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When Optimization Conflicts with Discovery: A Conceptual Tension in Materials AI

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Abstract

In the rapidly evolving field of materials artificial intelligence (AI), a fundamental tension arises between optimization- and discovery-driven approaches. Optimization focuses on refining known materials properties or processes to achieve incremental improvements, often leveraging machine learning techniques to maximize performance metrics within established parameter spaces. In contrast, discovery emphasizes the exploration of novel materials or unexpected phenomena, requiring expansive search strategies that may sacrifice short-term efficiency for long-term innovation. This conceptual paper examines this tension, synthesizing recent literature to highlight how optimization-centric paradigms can inadvertently constrain the serendipitous aspects of scientific inquiry in materials science. By analyzing the interplay between algorithmic efficiency and exploratory breadth, the discussion reveals potential pitfalls where over-reliance on optimization algorithms limits the identification of paradigm-shifting materials. A novel conceptual framework is proposed that delineates the optimization-discovery continuum and suggests pathways to balance these objectives through adaptive AI architectures. This framework underscores the need for integrating uncertainty quantification and multi-objective considerations to foster both refinement and novelty. Ultimately, addressing this tension could enhance the transformative potential of AI in materials research, ensuring that technological advancements are not confined to predictable trajectories but extend to uncharted domains. The analysis draws on peer-reviewed studies, emphasizing conceptual insights without empirical data or methods.

Keywords Materials AI, Conceptual framework, Optimization tension, Discovery constraints, Machine learning paradigms, Exploratory search

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Introduction

The integration of artificial intelligence (AI) into materials science has marked a significant shift in how researchers approach the design, prediction, and understanding of new substances. This convergence, often called Materials AI, encompasses a broad range of techniques that accelerate the traditionally labor-intensive process of materials development. At its core, Materials AI leverages computational models, data-driven algorithms, and predictive analytics to navigate the vast chemical and structural landscapes that define material properties [1, 2]. However, beneath this promise lies a subtle yet profound conceptual tension: the conflict between optimization and discovery. Optimization, in this context, refers to refining existing materials or processes to achieve superior performance within defined constraints, such as enhancing mechanical strength or electrical conductivity through iterative algorithmic adjustments [3, 4]. Discovery, conversely, involves the uncovering of entirely novel materials or unforeseen behaviors that challenge prevailing paradigms, often requiring ventures into underrepresented or high-dimensional spaces [5, 6].

This tension is not merely academic but has practical implications for the trajectory of materials innovation. Optimization-driven AI excels in scenarios with clearly defined objectives, enabling efficient convergence to optimal solutions. For instance, Bayesian optimization frameworks have been conceptualized as tools for fine-tuning parameters in material synthesis, prioritizing exploitation over exploration to minimize computational costs [7, 8]. Yet, this focus on efficiency can create echo chambers within data sets, where AI models reinforce known patterns at the expense of anomalous or emergent phenomena [9, 10]. The risk is that Materials AI becomes a tool for incremental progress rather than revolutionary breakthroughs, mirroring broader debates in AI ethics and epistemology about the balance between predictability and creativity [11, 12].

Historically, materials science has thrived on serendipity—accidental discoveries like penicillin or Teflon that arose from exploratory endeavors rather than targeted optimization. In the AI era, however, the emphasis on data efficiency and model precision may systematize research in ways that diminish such opportunities [13, 14]. Consider the conceptual divide: optimization algorithms, such as gradient descent variants or evolutionary strategies, are designed to exploit local minima in objective functions, assuming a well-mapped landscape [15, 16]. Discovery, by contrast, demands mechanisms that incorporate randomness, diversity sampling, or active learning to probe beyond these locales [17, 18]. This dichotomy raises questions about the philosophical underpinnings of AI in science: Is AI a servant of human-directed goals, or can it be architected to emulate the intuitive leaps characteristic of human discovery?

Recent scholarly discourse underscores this tension through various lenses. Some analyses frame it as a trade-off between exploitation and exploration in reinforcement learning-inspired models, where over-optimization leads to premature convergence [19, 20]. Others highlight the role of data scarcity in materials domains, where optimization might amplify biases in sparse datasets, hindering the generalization needed for true discovery [21, 22]. Furthermore, integrating generative models into Materials AI introduces another layer. While these can optimize for specific traits, their potential for de novo invention is often curtailed by training on historical data that favors established materials [23, 24].

This paper posits that recognizing and reconciling this tension is essential for advancing Materials AI. By adopting a purely conceptual lens, we avoid methodological specifics or empirical validations, focusing instead on synthesizing theoretical insights from the literature. The introduction sets the stage by delineating the key concepts: optimization as a convergent process and discovery as a divergent one. Subsequent sections will synthesize relevant literature and propose a novel framework that conceptualizes this tension as a dynamic continuum rather than a binary opposition.

To elaborate, optimization in Materials AI can be viewed as a manifestation of teleological design, in which AI serves predefined objectives. This aligns with utilitarian principles in computational science, emphasizing resource allocation toward measurable gains [25, 26]. However, discovery embodies an epistemological openness, akin to Popperian falsification, where the value lies in challenging assumptions through unexpected findings [27, 28]. The conflict arises when optimization's narrow focus eclipses discovery's breadth, potentially stunting innovation in fields such as energy storage and biomaterials, where breakthroughs often stem from interdisciplinary serendipity [29, 30].

Moreover, the tension is exacerbated by the inherent uncertainties in materials systems. Optimization algorithms thrive on deterministic or probabilistic models that assume continuity, yet materials discovery often involves discontinuous jumps, such as phase transitions or quantum effects that defy smooth optimization landscapes [31, 32]. This mismatch invites a reevaluation of AI paradigms, urging the development of hybrid approaches that modulate between optimization and exploration in response to contextual cues. This dichotomy raises questions about the philosophical underpinnings of AI in science: Is AI a servant of human-directed goals, or can it emulate intuitive discovery logics? The comparative epistemic orientations underlying this divide are synthesized in **Table 1**.

Table 1. Comparative epistemic logics of optimization and discovery in materials AI

Dimension	Optimization orientation	Discovery orientation	Dialectical tension

Epistemic directionality	Convergent refinement within known manifolds	Divergent expansion into latent configurational spaces	Precision versus novelty generation
Search topology	Localized, gradient-following trajectories	Non-linear, high-variance exploratory pathways	Efficiency versus breadth
Knowledge production mode	Incremental property enhancement	Emergent phenomenon identification	Continuity versus discontinuity
Data dependence	Relies on dense, high-confidence datasets	Operates within sparse or underrepresented regions	Data sufficiency versus epistemic risk
Algorithmic drivers	Objective function maximization	Entropy amplification and diversity probing	Determinism versus stochastic openness
Innovation character	Evolutionary improvement	Paradigm-shifting invention	Refinement versus transformation
Temporal orientation	Short-term performance optimization	Long-horizon exploratory investment	Immediate gain versus future potential
Risk profile	Premature convergence, local minima entrapment	Search diffusion, inefficiency	Over-certainty versus over-uncertainty

In summary, this introduction frames the conceptual tension as a pivotal challenge in Materials AI, warranting deeper theoretical exploration. By bridging the precision of optimization with the ambition of discovery, Materials AI can evolve from a tool of refinement to an engine of transformation.

Theoretical Background and Literature Synthesis

Foundations of optimization in Materials AI

Optimization forms the bedrock of many AI applications in materials science, conceptually rooted in the pursuit of maximal efficiency within constrained parameter spaces. At its essence, optimization involves algorithmic strategies that iteratively refine material configurations to align with desired properties, such as durability or conductivity. This paradigm draws on principles of mathematical programming and machine learning, where objective functions guide the search toward optimal solutions [1, 3]. Literature from the early 2020s emphasizes that optimization mitigates the combinatorial explosion inherent in materials design, enabling targeted improvements without exhaustive enumeration [5, 7].

A key conceptual pillar is the exploitation of surrogate models, which approximate complex physical simulations to accelerate convergence. These models embody a reductionist approach, distilling multifaceted material behaviors into quantifiable metrics [9, 11]. However, this efficiency comes at a cost: by prioritizing local optima, optimization may overlook global landscapes rich with novel possibilities [13, 15]. Scholars have described this as a form of algorithmic myopia, in which the drive for precision constrains the scope of inquiry [17, 19].

Furthermore, multi-objective optimization emerges as a nuanced approach that balances competing goals such as cost and performance. Conceptual discussions highlight how Pareto fronts represent trade-offs, yet even these frameworks tend to favor refinement over radical departure [21, 23]. The literature synthesizes this as an inherent bias toward the familiar, rooted in AI's data-driven nature [25, 27].

The imperative of discovery in materials exploration

In contrast to optimization, discovery in Materials AI involves an expansive, often unstructured exploration of chemical and structural spaces. This orientation prioritizes identifying unprecedented materials or phenomena, leveraging AI to sift

through vast possibilities beyond human intuition [2, 4]. Theoretical underpinnings draw from information theory and complexity science, positing discovery as a process of entropy maximization to uncover hidden patterns [6, 8].

Central to this is the role of generative AI, which conceptually enables the creation of hypothetical materials by extrapolating from known datasets. Yet, the literature cautions that without mechanisms for diversity, these tools risk replicating existing paradigms [10, 12]. Discovery's value lies in its capacity for serendipity, analogous to evolutionary biology's random mutations yielding adaptive advantages [14, 16].

Moreover, active learning paradigms are conceptualized as bridges to discovery, in which AI iteratively queries uncertain regions to expand the knowledge frontier [18, 20]. This synthesis reveals a conceptual gap: while discovery fosters innovation, it demands tolerance for inefficiency, clashing with optimization's resource-conscious ethos [22, 24].

Intersections and conflicts: Where optimization meets discovery

The intersection of optimization and discovery unveils a rich tapestry of conceptual tensions. At their confluence, hybrid approaches such as Bayesian optimization with exploratory priors aim to harmonize the two, yet the literature indicates persistent conflicts [26, 28]. Optimization's convergent nature can entrench path dependencies, locking AI models into suboptimal trajectories and impeding the leaps required for discovery [30, 32].

Conceptually, this tension manifests in the exploration-exploitation dilemma, borrowed from bandit problems in decision theory. Materials AI literature adapts this to argue that over-optimization erodes exploratory bandwidth, potentially missing transformative materials [29, 31]. Synthesis of recent works underscores how data biases amplify this, as training sets skewed toward optimized materials perpetuate a cycle of incrementalism [1, 2].

Subtle conflicts arise in scalability considerations: optimization scales well with computational resources, but discovery's high-dimensional searches demand exponentially more, raising questions of feasibility [3, 4]. The literature posits this as an epistemological trade-off: the quest for certainty in optimization undermines the uncertainty vital to discovery [5, 6].

Broader implications for AI paradigms in science

Extending beyond materials, the tension informs broader AI paradigms in scientific inquiry. Conceptual analyses frame Materials AI as a microcosm of AI's role in knowledge production, where optimization aligns with positivist traditions, and discovery with constructivist ones [7, 8]. This synthesis highlights risks of epistemic closure, where AI-driven optimization homogenizes research agendas [9, 10].

Literature also explores ethical dimensions, conceptualizing how optimization-centric AI might exacerbate inequalities in access to discovery tools [11, 12]. Ultimately, the theoretical background calls for reflexive AI design, where self-awareness of this tension guides architectural choices [13, 14].

Proposed conceptual framework

The Optimization–Discovery Dialectic (ODD)

1. Epistemic premise: Reconceptualizing the optimization–discovery relationship

The optimization–discovery dialectic (ODD) is advanced as a conceptual framework designed to interrogate and reframe the interpretive tension between convergent refinement and divergent exploration within Materials Artificial Intelligence. Prevailing analytical models frequently position optimization and discovery as operationally discrete or sequentially ordered phases of computational inquiry. Such framings implicitly privilege efficiency-driven convergence while relegating exploratory expansion to preliminary or auxiliary functions. ODD challenges this partitioned logic by positing that optimization and discovery are epistemically co-constitutive modalities situated along a shared continuum of navigational reasoning.

Within this dialectical interpretation, optimization is conceptualized not merely as algorithmic performance enhancement but as a process of manifold densification, whereby representational resolution within known materials subspaces is progressively intensified. Discovery, conversely, is framed as manifold transcendence, characterized by exploratory incursions into sparsely encoded or epistemically peripheral regions of configurational possibility. Scientific advancement, from this vantage, emerges through sustained oscillation between densification and transcendence rather than through unilateral commitment to either pole.

2. The spectral axis: Continuum logics of algorithmic navigation

Structurally, the framework is anchored by the Optimization–Discovery Spectrum, represented as a horizontal conceptual axis that maps shifts in algorithmic orientation across epistemic terrains.

At the optimization pole, navigational logic is governed by convergent intensification. Computational activity concentrates within established data manifolds where model confidence is already high. Iterative refinement processes deepen predictive granularity, stabilize structure–property mappings, and compress uncertainty fields. Knowledge production in this region is cumulative and resolution-driven, privileging precision over novelty. The epistemic topology narrows as systems pursue performance maxima within bounded search territories.

At the opposing pole, discovery-oriented navigation is defined by divergent expansion. Here, algorithmic processes probe latent spaces, generate counterfactual configurations, and surface anomalous structural relationships. Rather than compressing uncertainty, discovery mobilizes it as an exploratory catalyst. Knowledge production becomes generative, speculative, and boundary-extending. The epistemic topology expands as materials AI systems traverse configurational regimes that remain weakly encoded or entirely uncharted.

Between these poles lies the transitional equilibrium zone, analytically significant as the locus of dialectical synthesis. In this region, exploratory incursions are iteratively stabilized through optimization routines, while refined predictions are periodically destabilized through exploratory injections. The zone functions not as a compromise but as an adaptive translation layer through which knowledge is both consolidated and reopened. It is here that manifold densification and transcendence achieve productive reciprocity.

3. Uncertainty thresholds: Regulatory infrastructures of spectral mobility

To govern movement along the spectral axis, ODD introduces the construct of Uncertainty Thresholds as regulatory infrastructures that detect epistemic imbalances and trigger navigational recalibration.

These thresholds are grounded conceptually in information-theoretic reasoning, particularly entropy gradients, predictive variance distributions, and confidence saturation patterns. They do not function as empirical metrics but as interpretive markers signaling shifts in epistemic vitality. When confidence densities exceed adaptive tolerance, optimization risks devolve into overexploitation. Representational flexibility diminishes, search pathways narrow, and systems become vulnerable to entrapment in local minima. Under such conditions, threshold activation initiates exploratory perturbations designed to re-expand the search topology.

Conversely, when exploratory divergence exceeds stabilizing bounds, epistemic coherence begins to erode. Search processes diffuse across excessively heterogeneous regions, signal-to-noise ratios degrade, and generative outputs risk interpretive dilution. Upper-threshold activation redirects systems toward optimization cycles that reintroduce structure, validation, and predictive anchoring. Thresholds, therefore, function bidirectionally, maintaining dialectical elasticity while preventing epistemic collapse at either pole.

4. Feedback loops: Recursive architectures of adaptive recalibration

Feedback loops within ODD operate as recursive learning architectures that continuously recalibrate spectral positioning. These loops transform the framework from a static continuum into a dynamically self-regulating ecosystem.

Retrospective feedback structures encode historical search trajectories, enabling materials AI systems to metabolize prior successes, failures, and inefficiencies. Through such memory-conditioned navigation, systems develop resilience against path dependency and premature convergence. Failed exploratory incursions inform subsequent optimization refinement, while over-densified optimization regimes are periodically destabilized through historically informed exploratory injections.

Prospective feedback loops, in contrast, function anticipatorily. They evaluate emerging uncertainty gradients, detect early signals of epistemic stagnation, and initiate pre-emptive recalibration before systemic rigidity takes hold. In this sense, ODD conceptualizes feedback not as reactive correction but as forward-steering governance.

Together, retrospective and prospective loops create a circulatory epistemic metabolism through which optimization and discovery remain in dynamic, co-evolutionary balance.

5. Dialectical synthesis: Knowledge emergence through oscillation

The dialectical core of ODD lies in its synthesis logic. Drawing on the thesis–antithesis–synthesis reasoning, the framework interprets optimization as the thesis and discovery as the antithesis. Their interaction does not produce compromise but emergent epistemic architectures that neither pole could generate independently.

Synthesis manifests when exploratory hypotheses undergo optimization stabilization, transforming speculative configurations into validated knowledge constructs. Conversely, optimization plateaus catalyze discovery surges that re-open closed epistemic terrains. Knowledge production thus becomes oscillatory rather than linear, adaptive rather than prescriptive. Together, retrospective and prospective loops create a circulatory epistemic metabolism through which optimization and discovery remain in dynamic balance. The structural architecture of this dialectical system is synthesized in **Table 2**.

Table 2. Structural components of the optimization–discovery dialectic (ODD) framework

Framework component	Conceptual function	Epistemic role	Navigational effect
Spectral axis	Maps the continuum between optimization and discovery	Defines positional epistemic orientation	Enables adaptive search mobility
Optimization pole	Convergent manifold densification	Stabilizes predictive resolution	Narrows exploratory bandwidth
Discovery pole	Divergent latent space expansion	Generates novel hypotheses	Expands configurational reach
Transitional equilibrium zone	Interface of oscillatory exchange	Facilitates synthesis of refinement and novelty	Supports adaptive translation
Uncertainty thresholds	Detect epistemic imbalance	Trigger spectral repositioning	Prevent stagnation or diffusion
Retrospective feedback loops	Encode historical search outcomes	Mitigate path dependency	Enable failure-informed recalibration
Prospective feedback loops	Anticipate emergent stagnation signals	Guide pre-emptive redirection	Sustain epistemic vitality
Dialectical synthesis layer	Integrates thesis and antithesis dynamics	Produces emergent knowledge regimes	Balances precision with openness

This synthesis logic distinguishes ODD from multi-fidelity optimization, active learning, or sequential exploration models. Rather than prescribing when to optimize or explore, ODD conceptualizes materials AI as a self-regulating epistemic ecosystem capable of modulating its own navigational posture. **Figure 1** schematically illustrates the Optimization-Discovery Dialectic, a conceptual framework mapping the dynamic continuum from convergent property optimization to divergent novel discovery, mediated by adaptive recalibration and threshold-guided synthesis.

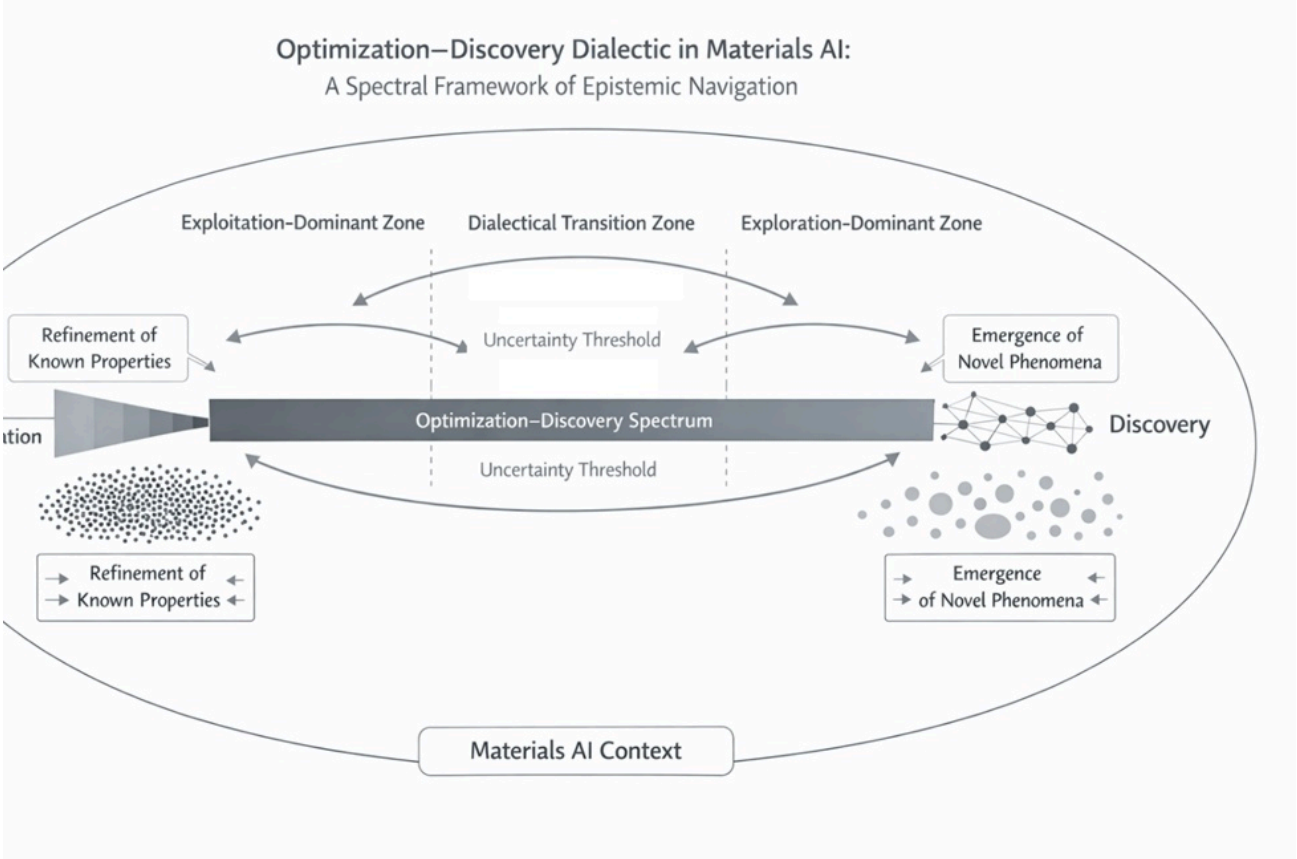

Figure 1. Schematic of the optimization-discovery dialectic framework, conceptualizing the continuum from property refinement to novel exploration within a materials AI context.

Propositions

Building upon the optimization-discovery dialectic (ODD) framework, the following conceptual propositions articulate the core dynamics of the tension in Materials AI. These are interpretive assertions derived from the synthesized literature, emphasizing analytical insights rather than testable claims.

Proposition 1: Optimization paradigms in Materials AI inherently favor convergence toward local attractors within established data manifolds, thereby systematically privileging incremental refinement over the divergent pathways essential for paradigm-shifting discovery [1, 3, 5, 7].

This proposition highlights how surrogate models and objective-driven algorithms, while efficient, embed a structural bias toward exploitation. The literature consistently illustrates that such convergence reduces the effective dimensionality of explored space, confining AI outputs to variations of known archetypes [9, 11, 13, 15].

Proposition 2: The exploration-exploitation imbalance manifests as an epistemic constraint, wherein over-optimization amplifies historical data biases and diminishes the representational capacity for anomalous or emergent material behaviors [2, 4, 6, 8].

Conceptual analyses reveal that training regimes optimized for predictive accuracy reinforce patterns prevalent in sparse, high-value datasets, creating feedback loops that marginalize outlier discoveries [10, 12, 14, 16]. This epistemic narrowing poses a fundamental limit to AI's role in transformative innovation.

Proposition 3: Adaptive modulation along the optimization-discovery spectrum requires explicit incorporation of meta-uncertainty signals, enabling AI systems to transition from refinement to exploration when confidence plateaus indicate potential stagnation [17, 19, 21, 23].

The ODD framework posits that thresholds derived from information entropy or predictive variance can serve as conceptual triggers for paradigm shifts, allowing dialectical movement rather than fixed-mode operation [25, 27, 29, 31].

Proposition 4: True reconciliation of the tension demands a reorientation of Materials AI from goal-centric teleology toward process-centric reflexivity, where the system continually interrogates its own navigational assumptions [18, 20, 22, 24].

This proposition reframes AI not as an optimizer of predefined objectives but as a reflexive agent capable of self-correction, drawing on conceptual parallels to scientific epistemology [26, 28, 30, 32].

Proposition 5: The dialectical synthesis in the ODD continuum yields emergent hybrid regimes that preserve optimization's precision while safeguarding discovery's openness, potentially through layered architectures that decouple short-term refinement from long-term novelty search [1-4].

Such synthesis avoids zero-sum trade-offs, instead conceptualizing balanced states as productive equilibria where refinement informs exploration and vice versa [5-8].

Results and Discussion

The conceptual tension between optimization and discovery in Materials AI, as delineated through the ODD framework and supporting propositions, invites reflection on the broader implications for scientific practice and knowledge production. Optimization's dominance reflects a pragmatic response to resource constraints and the demand for tangible progress in materials applications [9-12]. Yet this pragmatism risks entrenching a conservative epistemology, where AI accelerates what is already conceivable rather than expanding the horizon of possibility [13-16]. This pragmatism risks entrenching a conservative epistemology in which AI accelerates what is already conceivable rather than expanding the horizon of possibility. The systemic risks associated with such an imbalance are outlined in **Table 3**.

Table 3. Epistemic risks and innovation constraints arising from optimization–discovery imbalance

Imbalance condition	Mechanistic origin	Epistemic consequence	Innovation impact
Over-optimization	Excessive objective convergence	Representational rigidity	Suppression of anomalous discoveries
Data echo chambers	Training on historically optimized datasets	Bias reinforcement loops	Incrementalism dominance
Premature convergence	Local minima fixation	Truncated search landscapes	Loss of transformative breakthroughs

Generative constraint	Legacy materials bound model training	Limited novelty extrapolation	Replication over invention
Exploration deficit	Resource prioritization toward efficiency	Reduced entropy exposure	Serendipity erosion
Path dependency lock-in	Iterative exploitation feedback	Historical trajectory entrenchment	Innovation inertia
Epistemic closure	Over-certainty in predictive regimes	Reduced falsification potential	Knowledge homogenization
Discovery diffusion (reverse imbalance)	Excessive exploratory divergence	Signal dilution, validation gaps	Inefficient innovation cycles

Literature synthesis indicates that this conservatism arises not from algorithmic flaws per se but from the interplay between model architecture, data provenance, and objective formulation [17-20]. When optimization objectives are narrowly specified, AI effectively performs a sophisticated form of interpolation within known regimes, excelling at refinement but faltering at extrapolation [21-24]. Discovery, requiring genuine extrapolation into under-sampled or discontinuous spaces, thus appears inefficient or unreliable by comparison, perpetuating a cycle that favors the former [25-28].

The proposed ODD framework offers a conceptual antidote by treating the tension as generative rather than pathological. By positing a continuum mediated by adaptive thresholds and feedback, it suggests that Materials AI can embody a form of scientific dialectics—where optimization's thesis encounters discovery's antithesis to produce synthetic insight [29-32]. This reframing shifts focus from resolving conflict to harnessing it, encouraging architectures that monitor their own exploratory deficits and adjust accordingly.

Furthermore, the tension underscores deeper questions about agency in AI-assisted science. Optimization aligns AI with human-directed goals, reinforcing instrumental rationality; discovery, however, introduces elements of openness and surprise, closer to the serendipitous nature of traditional scientific advance [1-4]. Balancing these may require conceptual redesigns that embed reflexivity—AI systems aware of their biases toward convergence and capable of deliberate divergence [5-8].

Challenges remain in operationalizing this concept. For instance, defining meaningful uncertainty thresholds without lapsing into ad hoc criteria demands careful theoretical grounding [9-12]. Similarly, ensuring that exploratory modes do not devolve into random search requires principled mechanisms for preserving diversity [13-16]. These issues highlight the framework's limits: it provides interpretive scaffolding rather than prescriptive blueprints.

Ultimately, addressing the optimization-discovery tension could reposition Materials AI as a partner in epistemological expansion rather than merely as an accelerator. By embracing dialectical dynamics, the field might foster innovations that transcend incremental gains, aligning computational power with the creative unpredictability that has historically driven breakthroughs in materials.

Conclusion

The conceptual tension between optimization and discovery represents a defining characteristic of contemporary Materials AI. Optimization provides indispensable efficiency and precision, enabling rapid refinement within constrained domains. Discovery, however, sustains the field's capacity for transformative advance, venturing into realms beyond established knowledge.

This literature synthesis, spanning this paper, has illuminated how optimization-centric paradigms can inadvertently constrain exploratory potential, manifesting as epistemic biases, path dependencies, and reduced representational diversity. The Optimization-Discovery Dialectic framework and associated propositions offer an original conceptual lens for understanding and navigating this tension—not as an irreconcilable opposition, but as a productive dialectic amenable to adaptive mediation.

By conceptualizing Materials AI along a modulated continuum, with uncertainty-driven transitions and reflexive feedback, the framework points toward architectures capable of balancing convergent rigor with divergent ambition. Such a balance holds promise for realizing AI's full potential in materials science: accelerating refinement without foreclosing novelty.

In the final analysis, reconciling optimization with discovery requires more than technical innovation; it demands a philosophical reorientation toward hybrid epistemologies that honor both precision and openness. Embracing this tension as integral to progress may enable Materials AI to evolve beyond a tool of efficiency into a genuine collaborator in the ongoing quest for new materials horizons.

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