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Uncertainty and Reliability in Materials AI — Concepts, Language, and Decision Consequences

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Abstract

The integration of artificial intelligence (AI) and machine learning (ML) into materials science has accelerated the discovery and design of novel materials by enabling high-throughput prediction of properties from composition, structure, and processing parameters. However, the reliability of these predictions is frequently compromised by uncertainties stemming from limited datasets, model approximations, experimental noise, and intrinsic variability in materials systems. This narrative review synthesizes recent advances in understanding uncertainty and reliability in materials AI. It covers fundamental concepts such as aleatoric and epistemic uncertainty; methods for quantification, including Bayesian neural networks, ensembles, and Gaussian processes; inconsistencies in terminology and language across the literature; and the downstream consequences for decision-making in materials engineering, design, and deployment. Emphasis is placed on calibration of uncertainty estimates, domain-of-applicability assessment, and risk-aware applications in safety-critical contexts such as structural alloys and energy materials. By highlighting best practices and gaps, the review advocates for standardized frameworks to build trust and facilitate industrial translation of materials AI. Key challenges include data scarcity in high-performance materials and the need for physics-informed UQ to mitigate overconfidence in extrapolative predictions. This synthesis underscores the importance of robust uncertainty handling for responsible AI deployment in materials innovation.

Keywords Materials AI, Epistemic uncertainty, Uncertainty quantification, Machine learning, Reliability assessment, Decision consequences

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Introduction

The field of materials science is undergoing a profound methodological transformation driven by advances in artificial intelligence (AI) and machine learning (ML). These data-driven approaches enable the rapid exploration of vast chemical, compositional, and structural design spaces that are otherwise inaccessible through conventional experimental or computational pipelines [1-3]. By learning complex, non-linear relationships from curated experimental data, high-throughput simulations, and materials databases, ML models can predict a wide range of properties—including mechanical strength, electronic band gaps, thermal conductivity, and electrochemical stability—with orders-of-magnitude reductions in computational cost compared to traditional approaches [4, 5]. As a result, AI has become an increasingly central component of materials discovery workflows, spanning applications such as alloy design, energy storage materials, heterogeneous catalysis, and additive manufacturing, with the promise of compressing development timelines from decades to months [6, 7].

Despite these advances, the predictive success of materials AI has exposed a fundamental limitation: high accuracy alone does not guarantee reliability. ML predictions in materials science are frequently affected by multiple, interacting sources of uncertainty, including heterogeneous and biased data provenance, limited experimental validation, model misspecification, distributional shift between training and deployment regimes, and the intrinsic stochasticity of materials behavior across scales [8-10]. These factors undermine the trustworthiness of AI outputs, particularly when models are extrapolated beyond well-sampled regions of chemical or processing space. Consequently, uncertainty quantification (UQ) and reliability assessment have emerged as indispensable components of responsible and scientifically credible materials AI, enabling practitioners to contextualize predictions, assess risk, and prioritize validation efforts [11, 12].

The absence of robust uncertainty handling carries tangible consequences. Overconfident predictions can misguide material selection, obscure failure modes, and lead to inefficient allocation of experimental and computational resources [13, 14]. In engineering and safety-critical domains—such as aerospace structures, nuclear materials, and energy infrastructure—unacknowledged uncertainty may propagate into design decisions with severe technical, regulatory, or societal repercussions [6, 15]. In such contexts, uncertainty is not merely a statistical artifact but a decision-relevant property that governs whether AI-generated insights can be acted upon responsibly.

Compounding these challenges is the lack of conceptual and terminological consistency in how uncertainty and reliability are defined and operationalized within the materials AI literature. Terms such as aleatoric uncertainty, epistemic uncertainty, predictive uncertainty, confidence intervals, model confidence, and reliability are often used inconsistently or interchangeably across studies, disciplines, and modeling paradigms [2, 3]. This fragmentation hinders interdisciplinary communication between materials scientists, data scientists, and engineers, and complicates efforts to compare methods, benchmark performance, or establish best practices. More importantly, it obscures the link between quantified uncertainty and downstream decision-making, where different uncertainty types have distinct implications for model improvement, experimental design, and deployment readiness.

Against this backdrop, the present review provides a comprehensive, thematic synthesis of uncertainty and reliability in materials AI, drawing exclusively on peer-reviewed journal articles published. Rather than focusing on algorithmic novelty or benchmarking performance, the review emphasizes conceptual clarity, linguistic coherence, and decision relevance. Specifically, the objectives are threefold: (1) to clarify core concepts and sources of uncertainty in materials AI, including their origins and practical interpretations [8, 10, 16]; (2) to examine terminological inconsistencies and outline pathways toward conceptual and methodological standardization [2, 3]; and (3) to analyze how uncertainty shapes decision-making across materials discovery, design, validation, and deployment workflows [1, 7, 13]. By organizing the literature thematically, this review identifies synergies, unresolved gaps, and emerging best practices, aiming to support more trustworthy, interpretable, and actionable AI systems in materials science. **Figure 1** provides a conceptual overview of how uncertainty arises in materials AI, how it is quantified and evaluated for reliability, and how it ultimately shapes decision-making across materials discovery and deployment.

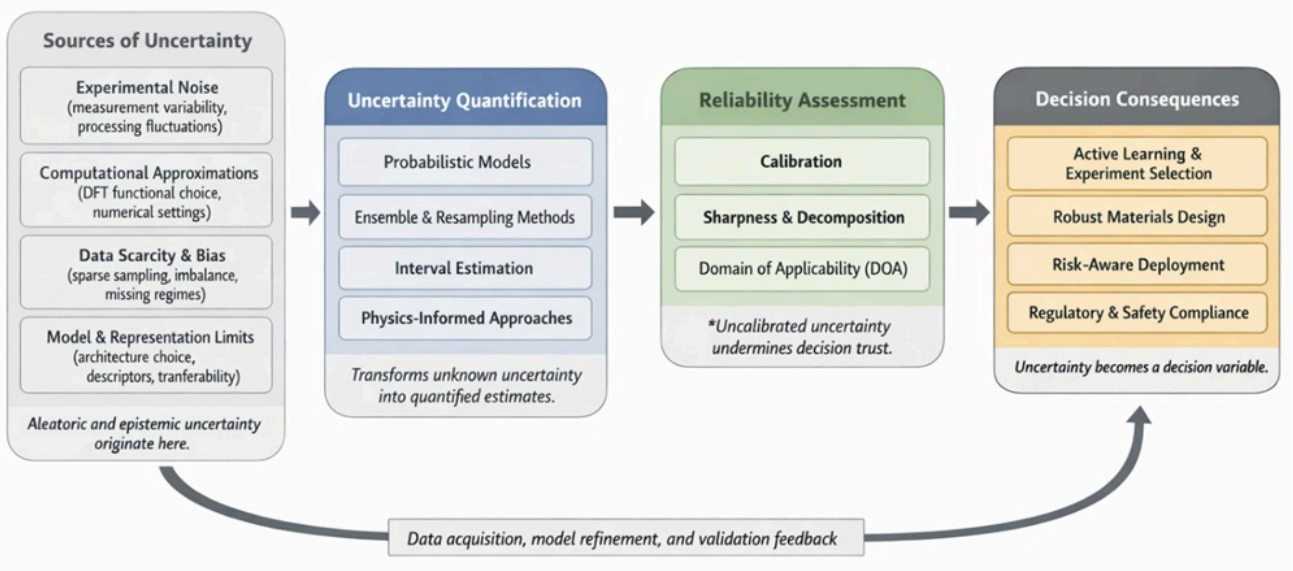

Figure 1. Conceptual pipeline connecting uncertainty sources, quantification methods, reliability assessment, and decision consequences in materials AI

Fundamental concepts of uncertainty in materials AI

Uncertainty in machine learning models applied to materials science is commonly classified into aleatoric and epistemic categories, reflecting fundamentally different origins and implications for model reliability and improvement. Aleatoric uncertainty refers to the irreducible randomness inherent in the data-generating process. In materials contexts, this includes experimental measurement noise in properties such as tensile strength or hardness, stochastic variability in microstructure formation during synthesis, and environmental fluctuations during testing [8, 9]. Because aleatoric uncertainty is intrinsic to the system or measurement process, it cannot be eliminated through additional data or model refinement. Still, it can be explicitly modeled to prevent overconfident predictions.

Epistemic uncertainty, by contrast, arises from incomplete knowledge about the underlying system or the limitations of the model used to represent it. In materials AI, epistemic uncertainty arises from factors such as insufficient or biased training data, incomplete coverage of compositional or processing spaces, suboptimal model architectures, and inadequate feature representations of materials' structure or chemistry [10, 11, 16]. Unlike aleatoric uncertainty, epistemic uncertainty is in principle reducible through targeted data acquisition, improved representations, or refined modeling assumptions. This distinction is particularly important in materials science, where data scarcity and domain complexity are pervasive and directly influence the trustworthiness of AI-driven predictions.

Epistemic uncertainty is especially pronounced in materials AI due to the high dimensionality and sparsity of materials design spaces. Many technologically relevant properties—such as creep resistance, fatigue life, corrosion behavior, or long-term stability—are costly and time-consuming to measure, resulting in limited labeled datasets that inadequately sample the relevant regimes [4, 5]. As a consequence, ML models may exhibit high apparent accuracy within narrow interpolation domains while remaining poorly constrained in extrapolative settings. Even large computational datasets are not immune to epistemic uncertainty: density functional theory (DFT)-generated data introduce systematic biases associated with exchange–correlation functionals, pseudopotentials, and numerical approximations, which propagate into ML predictions of formation energies, phase stability, or electronic properties [9, 10].

The situation is further complicated in hybrid workflows that combine experimental and computational data. While such approaches expand dataset size and diversity, they introduce heterogeneous uncertainty structures in which aleatoric experimental noise and epistemic simulation bias coexist and interact [17, 18]. Without explicit modeling, these mixed

sources can obscure the true confidence of predictions and confound model validation. As a result, uncertainty in materials AI is rarely attributable to a single source; rather, it emerges from the interaction of data limitations, modeling assumptions, and physical complexity across scales.

To address these challenges, probabilistic modeling approaches have gained prominence in materials AI. Bayesian neural networks (BNNs), for example, explicitly represent uncertainty by placing probability distributions over model parameters, enabling posterior predictive distributions that disentangle aleatoric and epistemic components [11, 16]. In practice, fully Bayesian inference remains computationally demanding for large-scale materials problems, motivating the use of approximate methods. Ensemble-based techniques—such as deep ensembles or bootstrap aggregation—estimate epistemic uncertainty by averaging predictions across independently trained models, offering scalable and empirically effective alternatives [11, 19]. Complementarily, heteroscedastic regression models directly predict input-dependent aleatoric variance, capturing property-dependent noise levels that are common in experimental materials data.

Sources of uncertainty specific to materials systems

Beyond these general categories, materials datasets introduce domain-specific sources of uncertainty that distinguish materials AI from applications in more homogeneous data domains. Experimental materials data are inherently variable due to sensitivity to processing histories, sample preparation, environmental conditions, and measurement protocols, leading to substantial aleatoric noise even under nominally identical conditions [4]. In many cases, metadata describing these factors is incomplete or unavailable, further complicating the attribution of uncertainty.

Computational materials datasets, while often larger and more systematic, inherit epistemic uncertainty from the approximations embedded in simulation methods. In DFT-based datasets, uncertainties arise from choices of exchange–correlation functionals, k-point sampling, basis sets, and convergence criteria, which may systematically bias predicted properties across material classes [9, 10]. When such data are treated as ground truth for ML training, these biases become embedded in the learned models, limiting transferability and interpretability.

Transferability itself constitutes a major source of epistemic uncertainty in materials AI. Models trained on specific material families—such as perovskites, oxides, or metallic alloys—often perform poorly when applied to chemically or structurally distinct systems, particularly in extrapolation regimes relevant to discovery [5, 18]. This challenge is exacerbated by data imbalance and long-tailed distributions of material properties, commonly observed in materials databases such as JARVIS and the Materials Project, where well-studied compounds dominate and rare or extreme-property materials are underrepresented [2].

Finally, representation choices play a critical but often underappreciated role in shaping uncertainty. Feature engineering decisions—ranging from handcrafted descriptors of composition and symmetry to learned graph-based representations—implicitly encode assumptions about what aspects of materials structure are relevant [4, 5]. Inadequate or overly coarse representations can introduce additional epistemic uncertainty by constraining the model's hypothesis space, leading to confident but physically uninformative predictions. Recognizing and accounting for these representation-induced uncertainties is therefore essential for building reliable and interpretable materials AI systems.

Methods for uncertainty quantification in materials machine learning

A wide range of uncertainty quantification (UQ) techniques has been adapted from statistical learning and probabilistic modeling to address the distinctive challenges of materials machine learning. Among the earliest and most established approaches, Gaussian process regression (GPR) offers closed-form predictive uncertainty estimates derived from Bayesian principles, making it attractive for small-to-moderate materials datasets where data efficiency and interpretability are critical [7]. However, the cubic computational scaling of GPR with dataset size limits its applicability to large materials databases, motivating the development of hybrid approaches that combine GPR kernels with neural network feature extractors or sparse approximations [7].

As scalable alternatives, nonparametric interval estimation methods, such as quantile regression and direct prediction-interval modeling, have gained prominence in materials applications [11, 19]. These approaches construct uncertainty bounds without assuming Gaussian error distributions, an important advantage given the skewed, heteroscedastic, and long-tailed nature of many material property distributions. By directly modeling conditional quantiles, these methods provide flexible prediction intervals that better reflect experimental variability and regime-dependent noise, particularly for properties such as fracture toughness, fatigue life, or degradation rates.

Recent work has also emphasized integrating physical knowledge into uncertainty-aware learning. Physics-informed neural networks (PINNs) incorporate governing equations, constitutive relations, or conservation laws as inductive biases that constrain the model's hypothesis space [14, 18]. In materials contexts, such constraints can reduce epistemic uncertainty by ruling out physically implausible solutions, especially in multiscale modeling scenarios where data are sparse and physical priors are well established. While PINNs do not eliminate uncertainty, they reshape its structure, shifting uncertainty from physically constrained regions toward under-specified boundary conditions or poorly observed regimes.

Conformal prediction frameworks have emerged as a complementary paradigm, offering distribution-free, finite-sample guarantees on the coverage of prediction intervals [19]. This property is particularly appealing for materials decision-making under safety or regulatory constraints, where guarantees on worst-case performance may be more valuable than asymptotic Bayesian optimality. Conformal methods are model-agnostic and can be layered atop existing predictors, making them attractive for deployment in materials screening pipelines where reliability assurances are required without re-engineering the underlying model.

Calibration and the role of post-hoc adjustment

Accurate uncertainty estimation alone is insufficient if predicted uncertainties are poorly calibrated. In practice, many materials ML models exhibit systematic miscalibration, where nominal confidence levels fail to correspond to observed error frequencies. Such misalignment undermines the practical utility of uncertainty estimates, particularly in ranking or decision-support settings. Post-hoc calibration techniques—including temperature scaling, isotonic regression, and bootstrap-based recalibration—have therefore become integral components of reliable materials AI workflows [19, 20].

Calibration is especially critical in materials science because uncertainty often varies strongly across compositional, structural, or processing regimes. Models that appear well-calibrated on average may still exhibit localized overconfidence in sparsely sampled regions, leading to misleading predictions during materials exploration. As a result, calibration must be evaluated not only globally but also in relation to domain coverage and data density.

Reliability assessment and evaluation metrics

Reliability in materials ML extends beyond point prediction accuracy to encompass multiple complementary dimensions, including calibration quality, uncertainty sharpness, and domain of applicability (DOA). Standard quantitative metrics include negative log-likelihood, expected calibration error (ECE), and empirical coverage probability of prediction intervals, each capturing distinct aspects of predictive trustworthiness [11, 19]. Sharpness metrics assess whether uncertainty bounds are informative rather than trivially wide, while coverage metrics evaluate whether stated confidence levels are empirically justified.

Domain-of-applicability analysis plays a particularly central role in materials discovery, where extrapolation beyond known chemical or processing regimes is common. Techniques such as kernel density estimation, Mahalanobis distance, or latent-space distance measures identify regions of input space where model predictions are well supported by training data [6, 13]. By flagging predictions made outside the DOA, these methods help prevent spurious discoveries and reduce wasted experimental effort. **Table 1** summarizes the relationships between uncertainty sources, commonly used quantification approaches, reliability evaluation metrics, and their implications for materials decision-making.

Table 1. Mapping uncertainty types, quantification methods, reliability metrics, and decision implications in materials AI

Uncertainty type/Source	Typical UQ methods	Reliability metrics	Decision implications in materials AI
Aleatoric (experimental noise, process variability)	Heteroscedastic regression, quantile regression	Coverage probability, sharpness	Sets irreducible error bounds; informs safety margins and tolerance design
Epistemic (data scarcity, model limits)	Bayesian neural networks, ensembles, GPR	Ensemble variance, mutual information	Guides data acquisition, active learning, and model improvement
Computational bias (DFT approximations)	Multi-fidelity models, Bayesian calibration	Calibration error, cross-domain validation	Limits transferability; informs confidence in simulation-trained models
Extrapolation / OOD regimes	DOA analysis, conformal prediction	OOD detection rate, coverage under shift	Prevents spurious discoveries and unsafe deployment
Representation uncertainty	Latent-space analysis, ensemble diversity	Stability across representations	Flags are physically uninformative but confident predictions

Advanced decomposition techniques further separate uncertainty components to guide targeted improvements. Ensemble variance and mutual-information-based methods distinguish epistemic uncertainty from aleatoric contributions, enabling informed decisions about whether to prioritize data acquisition, model refinement, or experimental validation [6, 10]. Complementarily, cross-validation strategies and explicit out-of-distribution (OOD) detection serve as stress tests of model reliability in realistic deployment scenarios [2, 4].

Language and terminology in uncertainty and reliability literature

Despite methodological progress, the materials AI literature remains fragmented in its use of terminology for uncertainty and reliability. The term uncertainty is frequently conflated with error, variance, or model confidence, while reliability may variously denote robustness to noise, reproducibility across datasets, or subjective trust in predictions [2, 3]. Such ambiguity obscures essential conceptual distinctions, hindering rigorous interpretation and comparison of studies.

A recurring source of confusion lies in the interchangeable use of confidence intervals (frequentist) and credible intervals (Bayesian), often without explicit acknowledgment of their differing statistical interpretations [11, 16]. Similarly, phrases such as ‘uncertainty-aware design,’ ‘reliable ML,’ or ‘trustworthy AI’ are widely used in materials-specific contexts but lack consistent operational definitions, complicating their translation into industrial practice or standards development [4, 10].

Recent reviews and position papers emphasize the need for terminological standardization, advocating clear separation between total predictive uncertainty and its aleatoric and epistemic components, as well as explicit alignment with probabilistic theory [2, 3]. In the materials domain, such clarity is particularly important given the field’s interdisciplinary nature, spanning materials science, statistics, physics, and AI. The development of shared glossaries and unified conceptual frameworks has therefore been identified as a prerequisite for reproducible, interpretable, and actionable uncertainty-aware materials AI.

Decision consequences in materials design and applications

Uncertainty plays a decisive role in how AI-generated predictions are translated into actionable decisions in materials engineering. In early-stage discovery workflows, uncertainty quantification (UQ) directly shapes experimental strategy by guiding active learning and sequential design. Rather than selecting candidates solely on predicted performance, uncertainty-aware workflows prioritize materials that maximize information gain, enabling efficient exploration of vast

design spaces under limited experimental budgets [6, 13]. This paradigm has proven particularly effective in high-dimensional compositional systems, where naive exploitation of point predictions can lead to premature convergence to suboptimal regions.

In materials design and optimization, uncertainty propagation across multiscale models is essential for ensuring robust performance under variability. Properties such as creep resistance, fatigue life, and thermal stability are sensitive to microstructural heterogeneity and processing fluctuations, making deterministic optimization insufficient [14, 15]. By explicitly accounting for uncertainty, designers can evaluate trade-offs between nominal performance and robustness, a requirement in applications such as turbine blade alloys or structural components subjected to extreme operating conditions.

The consequences of ignoring uncertainty are well documented. Overconfident ML predictions can lead to optimistic material selections that fail during prototyping or deployment, resulting in increased development costs, delayed timelines, or safety incidents. In high-temperature alloys, for example, mispredictions of creep behavior due to unacknowledged epistemic uncertainty may only manifest after long-term testing, at substantial economic and technical cost [8, 10]. In regulated domains such as aerospace and nuclear engineering, certification frameworks increasingly demand quantified risk assessments that explicitly incorporate uncertainty, rendering uncertainty-agnostic AI outputs insufficient for compliance [15].

Empirical case studies underscore the practical benefits of uncertainty-aware decision-making. In perovskite photovoltaics, calibrated UQ has been shown to reduce false positives in stability screening, accelerating experimental validation while minimizing wasted effort on unstable compositions [7, 18]. Similarly, in additive manufacturing, uncertainty-aware defect prediction enables proactive process optimization, reducing the likelihood of structural weaknesses and improving quality control [5]. Across these applications, uncertainty serves not merely as an auxiliary metric but as a control variable that governs decision confidence and validation strategy.

Challenges, integration, and emerging directions

Despite demonstrated benefits, integrating UQ into materials AI pipelines remains challenging. Scalability limitations hinder the widespread adoption of Bayesian neural networks for large, high-dimensional materials datasets, while mixed-variable inputs—combining composition, processing parameters, and structural descriptors—complicate uncertainty modeling [1, 10, 21]. The integration of UQ with generative models for inverse design introduces additional complexity, as uncertainty must be propagated through both the generation and evaluation stages of the design loop.

Benchmarking consistency represents another open challenge. Different studies evaluate UQ performance using heterogeneous metrics and datasets, making cross-property or cross-method comparisons difficult. Moreover, hybrid physics–ML approaches, while promising for improving generalization, raise unresolved questions about how uncertainty should be partitioned between physical constraints and data-driven components [14, 18].

Addressing these challenges requires sustained interdisciplinary collaboration among materials scientists, statisticians, and AI researchers. Standardized terminology, shared benchmarks, and modular UQ components embedded within commonly used materials informatics platforms are increasingly recognized as prerequisites for broader adoption [2, 3]. Looking ahead, emerging directions include real-time UQ in autonomous laboratories, uncertainty-aware decision-support systems, and frameworks that explicitly quantify economic, environmental, and safety trade-offs alongside predictive uncertainty [1, 6, 7].

Results and Discussion

This review synthesizes recent progress in uncertainty and reliability for materials AI, highlighting both conceptual advances and persistent limitations. Aleatoric uncertainty, arising from inherent randomness in synthesis and

measurement, and epistemic uncertainty, stemming from data scarcity and model limitations, represent distinct but interacting sources that must be disentangled to support trustworthy predictions [8, 22]. Probabilistic approaches such as Bayesian neural networks and ensemble methods enable this separation in principle. Yet, their application to high-dimensional materials spaces—such as complex alloys or defect-rich microstructures—remains computationally demanding and sensitive to modeling assumptions [1, 23].

Terminological inconsistency continues to impede progress. Core concepts such as “prediction interval,” “credible interval,” and “uncertainty estimate” are frequently used without formal distinction, leading to ambiguity in interpretation and comparison across studies [11, 16]. Similarly, reliability is variably defined in terms of calibration, sharpness, robustness, or domain coverage, reflecting a lack of consensus on evaluation priorities. Community-driven standardization efforts, including shared glossaries aligned with statistical theory, are therefore essential for improving reproducibility and interdisciplinary communication [17, 24].

The decision consequences of uncertainty are particularly acute in materials engineering. In discovery settings, uncertainty-guided active learning demonstrably reduces experimental cost and accelerates convergence for properties such as formation energy and bandgap [19, 25]. In safety-critical applications—including creep-resistant alloys and energy storage materials—miscalibrated or ignored uncertainty can lead to structural failure, regulatory delays, or inefficient designs, with significant downstream impacts [12, 15]. Physics-informed and multi-fidelity approaches mitigate some extrapolation risks by embedding conservation laws and hierarchical information, yet they remain challenged by heterogeneous integration of experimental–computational data [6, 20].

Calibration emerges as a central pillar of reliability. Uncertainties that are numerically precise but empirically miscalibrated undermine decision trust, particularly for sparse-data properties such as fatigue life or irradiation damage. Post-hoc calibration techniques and conformal prediction frameworks improve empirical coverage and provide defensible uncertainty bounds, enhancing confidence in downstream decisions [18, 26]. Complementarily, domain-of-applicability assessment and out-of-distribution detection prevent deployment in unsupported regimes, a recurring risk in inverse and generative materials design [9, 27].

No single UQ method dominates across all material properties or data regimes. Hybrid models combining Gaussian processes with neural architectures, as well as variational inference techniques, offer scalable compromises, but benchmark studies consistently demonstrate property-dependent performance trade-offs [2, 4]. Data scarcity in emerging materials classes, including rare-earth systems and high-entropy alloys, further amplifies epistemic uncertainty, motivating the use of transfer learning and data augmentation strategies [10, 21]. Importantly, industrial adoption remains sensitive to language and interpretability, as practitioners require uncertainty estimates that are not only statistically sound but operationally actionable for risk assessment [13, 28].

Case studies reinforce these conclusions. In perovskite solar cells, uncertainty-aware screening reduces false discovery rates and accelerates stability validation [3, 29]. In additive manufacturing, uncertainty-informed defect prediction supports process optimization and quality assurance [5, 30]. Across domains, misalignment in terminology and expectations between AI developers and materials engineers continues to slow translation, underscoring the need for shared conceptual frameworks [7, 31].

Beyond technical considerations, broader implications emerge. The deployment of unreliable AI models in high-stakes materials contexts raises ethical and accountability concerns, particularly when decisions affect safety, sustainability, or public trust [14, 32]. Economically, uncertainty-aware pipelines reduce wasted experimentation and improve resource efficiency across R&D ecosystems [33, 34]. Taken together, the evidence synthesized in this review underscores that robust uncertainty quantification is not merely an adjunct to predictive accuracy but a foundational requirement for risk-aware, responsible, and sustainable materials innovation [35, 36].

Conclusion

This narrative review has elucidated the core concepts of uncertainty in materials AI, highlighted terminological inconsistencies, and examined their profound impacts on decision-making. Aleatoric and epistemic uncertainties require tailored quantification methods like BNNs, ensembles, and GPR, while standardized language is critical for cross-disciplinary efficacy. The consequences of decisions span accelerated discovery, risk mitigation in engineering, and the avoidance of costly failures.

Future directions include developing scalable, physics-informed UQ for large datasets, creating unified benchmarks for materials-specific properties, and integrating real-time UQ in autonomous laboratories. Emphasis on calibration, domain applicability, and interpretable metrics will build greater trust. Community efforts toward glossaries, open datasets, and regulatory guidelines will facilitate industrial adoption. Ultimately, advancing uncertainty handling will realize the full potential of materials AI for innovative, reliable solutions.

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