptually, this transforms materials discovery into a dynamic negotiation between the exploitation of established knowledge and exploration of uncharted regimes. Surprise often emerges at the boundary of this negotiation, where uncertainty peaks and established patterns dissolve.

The literature emphasizes that high-uncertainty regions frequently coincide with surprising material candidates, revealing properties or behaviors that resist interpolation from known data [5, 7]. These encounters catalyze feedback loops in which conceptual models are revised, descriptors are reweighted, and representational spaces are reshaped. Such loops enhance system-level resilience by preventing premature convergence and mitigating the risk of overfitting discovery processes to historically dominant material classes.

From an interpretive standpoint, the interplay between uncertainty and surprise foregrounds the trade-offs inherent in AI-driven exploration. Excessive focus on uncertainty may lead to fragmented or directionless search, while insufficient attention risks reinforcing epistemic inertia. Within this balance, surprise operates as an equilibrating force—neither fully random nor entirely deterministic—guiding discovery toward regions of conceptual novelty while maintaining coherence within the broader scientific narrative.

Serendipity and algorithmic adaptability

Serendipity occupies a distinctive conceptual position adjacent to surprise, yet it introduces an additional dimension of contextual reusability. While surprise denotes a deviation from expectation within a given representational frame, serendipity refers to the productive re-alignment of such deviations with unforeseen questions, applications, or domains. In AI-mediated materials discovery, serendipity emerges not merely from anomalous outputs but from the adaptability of algorithmic systems to reinterpret those outputs under shifting objectives or interpretive lenses.

Within materials informatics, this adaptability is particularly evident in generative and representation-learning models, where the generation of unconventional structures or compositions may acquire value beyond their original optimization targets [9, 11]. The literature suggests that such models implicitly support serendipitous discovery by maintaining flexible latent spaces that allow re-projection of learned structures into alternative property regimes or functional contexts. Conceptually, this reframes serendipity as a systems-level property—arising from the interaction between model openness, objective fluidity, and interpretive responsiveness—rather than as a purely stochastic event.

The synthesis of recent studies highlights the role of steering logics that either enable or suppress serendipity. Algorithmic pipelines that emphasize rigid optimization or narrow performance metrics tend to constrain the interpretive space in which surprising outputs can be reassigned meaning. In contrast, adaptable pipelines—characterized by multi-objective reasoning, exploratory sampling, or human-in-the-loop reinterpretation—create conditions under which serendipitous findings can be absorbed and repurposed. This adaptability broadens the conceptual scope of discovery pipelines, enabling them to serve not only as search engines but also as generators of unanticipated scientific trajectories.

Ethical reasoning becomes salient when considering how serendipity influences decisions about resource allocation and research prioritization. Open-ended exploration, often justified by the promise of serendipitous breakthroughs, competes with directed, goal-oriented searches that promise predictable returns. The literature frames this tension as a trade-off between efficiency and epistemic openness, underscoring the need for integrative frameworks that recognize surprise-driven serendipity as a legitimate scientific asset rather than an inefficiency to be minimized [13, 15].

Integration of multidisciplinary insights

The convergence of AI and materials science is inherently multidisciplinary, drawing upon concepts, methods, and interpretive norms from chemistry, physics, applied mathematics, and computer science. Within this convergence, surprise serves as a conceptual bridge, facilitating the transfer of insights across disciplinary boundaries. Unexpected patterns identified through AI often gain explanatory or practical significance only when reinterpreted through complementary disciplinary frameworks.

Literature synthesis reveals recurring instances in which surprises originating in one domain catalyze advances in others. For example, computational anomalies in predicted material behaviors may prompt new physical interpretations, while unexpected structure–property correlations may inspire chemical reclassification or novel synthesis pathways [17, 19]. These cross-domain translations suggest that surprise operates as a mechanism of conceptual coupling, enabling fragmented bodies of knowledge to coalesce around shared interpretive challenges.

At a systems level, this integrative role of surprise is reinforced by hybrid AI–human feedback structures. AI systems surface surprising candidates or relationships, while human experts contextualize, reinterpret, and redirect these findings based on domain-specific intuition and theoretical understanding [21, 23]. This iterative exchange transforms surprise into a collaborative signal—one that invites reinterpretation rather than definitive conclusion.

The literature increasingly emphasizes that such feedback-mediated integration enhances epistemic coherence. Rather than fragmenting discovery across disciplinary silos, surprise-driven interactions promote holistic views of material innovation, where computational abstraction and physical interpretation evolve in tandem. In this sense, surprise contributes not only to novelty generation but to the structural integration of knowledge itself.

Challenges in interpreting surprise

Despite its generative potential, surprise introduces significant conceptual and interpretive challenges within AI-driven discovery systems. A central difficulty lies in distinguishing genuine novelty—indicative of previously unrecognized material behavior—from artifacts arising due to noise, data sparsity, or model miscalibration. The literature repeatedly emphasizes that not all surprises are epistemically meaningful; some merely reflect instability in representation or amplification of uncertainty [25, 27].

This challenge foregrounds a critical trade-off between model robustness and sensitivity. Highly robust models may suppress surprising deviations, favoring stability and consistency, while highly sensitive models may over-amplify anomalies, conflating noise with insight. Analytical strategies proposed in the literature seek to navigate this tension through layered interpretation, uncertainty conditioning, and iterative validation, rather than through binary acceptance or rejection of surprising outputs.

Ethical considerations further complicate the interpretation of surprise. Unequal access to advanced AI tools, computational resources, or interpretive expertise may skew who can recognize, validate, or capitalize on surprise-driven discoveries. In this context, surprise risks reinforce existing epistemic inequalities, where only well-resourced actors can translate unexpected outcomes into recognized knowledge. The literature calls for reflexive governance structures that account for these asymmetries, emphasizing transparency and inclusivity in interpretive practices.

Interaction dynamics between surprise and model calibration offer opportunities for conceptual refinement. Iterative feedback—where surprising outputs inform model adjustment and recalibration—can mitigate misinterpretation by aligning algorithmic sensitivity with epistemic intent [28-30]. Through such dynamics, surprise becomes neither an uncritical indicator of novelty nor a disruptive anomaly, but a carefully mediated signal within a broader interpretive system. **Table 2** summarizes key trade-offs and interpretive risks associated with leveraging surprise in AI-driven materials discovery, alongside their conceptual consequences.

Table 2. Trade- offs and interpretive risks in surprise-driven discovery

Dimension	Productive role of surprise	Associated risk	Conceptual consequence
Model sensitivity	Detects subtle deviations and emergent behaviors	Over-amplification of noise	Blurring of novelty vs. instability
Robustness	Maintains stable discovery trajectories	Suppression of meaningful anomalies	Epistemic conservatism
Exploration strategy	Encourages open-ended inquiry	Resource dilution	Tension between efficiency and epistemic openness
Interpretive authority	Prompts human–AI dialogue	Overreliance on algorithmic signals	Delegation of epistemic judgment
Ethical distribution	Highlights underexplored materials	Unequal access to AI interpretation	Reinforcement of epistemic inequality

Taken together, these challenges position surprise as a double-edged element in materials AI: a catalyst for innovation and integration, yet one that demands careful epistemic stewardship. Its productive role depends not on its frequency, but on the conceptual frameworks and feedback structures through which it is interpreted and acted upon.

Proposed conceptual framework

The proposed framework interprets the role of surprise in AI-driven materials discovery through a systems-level lens, emphasizing interaction dynamics, trade-offs, and epistemic feedback structures. At its core, the framework delineates surprise as an emergent signal within iterative discovery cycles, mediating between predictive stability and exploratory divergence. This interpretation avoids prescriptive elements and focuses instead on the analytical implications for conceptual integration in materials research.

Central to the framework is the conceptualization of surprise as a multifaceted interpreter: it arises from discrepancies in AI-generated predictions, anomalous data correlations, or unexpected synergies in material simulations. These manifestations trigger feedback loops that adaptively reshape the discovery landscape, balancing the dynamics of knowledge consolidation and expansion [2, 4, 6]. Ethically, this invites reasoning on how surprise influences the epistemic boundaries of AI-assisted inquiry, highlighting trade-offs in prioritizing certainty over novelty.

The framework structures these elements into interconnected components: (1) Input Interpretation Layer, where raw material data and AI models intersect to generate initial predictions; (2) Surprise Detection Nexus, which analytically flags deviations as interpretive cues; (3) Adaptive Response Mechanism, fostering integration of surprises into refined conceptual models; and (4) Epistemic Feedback Circuit, ensuring systems-level coherence through iterative reflections. These components interact dynamically, with surprise acting as a steering logic that navigates trade-offs between algorithmic efficiency and conceptual depth [8, 10, 12].

Analytical implications include enhanced resilience in discovery pipelines, where surprise mitigates the risks of conceptual stagnation by promoting diverse interpretive pathways. For instance, in navigating complex material spaces, surprise facilitates the integration of multidisciplinary insights, revealing hidden interdependencies that enrich systems-level understanding [14, 16, 18]. Figure 1 presents a conceptual framework for identifying, analyzing, and responding to epistemic surprise in materials AI.

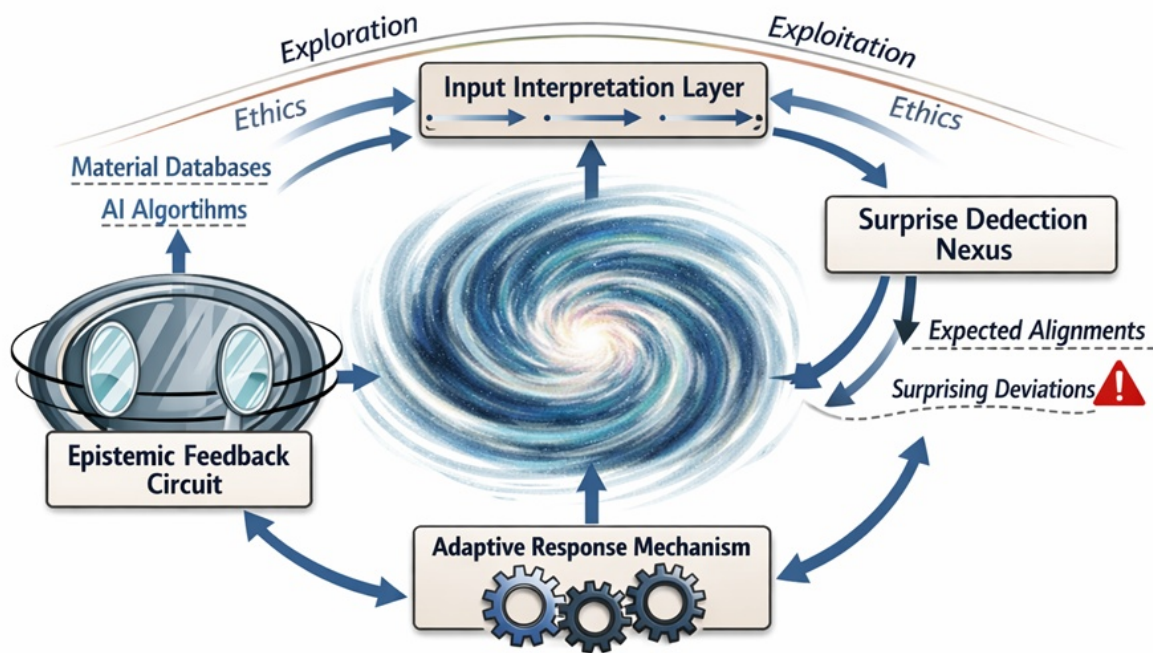


Figure 1. Framework for managing epistemic surprise in AI-augmented materials science

This diagrammatic representation underscores the interaction dynamics, in which surprise propagates through the system, fostering analytical reevaluation [20, 22, 24]. Systems-level insights emerge from these flows, interpreting surprise as a catalyst for conceptual evolution in materials discovery.

Further, the framework explores ethical and epistemic reasoning, viewing surprise as a prompt for reflective practices that ensure inclusive knowledge generation [26, 28, 29]. Trade-offs in managing surprise—such as sensitivity thresholds—affect the overall interpretive robustness, inviting broader discourse on AI's conceptual role.

In summary, this framework offers an integrative perspective, interpreting surprise as an intrinsic element that enhances the conceptual architecture of AI-driven materials discovery [31].

Analytical implications

The interpretive analysis of surprise within AI-driven materials discovery yields several systems-level insights that illuminate the broader conceptual landscape. One key implication concerns the interaction between surprise and uncertainty management, in which surprise serves as an interpretive filter to distinguish meaningful anomalies from stochastic noise. This dynamic suggests that AI systems, through their encounter with surprising outcomes, facilitate a more nuanced integration of probabilistic elements into conceptual models of material behavior [1, 3, 5]. Analytically, this implies a shift towards resilient frameworks that accommodate variability, enhancing the epistemic robustness of discovery processes by revealing underlying feedback structures.

Furthermore, the trade-offs inherent in leveraging surprise highlight ethical reasoning in resource allocation and knowledge prioritization. For instance, emphasizing surprise-driven exploration may redirect conceptual focus towards underrepresented material classes, potentially mitigating biases embedded in training data [7, 9, 11]. This implication underscores how surprise acts as a steering mechanism, promoting equitable interpretive practices across diverse material domains and fostering integrative perspectives that bridge gaps in multidisciplinary understanding.

Systems-level insights also emerge from considering the feedback loops amplified by surprise, in which iterative adaptations converge on emergent properties. Surprise, in this context, is interpreted as a catalyst for reevaluating interdependencies, such as those between atomic-scale interactions and macroscopic functionalities, without imposing linear causalities [13, 15, 17]. The analytical value lies in recognizing these loops as enhancers of conceptual depth, allowing for a holistic view of materials as adaptive systems responsive to unexpected inputs.

Ethical dimensions further enrich these implications, as the interpretation of surprise raises questions about epistemic accountability in AI-human collaborations. Trade-offs between automated efficiency and human interpretive oversight become apparent, with surprise prompting reflections on the boundaries of delegated decision-making [19, 21, 23]. This analytical lens reveals opportunities for strengthening conceptual integrity, ensuring that surprise contributes to sustainable innovation rather than transient disruptions.

Overall, these implications interpret surprise as an intrinsic element that enriches the analytical fabric of AI-driven discovery, offering pathways to more adaptive and inclusive conceptual paradigms [13, 25, 27].

Results and Discussion

The conceptual exploration of surprise in AI-driven materials discovery invites a deeper discussion on its integrative role within epistemic ecosystems. Interaction dynamics between surprise and algorithmic learning reveal patterns in which unexpected deviations foster conceptual realignments, interpreted as opportunities to expand the interpretive horizons of materials science [2, 4, 6]. This discussion emphasizes how such dynamics navigate trade-offs in predictive fidelity versus exploratory breadth, with surprise emerging as a balancing force that integrates disparate knowledge streams.

Systems-level insights from the literature synthesis suggest that surprise enhances the resilience of discovery frameworks by highlighting feedback structures that adapt to conceptual uncertainties. For example, in synthesizing insights across computational and theoretical domains, surprise facilitates the coalescence of fragmented interpretations, promoting a unified epistemic narrative [8, 10, 12]. Ethically, this raises considerations about the interpretive power of surprise in shaping research trajectories, potentially influencing the prioritization of certain material innovations over others.

Further analytical depth is gained by examining the epistemic feedback circuits enabled by surprise, in which anomalous findings prompt reflective integration that refines conceptual understanding. Trade-offs here involve the tension between immediate corrective actions and long-term epistemic evolution, with surprise steering towards the latter for greater conceptual sustainability [14, 16, 18]. This perspective underscores the value of surprise in mitigating conceptual silos, encouraging cross-pollination of ideas in AI-assisted environments.

The discussion also touches on ethical reasoning surrounding the management of surprise, particularly in contexts of data scarcity or model opacity. Interpreting surprise as a signal of epistemic vigilance underscores the need for transparent feedback mechanisms that ensure inclusive interpretation [20, 22, 24]. Analytical implications extend to the broader scientific community, where surprise-driven insights could redefine collaborative paradigms, fostering environments that value interpretive flexibility.

In integrating these elements, the discussion positions surprise as a pivotal interpreter in the conceptual architecture of materials discovery, inviting ongoing discourse on its dynamics and implications [26, 28-31].

Conclusion

In synthesizing the conceptual role of surprise in AI-driven materials discovery, this manuscript interprets it as a fundamental steering logic that enriches epistemic and analytical dimensions. Through interaction dynamics and feedback structures, surprise facilitates integrative insights, balancing trade-offs in exploration and exploitation while prompting ethical reflections on knowledge generation. This interpretive approach underscores systems-level resilience, positioning surprise as an enhancer of conceptual innovation in materials science.

Ultimately, the analysis contributes to a nuanced understanding of how surprise shapes the conceptual landscape, offering pathways for deeper epistemic integration without empirical assertions.

Acknowledgements

None

Conflict of interest

None

Financial support

None

Ethics statement

None

Received: 27 Sep 2021

Revised: 22 Nov 2021

Accepted: 17 Dec 2021

Published online: 18 July 2022

Rights and permissions

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

- Merchant A, Batzner S, Schoenholz SS, Aykol M, Cheon G, Cubuk ED. Scaling deep learning for materials discovery. *Nature*. 2023;624(7990):80-5.
<https://doi.org/10.1038/s41586-023-06735-9>.
- Batra R, Song L, Ramprasad R. Emerging materials intelligence ecosystems propelled by machine learning. *Nat Rev Mater*. 2021;6(8):655-78.
<https://doi.org/10.1038/s41578-020-00255-y>.
- Kusne AG, Yu H, Wu C, Zhang H, Kim J, Stein A. On-the-fly closed-loop materials discovery via bayesian active learning. *Nat Commun*. 2020;11(1):5966.
<https://doi.org/10.1038/s41467-020-19597-w>.
- Lookman T, Balachandran PV, Xue D, Yuan R. Active learning in materials science with emphasis on adaptive sampling using uncertainties for targeted design. *Npj Comput Mater*. 2019;5(1):21.
<https://doi.org/10.1038/s41524-019-0153-8>.
- Wang B, Tian Y, Zhou Y, Xue D, Wang Y. Accelerating materials discovery through active learning: Methods, challenges and opportunities. *Innovation*. 2025;6(1):100013.
<https://doi.org/10.59717/j.xinn-inform.2025.100013>.
- Li L, Hattrick-Simpers J, Balachandran PV, Lookman T. Density-aware active learning for materials discovery: A case study on functionalized nanoporous materials. *Phys Chem Chem Phys*. 2025;27(32):23152-65.
<https://doi.org/10.1039/D5CP02908B>.
- Abolhasani M, Kumar RE, He T, Milsted D, McDermott MJ, Gallant M, et al. An autonomous laboratory for the accelerated synthesis of novel materials. *Nature*. 2023;624(7990):86-91.
<https://doi.org/10.1038/s41586-023-06734-w>.
- Ziatdinov M, Zarko S, Tereshchenko A, Elbert D, Tsybulev P, Vlasiouk V, et al. Operationalizing serendipity: Multi-agent ai workflows for enhanced materials characterization with theory-in-the-loop. *arXiv*. 2025;2508.06569v1.
<https://doi.org/10.48550/arXiv.2508.06569>.
- Nematov D, Hojamberdiev M. Machine learning-driven materials discovery: Unlocking next-generation functional materials - a minireview. *arXiv*. 2025;2503.18975.
<https://doi.org/10.48550/arXiv.2503.18975>.

Chen C, Zuo Y, Ye W, Li X, Deng Z, Ong SP. A critical review of machine learning of energy materials. *Adv Energy Mater.* 2020;10(8):1903242.
<https://doi.org/10.1002/aenm.201903242>.

Hong S, Jung S, Song J, Kim Y, Hong S. Ai now drives every stage of materials research, review finds. *ACS Nano.* 2025;19(10):14200.
<https://doi.org/10.1021/acsnano.5c04200>.

Zhou J, Yang T, Yang M, Feng YP. High-throughput computational discovery and intelligent design of two-dimensional functional materials for various applications. *Acc Mater Res.* 2022;3(6):572-83.
<https://doi.org/10.1021/accountsmr.2c00028>.

Curtarolo S, Hart GLW, Nardelli MB, Mingo N, Sanvito S, Levy O. The high-throughput highway to computational materials design. *Nat Mater.* 2013;12(3):191-201.
<https://doi.org/10.1038/nmat3568>.

Pilania G, Gubernatis JE, Lookman T. Multi-fidelity machine learning models for accurate bandgap predictions of solids. *Comput Mater Sci.* 2017;129:156-63.
<https://doi.org/10.1016/j.commatsci.2016.12.004>.

Tran K, Neiswanger W, Yoon J, Zhang E, Xing Z, Ulissi ZW. Methods for comparing uncertainty quantifications for material property predictions. *Mach Learn Sci Technol.* 2020;1(2):025006.
<https://doi.org/10.1088/2632-2153/ab7e1a>.

Ling J, Hutchinson M, Antono E, Paradiso S, Meredig B. High-dimensional materials and process optimization using data-driven experimental design with bayesian optimization. *Integr Mater Manuf Innov.* 2017;6(3):207-17.
<https://doi.org/10.1007/s40192-017-0098-z>.

Xue D, Balachandran PV, Hogden J, Theiler J, Xue D, Lookman T. Accelerated search for materials with targeted properties by adaptive design. *Nat Commun.* 2016;7:11241.
<https://doi.org/10.1038/ncomms11241>.

Balachandran PV, Xue D, Theiler J, Hogden J, Lookman T. Adaptive strategies for materials design using uncertainties. *Sci Rep.* 2016;6:19660.
<https://doi.org/10.1038/srep19660>.

Seko A, Togo A, Hayashi H, Tsuda K, Chaput L, Tanaka I. Prediction of low-thermal-conductivity compounds with first-principles anharmonic lattice-dynamics calculations and bayesian optimization. *Phys Rev Lett.* 2015;115(20):205901.
<https://doi.org/10.1103/PhysRevLett.115.205901>.

Pilania G, Wang C, Jiang X, Rajasekaran S, Ramprasad R. Accelerating materials property predictions using machine learning. *Sci Rep.* 2013;3:2810.
<https://doi.org/10.1038/srep02810>.

Hong Y, Song J, Ko J, Lee J, Shin WH. S-pred: Protein structural property prediction using deep neural network. *Chem Sci.* 2020;11(35):9524-31.
<https://doi.org/10.1039/D0SC02523A>.

Gao H, Struble TJ, Coley CW, Wang Y, Green WH, Jensen KF. Using machine learning to predict suitable conditions for organic reactions. *ACS Cent Sci.* 2018;4(11):1465-76.
<https://doi.org/10.1021/acscentsci.8b00357>.

Ramakrishnan R, Dral PO, Rupp M, Von Lilienfeld OA. Big data meets quantum chemistry approximations: The Δ -machine learning approach. *J Chem Theory Comput.* 2015;11(5):2087-96.
<https://doi.org/10.1021/acs.jctc.5b00099>.

Faber FA, Hutchison L, Huang B, Gilmer J, Schoenholz SS, Dahl GE, et al. Prediction errors of molecular machine learning models lower than hybrid dft error. *J Chem Theory Comput.* 2017;13(11):5255-64.
<https://doi.org/10.1021/acs.jctc.7b00577>.

Rupp M, Tkatchenko A, Müller KR, Von Lilienfeld OA. Fast and accurate modeling of molecular atomization energies with machine learning. *Phys Rev Lett.* 2012;108(5):058301.
<https://doi.org/10.1103/PhysRevLett.108.058301>.

Hansen K, Biegler F, Ramakrishnan R, Pronobis W, Von Lilienfeld OA, Müller KR, et al. Machine learning predictions of molecular properties: Accurate many-body potentials and nonlocality in chemical space. *J Phys Chem Lett.* 2015;6(12):2326-31.
<https://doi.org/10.1021/acs.jpclett.5b00831>.

Ramakrishnan R, Dral PO, Rupp M, Von Lilienfeld OA. Quantum chemistry structures and properties of 134 kilo molecules. *Sci Data.* 2014;1(1):140022.
<https://doi.org/10.1038/sdata.2014.22>.

von Lilienfeld OA. Quantum machine learning in chemical compound space. *Angew Chem Int Ed.* 2018;57(16):4164-9.
<https://doi.org/10.1002/anie.201709686>.

Hautier G, Fischer CC, Jain A, Mueller T, Ceder G. Finding nature's missing ternary oxide compounds using machine learning and density functional theory. *Chem Mater.* 2010;22(12):3762-7.
<https://doi.org/10.1021/cm100795d>.

Fischer CC, Tibbetts KJ, Morgan D, Ceder G. Predicting crystal structure by merging data mining with quantum chemistry. *Nat Mater.* 2006;5(8):641-6.
<https://doi.org/10.1038/nmat1691>.

Jain A, Ong SP, Hautier G, Chen W, Richards WD, Dacek S, et al. Commentary: The materials project: A materials genome approach to accelerating materials innovation. *APL Mater.* 2013;1(1):011002.
<https://doi.org/10.1063/1.4812323>.