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Scientific Decision-Making with Materials AI — How Models Actually Influence Action: A Review Study

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Abstract

The integration of artificial intelligence (AI) and machine learning (ML) in materials science has revolutionized traditional approaches to material discovery, design, and application. This narrative review explores how AI models not only predict material properties but also influence scientific decision-making by providing actionable insights, optimizing experimental strategies, and enabling inverse design paradigms. Drawing on recent advancements, we examine the transition from data-driven prediction to AI-assisted decision-making, highlighting case studies in porous materials, optoelectronics, and polymeric membranes. The review addresses challenges such as data scarcity, model interpretability, and integration with experimental workflows, while proposing future directions for AI to enhance human decision-making in materials research. Ultimately, AI is positioned as a collaborative tool that augments scientific intuition, accelerating innovation in sustainable and high-performance materials.

Keywords Artificial intelligence, Materials discovery, Machine learning, Inverse design, Decision-making, Predictive modeling

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Introduction

Scientific decision-making with Materials AI — How models actually influence action

From experimental iteration to algorithmic mediation

Materials science has traditionally progressed through iterative experimental cycles supported by theoretical modeling and empirical reasoning. Discovery pathways were shaped by laboratory trial-and-error processes, incremental parameter adjustments, and the interpretive judgment of domain experts. Whether in metallurgy, ceramics, polymers, or semiconductor engineering, materials development relied heavily on sequential experimentation guided by accumulated scientific intuition [1-4].

While this empirically grounded paradigm yielded transformative innovations, it was inherently constrained by time, cost, and experimental throughput. Exploration of compositional and structural design spaces remained selective rather than exhaustive, bounded by the practical limitations of synthesis feasibility, instrumentation access, and human cognitive bandwidth. As a result, vast regions of potentially valuable materials landscapes remained underexplored or entirely inaccessible [5-7].

The integration of artificial intelligence (AI) and machine learning (ML) has fundamentally reconfigured this epistemic structure. Materials research is no longer governed solely by hypothesis-driven experimentation but increasingly mediated by predictive inference systems capable of screening millions of candidate materials computationally before laboratory validation. In this context, AI functions not merely as an analytical accelerator but as a strategic intermediary that reshapes how scientific attention, resources, and risk are distributed across discovery pipelines [6-9].

Evolution of AI in materials science

Early predictive applications

The initial incorporation of AI into materials science focused on predictive modeling. Supervised learning algorithms were trained on computational and experimental datasets to estimate material properties, including band gaps, elastic moduli, thermal conductivity, and formation energies. These early systems provided valuable forecasting capabilities, enabling researchers to anticipate performance outcomes without immediate experimental verification.

However, decision influence at this stage remained largely interpretive. AI outputs informed understanding and guided discussion, but rarely dictated experimental direction. Scientists retained primary agency in determining which materials to synthesize, test, or discard [10-13].

Expansion into design space navigation

As high-throughput computational infrastructures and open materials databases expanded, AI systems began operating within combinatorially vast chemical and structural design spaces. The role of models evolved from isolated property prediction toward large-scale candidate screening and prioritization.

In this phase, AI systems began to function as navigational engines. Rather than evaluating one material at a time, models ranked thousands or even millions of hypothetical compounds based on predicted performance, stability, and feasibility. This ranking capability introduced a new layer of decision mediation, influencing which materials advanced to synthesis and which remained computational abstractions [14-17].

Emergence of generative and foundation models

Recent advances in generative modeling architectures have extended AI's role beyond evaluation into the realm of creation. Variational autoencoders, generative adversarial networks, diffusion models, and emerging foundation systems can propose entirely new material compositions and structures.

These systems generate candidates that may not yet exist in experimental databases, expanding the horizon of conceivable materials. Consequently, AI is no longer confined to optimizing known systems but actively participates in defining future discovery pathways. The conceptual boundary between scientific imagination and computational generation is increasingly blurred [16-19].

AI as a scientific decision infrastructure

As AI capabilities have matured, their role in materials science has shifted from supporting analysis to embedded decision infrastructure. Models now operate across multiple layers of scientific action, influencing not only how materials are evaluated but how research itself is organized and executed.

At the strategic level, AI insights inform research portfolio planning, identifying high-potential domains for investment. At the experimental level, predictive rankings determine which candidates are synthesized or tested. At the translational stage, models help assess scalability, manufacturability, and deployment feasibility.

This multi-layered integration positions AI as a governance mechanism within materials innovation ecosystems. Scientific workflows increasingly incorporate algorithmic recommendations as operational decision inputs rather than optional

analytical supplements [20-22].

Domains of decision influence

Predictive analytics as experimental gatekeeping

Property prediction remains one of the most visible domains of AI influence. Predictive models act as filters, determining which materials warrant experimental validation. By forecasting performance metrics in advance, AI enables laboratories to allocate resources toward the most promising candidates.

This predictive gatekeeping enhances efficiency but also introduces directional bias. Materials falling outside high-confidence prediction zones may be deprioritized, potentially constraining exploratory diversity and serendipitous discovery [23-26].

Inverse design and target-driven discovery

Inverse design frameworks represent a conceptual inversion of traditional materials research. Rather than evaluating the properties of existing materials, scientists define desired functional targets and use AI systems to identify candidate structures that can achieve them.

This goal-oriented paradigm embeds algorithmic reasoning directly into ideation processes. AI systems become partners in formulating discovery hypotheses, proposing structural solutions aligned with performance objectives [27-29].

Autonomous and closed-loop experimentation

Integration of AI with robotics and high-throughput instrumentation has enabled the emergence of autonomous experimentation platforms. In these environments, models iteratively propose experiments, analyze resulting data, and refine subsequent experimental decisions.

Such closed-loop systems transform laboratories into adaptive learning ecosystems. Human researchers increasingly supervise rather than manually direct experimental sequencing, marking a shift toward hybrid human–machine discovery architectures [8, 28, 29].

Data expansion and the scaling of search spaces

The rapid expansion of computational repositories, experimental archives, and simulation datasets has amplified the scale of searchable materials design spaces. AI systems extract latent correlations across these data environments, identifying patterns that would remain undetectable through manual analysis.

This capability has accelerated the discovery of functional materials across domains such as optoelectronics, catalysis, and high-entropy alloy systems. By navigating ultra-high-dimensional search terrains, AI extends the exploratory reach of materials science beyond traditional feasibility constraints.

Uncertainty as a regulator of scientific action

Beyond prediction, uncertainty quantification plays a central role in moderating AI-guided decision-making. Confidence estimates indicate whether model outputs warrant experimental validation or require additional data acquisition.

In this sense, uncertainty functions as a governance signal within discovery pipelines. It regulates risk exposure, prioritizes data generation, and shapes the sequencing of experimental investment. Decision-making becomes not only performance-driven but confidence-conditioned.

Ethical and epistemic implications

As AI systems assume greater influence over scientific direction, ethical and epistemic considerations become increasingly salient. Questions arise regarding transparency, interpretability, and accountability in model-mediated decisions.

Opaque predictive systems may guide high-stakes materials deployment without a fully interpretable mechanistic justification. Dataset biases may propagate through predictive pipelines, shaping discovery priorities in ways that remain scientifically invisible yet operationally consequential.

Responsible integration of AI, therefore, requires reflexive governance frameworks that address not only technical performance but epistemic reliability and societal accountability.

Scope and structure of this review

This narrative review examines how AI systems shape scientific and industrial decision-making across the materials lifecycle. The analysis is organized thematically rather than methodologically, focusing on interpretive and infrastructural dimensions of model influence.

Three primary domains structure the discussion:

1. Predictive analytics as experimental gatekeeping
2. Generative and inverse design as ideation engines
3. Autonomous platforms as operational decision systems

By synthesizing recent literature, the review seeks to illuminate how AI models move beyond passive prediction to actively shape scientific action, research prioritization, and innovation trajectories in contemporary materials science. **Figure 1** summarizes the model-mediated decision pathways that translate predictive outputs into scientific action.

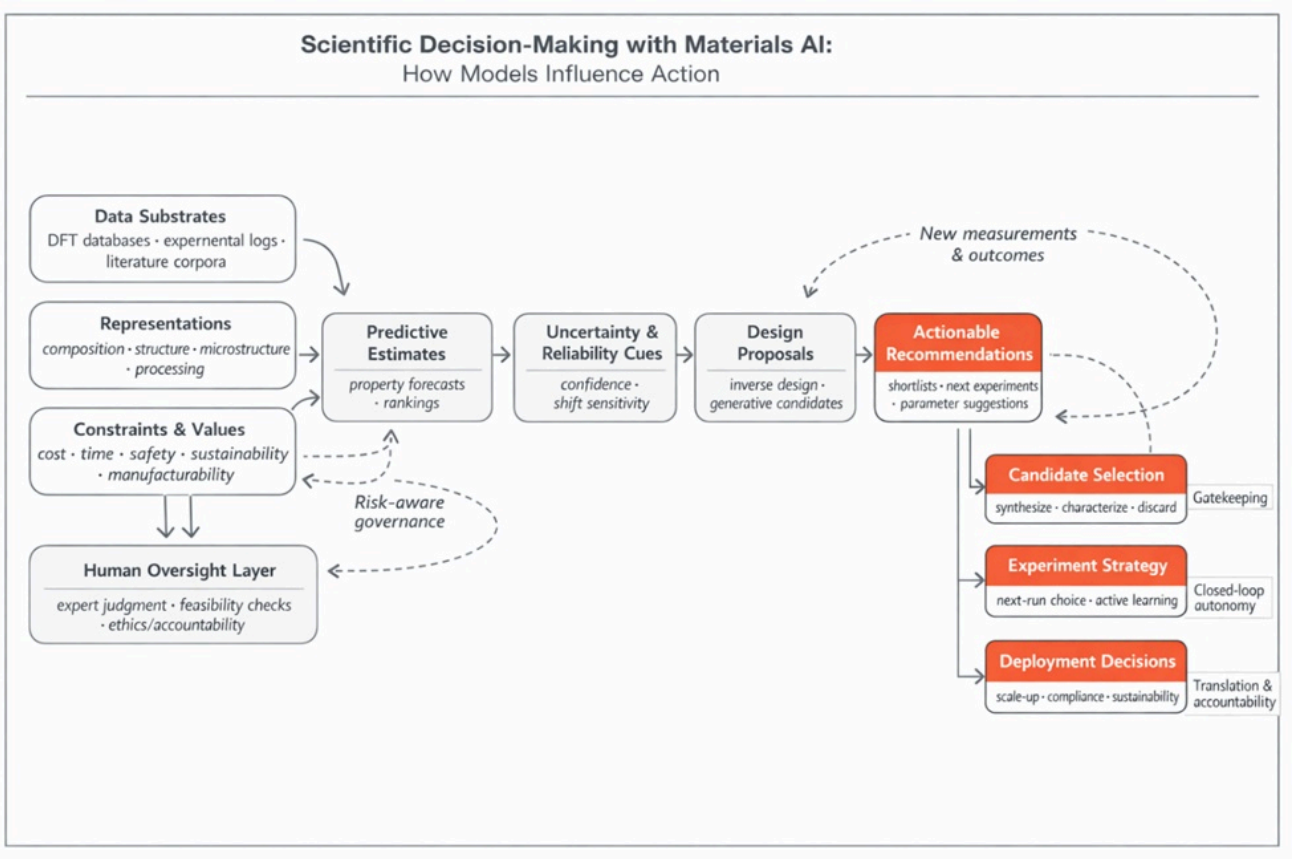

Figure 1. Model-mediated scientific action in materials AI: from prediction outputs to decision pathways

Table 1 summarizes the primary mechanisms through which materials AI translates prediction into action across the research pipeline.

Table 1. How materials AI influences scientific action across the research pipeline

Decision stage in materials workflow	What the AI model provides	How it changes action (not just understanding)	Typical materials-domain examples you already use	Common failure mode/risk	Practica you disc
Problem framing and research direction	Pattern discovery in large corpora and databases; emerging "opportunity zones"	Redirects what teams consider worth pursuing; narrows/expands research portfolio	Optoelectronics and high-throughput screening; database-driven hypothesis generation	Agenda bias toward well-represented materials families	Da diver governan ben trans
Candidate screening and prioritization	Ranked candidate lists; feasibility-informed shortlists	Determines *which* candidates enter synthesis/characterization queues	Porous materials screening for gas separation; optoelectronic candidates for validation	Over-filtering and lost serendipity; bias amplification	Inject e quotas "novel human r

Experiment planning and resource allocation	Recommendations for next experiments; active learning choices	Allocates time, budget, and instrument access; reduces trial-and-error	Nanomaterials under small-data regimes; active learning for acquisition	Premature convergence on “safe” regions; feedback loops	Exp safe uncerta samplir reset s
Inverse design and target-driven discovery	Proposed structures/materials meeting target specs	Moves ideation from human-first to model-assisted; shifts synthesis toward model-generated candidates	Polymeric membranes with predicted selectivity/permeability; inverse design pipelines	Proposes impractical or non-synthesizable candidates	Synth constrai rules; hy AI sc
Generative “what-if” exploration	Counterfactual variants; design alternatives and trade-off surfacing	Enables pre-experimental decision rehearsal; guides which modifications to attempt	Battery composition exploration; functional materials design proposals	Opaque rationales; “creative but wrong” candidates	Exp constra interp cons deploym stakes
Risk management and validation gating	Confidence/uncertainty signals; reliability cues	Decides whether to validate, defer, or collect more data	Safety-relevant structural materials; deployment decisions	Miscalibrated confidence; false security	Cali uncerta out-of- detecti p
Translation and scale-up considerations	Early manufacturability/stability flags; process sensitivity insights	Influences go/no-go for scale-up and deployment	Industrial filtration/membrane deployment; energy materials translation	Lab-to-fab mismatch; context shift	Hybrid con monitor validation
Ethical governance and accountability	Interpretability artifacts; traceability; bias indicators	Shapes what is acceptable to deploy; changes institutional decision thresholds	High-stakes applications (biomedical/structural)	“Black-box authority” without accountability	XAI in docun human- gove

Main Text

Decision support

Data as the epistemic substrate of materials AI

Artificial intelligence in materials science is fundamentally grounded in data-driven learning. Unlike traditional physics-first modeling approaches, AI systems derive inferential capacity from exposure to large datasets linking composition, structure, processing conditions, and functional properties. Through statistical pattern recognition and representation learning, these models identify latent correlations that may not be explicitly encoded within established theoretical frameworks.

Materials datasets—sourced from high-throughput density functional theory calculations, experimental repositories, and combinatorial screening platforms—serve as the epistemic substrate for AI reasoning. Within these environments, models

learn to associate crystallographic features, elemental distributions, and microstructural attributes with performance metrics such as conductivity, catalytic activity, or mechanical strength.

This data-centric paradigm enables predictive capabilities that extend beyond human-scale analytical capacity. However, the significance of these systems lies not solely in their forecasting accuracy but in their ability to transform predictive outputs into actionable scientific direction.

Early predictive systems: Informing but not directing action

Initial deployments of machine learning in materials science focused on property prediction tasks. Algorithms such as random forests, support vector machines, and early neural network architectures were trained to estimate materials' behavior across diverse domains, including electronic structure, thermodynamic stability, and optical performance.

In this phase, AI primarily served as a decision-support tool rather than a decision driver. Predictions provided probabilistic guidance that researchers could integrate into broader interpretive reasoning processes. Experimental agendas remained human-directed, with AI serving as an efficiency-enhancing analytical layer.

Illustrative applications included predicting topological semimetals, in which Gaussian process models screened candidate compounds and identified promising structures for experimental validation. Such systems reduced exploratory uncertainty and minimized trial-and-error experimentation, yet ultimate decision authority remained anchored in expert evaluation.

Transition to decision-centric modeling

The shift from predictive analytics to decision support emerged as AI systems began incorporating uncertainty estimation and multi-objective optimization capabilities. Rather than providing single-point forecasts, models started delivering probabilistic performance landscapes that accounted for prediction confidence, trade-offs, and feasibility constraints.

This transition marked a critical epistemic inflection. AI outputs no longer answered only the question "What will happen?" but increasingly addressed "What should be done next?"

In architectured porous materials, for example, convolutional neural networks and graph neural networks have been deployed to evaluate structural topologies while simultaneously recommending design parameters. These recommendations influence material selection decisions in applications such as gas separation, catalysis, and energy storage.

Similarly, optoelectronic materials discovery pipelines now integrate high-throughput screening with AI-guided prioritization. Here, predictive ranking systems determine which materials advance to synthesis, effectively governing research resource allocation.

Generative reasoning and "What-If" decision simulation

A defining development in AI-mediated decision-making is the rise of generative modeling frameworks. Variational autoencoders, generative adversarial networks, and related architectures enable the simulation of hypothetical materials scenarios before experimental realization.

These systems facilitate structured "what-if" exploration, allowing scientists to evaluate potential outcomes of compositional or structural modifications without physical synthesis. By generating candidate materials aligned with specified functional targets, generative AI transforms speculative reasoning into computationally testable propositions.

In battery materials research, for instance, generative workflows have accelerated compositional optimization by proposing chemistries that balance energy density, thermal stability, and lifecycle durability. This capability compresses

experimental iteration cycles and enables more strategically targeted validation efforts.

Thus, generative AI does not merely predict the future—it allows researchers to simulate alternative decision pathways before committing laboratory resources.

AI-Driven inverse design: Reshaping material discovery strategies

Conceptual inversion of the discovery paradigm

Inverse design is among the most transformative manifestations of AI's decision-making influence. Traditional materials research follows a forward modeling paradigm: researchers synthesize or hypothesize a material and subsequently evaluate its properties.

Inverse design inverts this logic. Scientists begin with target performance criteria—such as permeability thresholds, band gap ranges, or catalytic efficiencies—and employ AI systems to identify structures capable of fulfilling those objectives.

This reversal shifts AI from evaluative analyst to ideation partner. Models actively participate in defining candidate materials rather than merely assessing them.

Navigating vast chemical design spaces

The utility of inverse design is particularly evident in expansive chemical spaces where conventional search strategies are computationally or experimentally infeasible. Polymeric materials provide a notable example. Machine-learning–assisted inverse design frameworks have identified novel membrane chemistries optimized for selective gas separation and environmental remediation.

By simultaneously forecasting permeability–selectivity trade-offs and structural feasibility, AI systems guide synthesis decisions with unprecedented precision. This reduces exploratory inefficiency while expanding the set of viable candidate solutions.

Generative models as discovery engines

Generative architectures play a pivotal role in operationalizing inverse design. By learning statistical distributions from existing materials datasets, these systems produce new candidate structures aligned with defined performance targets.

In the field of functional materials discovery, generative AI has proposed advanced compounds for catalysis, sensing, and electronic applications. Conditional generative models further refine this capability by constraining outputs to synthesizable or application-relevant domains.

One prominent application lies in drug-like materials and biofunctional compounds, where generative models have accelerated anticancer material discovery by recommending structurally plausible and experimentally tractable candidates. Here, AI directly informs the prioritization of synthesis and the biomedical exploration pathways.

Integration with autonomous experimentation

The convergence of inverse design, robotics, and high-performance computing has enabled the emergence of AI-directed experimental ecosystems. Autonomous laboratories integrate generative design engines with robotic synthesis and real-time characterization systems.

Within these environments, AI systems propose candidate materials, experimental platforms execute synthesis and testing, and resulting data feed back into model refinement loops. Decision-making becomes iterative, adaptive, and increasingly machine-mediated.

Such infrastructures are particularly impactful in energy materials and biomedical systems, where discovery timelines and optimization complexity are substantial.

Uncertainty quantification and interpretability: Enhancing trust in AI decisions

Uncertainty as a decision governance mechanism

A critical determinant of AI's influence on scientific action is its capacity to express predictive uncertainty. Confidence estimation enables researchers to evaluate the reliability of model recommendations before committing experimental resources.

Advanced probabilistic models provide prediction intervals, variance estimates, confidence distributions, and performance forecasts. These signals inform whether a candidate warrants synthesis, further simulation, or additional data acquisition.

In materials intelligence workflows, uncertainty-aware optimization has enabled performance-driven yet risk-moderated design strategies that balance exploratory breadth with validation efficiency.

Interpretability and explainable AI

Interpretability mechanisms further enhance trust in AI-guided decisions. Explainable AI techniques illuminate how models derive predictions, revealing feature contributions, structural sensitivities, and drivers of latent representations.

In solid-state materials research, interpretable feature mapping has clarified structure–property relationships, enabling scientists to understand why certain crystal motifs or compositional patterns yield superior performance.

This transparency influences downstream actions, including targeted material modification, compositional tuning, and processing optimization.

Hybrid Physics–AI decision frameworks

Hybrid modeling approaches that integrate physics-based constraints with machine learning inference have emerged as powerful decision-support systems. By embedding thermodynamic laws, symmetry constraints, and mechanistic priors into AI architectures, these frameworks enhance both predictive reliability and interpretive coherence.

Applications in composite structures and structural materials engineering demonstrate how hybrid models guide design decisions while maintaining alignment with safety, durability, and sustainability requirements.

Such systems position AI not as an opaque oracle but as a scientifically grounded collaborator.

Case studies: AI models in action across materials domains

Membrane and separation technologies

In membrane science, AI-guided inverse design has enabled the discovery of high-performance polymeric systems optimized for gas separation and water purification. Models simultaneously evaluate permeability, selectivity, and manufacturability, informing synthesis prioritization.

This has accelerated the deployment of environmental materials and reduced development timelines in industrial filtration applications.

Nanomaterials discovery under data scarcity

Nanomaterials research often operates under small-data constraints. AI systems employing active learning strategies have demonstrated the ability to guide experimental sequencing efficiently, determining which measurements yield

maximal informational gain.

Such decision-guided data acquisition optimizes resource allocation and accelerates nanoscale materials characterization.

Generative AI in energy storage materials

Generative transformer-based models and related architectures have influenced decision-making in the field of battery and supercapacitor materials. By predicting and designing electrode structures and electrolyte chemistries, AI systems guide development from laboratory prototypes to industrial-scale considerations.

These applications highlight AI's capacity to shape the full innovation pipeline rather than isolated discovery stages.

Challenges in AI-influenced decision-making and mitigation strategies

Data scarcity and generalizability constraints

Despite significant progress, data limitations remain a persistent challenge. Sparse, noisy, or domain-specific datasets can limit model generalizability, leading to decisions grounded in incomplete information.

Transfer learning strategies mitigate these constraints by leveraging knowledge from adjacent materials domains, enabling cross-system inference and broader applicability.

Bias and interpretability risks

Dataset bias can propagate through predictive pipelines, skewing AI-guided discovery priorities. In optoelectronic materials research, biased training distributions have been shown to influence candidate ranking outcomes.

Mitigation strategies include physics-informed modeling, dataset diversification, and the integration of explainable AI to ensure recommendations remain scientifically grounded.

Scalability in autonomous systems

Scaling AI decision-making into autonomous laboratory environments introduces logistical and infrastructural challenges. Experimental throughput, instrumentation compatibility, and synthesis feasibility must align with algorithmic recommendations.

Hybrid human–AI governance models are emerging as pragmatic solutions that combine computational optimization with expert oversight.

Future directions in decision-centric materials AI

Future trajectories point toward increasingly integrated AI ecosystems where prediction, generation, experimentation, and deployment operate within unified decision architectures.

Advances in foundation models, multimodal data fusion, and physics-constrained learning are expected to further AI's capacity to influence scientific action responsibly and transparently.

Emerging trends: AI as a collaborative decision-maker

Emerging trends position AI as a collaborative tool in decision-making. Foundation models, trained on vast datasets, enable intuitive queries and adaptive recommendations, influencing actions in real-time [9]. In biomedicine, AI decisions optimize drug-delivery materials, blending predictive modeling with ethical considerations [8].

The integration of AI with quantum computing promises faster decisions, while ethical frameworks ensure equitable influence on action [11]. These trends signal a future where AI augments human expertise, driving sustainable materials innovation [4].

Results and Discussion

The integration of AI models into scientific decision-making in materials science represents a transformative leap, yet it is not without its complexities and debates [1, 3, 6]. One central discussion revolves around the balance between AI-driven automation and human oversight. While AI excels at processing vast datasets and identifying patterns that elude human intuition, such as predicting material properties for architecturally porous materials [1], it often lacks the contextual understanding that scientists bring to decision-making [12]. For instance, in inverse design applications for polymeric membranes, AI models may propose structures that optimize specific metrics, such as permeability. Still, they might overlook practical constraints, such as manufacturability or environmental impact [7, 19]. This raises questions about accountability: when AI influences actions such as selecting synthesis routes, who bears responsibility for failures—the model developers, the users, or the algorithms themselves [11, 15]?

Another key point of contention is the role of data quality and bias in shaping AI-influenced decisions [2, 10]. Materials AI relies heavily on repositories and platforms that may contain incomplete or biased data, leading to skewed recommendations [4]. In optoelectronic material discovery, for example, ML models trained on historical datasets might perpetuate biases toward well-studied materials, thereby underexploiting novel compounds [5, 8]. Scholars argue that this could hinder diversity in materials innovation, particularly in emerging fields like sustainable energy storage [16, 18]. Mitigation strategies, such as incorporating active learning and transfer learning, have been proposed to refine decision-making by iteratively improving model accuracy [17, 22]. However, the discussion extends to ethical implications: AI decisions in critical sectors, such as healthcare, must prioritize fairness and transparency to avoid exacerbating inequalities [14, 26].

Interpretability remains a pivotal topic of discussion, as opaque "black-box" models can undermine trust in AI-guided actions [13, 23]. In generative AI for materials design, while models like VAEs enable creative exploration [9, 21], their lack of explainability can deter adoption in decision-critical environments [25, 28]. Recent advancements in XAI techniques aim to address this by providing insights into model reasoning, thereby enhancing the reliability of decisions in composite structures and nanomaterials [12, 29]. Yet, critics contend that full interpretability might come at the cost of performance, creating a trade-off that influences how AI is deployed in real-world scientific workflows [8, 20].

Furthermore, the scalability of AI in shaping action across multidisciplinary domains continues to spark debate [27]. In membrane technology and chemistry, AI has demonstrated success in small-data regimes [10, 17], but scaling to complex systems like chemical, biological, or nuclear materials requires robust integration with experimental robotics [6, 15]. This discussion highlights the need for hybrid approaches that combine AI with domain expertise, ensuring that models not only predict but also adapt to dynamic decision contexts [18, 24].

Limitations of current AI models in decision-making

Despite their promise, AI models exhibit limitations that affect their influence on scientific action [3, 11]. Data scarcity in niche materials domains often leads to overfitting, resulting in unreliable decisions [2, 7]. For example, in high-entropy alloys or biomimetic materials, models may generate implausible structures, prompting misguided experimental pursuits [4, 22]. Additionally, computational demands pose barriers, as advanced models require significant resources, influencing decisions toward simpler, less optimal alternatives [6, 16].

Generalization across materials classes is another constraint, with models trained on one domain struggling in others [5, 12]. This limits AI's potential to influence action in interdisciplinary applications, such as combining optoelectronics with

structural composites [8, 19]. Moreover, the absence of standardized benchmarks complicates comparisons, affecting how scientists decide on model adoption [13, 25].

Conclusion

In conclusion, AI models have profoundly influenced scientific decision-making in materials science by shifting from mere prediction to active guidance in discovery, design, and application. Through a thematic exploration, this review has demonstrated how tools such as ML-driven inverse design and generative models enable action, accelerating innovation across porous materials to optoelectronics. By providing uncertainty-aware recommendations and interpretable insights, AI augments human decision-making, reducing inefficiencies and fostering sustainable advancements.

However, challenges such as bias, interpretability, and scalability must be addressed to maximize AI's impact. Future directions include developing foundation models tailored to materials, integrating AI with quantum computing for faster simulations, and establishing ethical guidelines to ensure equitable decision-making. Collaborative efforts between AI experts and materials scientists will be crucial, potentially leading to autonomous labs where models independently decide which experiments to run. Ultimately, as AI evolves, it will redefine scientific research, driving a new era of intelligent materials innovation.

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