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Objective Functions Shape Materials Futures: A Conceptual Study of Optimization Targets in AI-Driven Design

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Abstract

In AI-driven materials design, the formulation of objective functions fundamentally shapes innovation trajectories by defining priorities across vast design spaces. This conceptual manuscript examines how optimization targets steer the discovery and refinement of materials, shaping emergent properties, scalability pathways, and integration into technological and societal systems. By synthesizing advancements in surrogate modeling, Bayesian optimization, generative architectures, and multi-objective strategies from recent literature, the analysis shows that single-objective formulations often constrain exploration to narrow performance peaks. In contrast, multi-objective configurations introduce intricate interaction dynamics, trade-offs, and feedback structures that diversify possible material outcomes. The proposed objective function nexus (OFN) framework conceptualizes objective functions as an interconnected system in which primary metrics, auxiliary constraints, weighting schemes, and iterative evaluations create steering logics that channel computational effort toward distinct horizons—ranging from high-performance specialized materials to scalable, sustainable alternatives. Analytical implications underscore nonlinear effects arising from objective interactions, such as the amplification of certain property clusters at the expense of others. At the same time, systems-level insights reveal how these choices encode epistemic priorities and value-laden selections. Trade-offs between competing goals, including performance versus manufacturability or cost versus environmental impact, manifest as dynamic tensions that reshape accessible design spaces over iterative cycles. By interpreting these dynamics interpretively, the framework illuminates how objective function design not only navigates but actively sculpts the futures of materials science, inviting reflective consideration of the priorities embedded in optimization practices.

Keywords Materials discovery, AI-driven materials design, Multi-objective optimization, Conceptual frameworks, Objective functions, Optimization trade-offs

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Introduction

The advent of artificial intelligence (AI) has profoundly transformed materials science, enabling systematic navigation of vast chemical, structural, and processing spaces that traditional experimental and computational approaches could scarcely address [1]. Data-driven models now support property prediction, inverse design, and accelerated discovery across diverse materials classes, ranging from structural alloys to energy storage systems. At the core of these AI-enabled methodologies lie objective functions—mathematical expressions that quantify the desirability of candidate materials relative to predefined targets such as mechanical strength, electronic conductivity, thermal stability, cost efficiency, or lifecycle environmental impact. These functions serve not merely as evaluative tools but as directive

mechanisms that delineate the boundaries and contours of explorable design spaces, thereby exerting a decisive influence on which material configurations are pursued and ultimately realized.

Recent developments—including surrogate-assisted optimization, Bayesian learning frameworks, and deep generative models—underscore the centrality of objective functions in guiding AI-driven discovery processes [2]. In these approaches, objective functions operationalize abstract design goals into computable criteria that govern exploration–exploitation balance, candidate ranking, and iterative refinement. Yet, despite their operational prominence, the conceptual ramifications of objective function specification remain underexplored. Objective functions implicitly encode assumptions about what constitutes “success” in materials research, prioritizing certain attributes while de-emphasizing others. These prioritizations shape not only immediate optimization outcomes but also longer-term innovation trajectories, influencing scalability, manufacturability, and alignment with broader societal goals such as sustainability and resource efficiency.

The consequences of these choices become evident when contrasting different optimization strategies. An objective focused narrowly on maximizing a single property metric may converge toward exotic compositions or finely tuned microstructures that exhibit peak performance under controlled laboratory conditions, yet prove ill-suited for industrial deployment due to synthesis complexity, cost barriers, or supply-chain constraints. In contrast, objective formulations that incorporate multiple, often conflicting, criteria—such as performance, durability, manufacturability, and environmental impact—introduce structured trade-offs that more closely mirror real-world constraints. Such multi-objective landscapes expose interaction dynamics in which improvements along one axis induce compromises along others, revealing Pareto fronts rather than singular optima. Iterative engagement with these trade-offs can yield materials with balanced performance profiles while simultaneously reshaping the optimization horizon.

Beyond operational considerations, objective functions carry an important epistemic dimension. They are constructed from available datasets, measurement practices, and domain knowledge, and therefore inherit the limitations, biases, and blind spots of those inputs. What is measured becomes what is optimized; what is optimized becomes what is systematically explored and valued. As a result, entire classes of materials or performance attributes may remain marginalized simply because they fall outside the quantified scope of the objective. This selective visibility constrains not only optimization outcomes but also the kinds of scientific knowledge that are produced through AI-mediated workflows.

Ethical considerations emerge from this same mechanism. Objective functions that implicitly privilege economic efficiency or peak performance may marginalize sustainability, environmental impact, or long-term resilience, embedding narrow value systems into ostensibly neutral algorithms. Such encoding raises questions about the societal values being operationalized within AI-driven materials design pipelines. It highlights that objective function design is not a neutral technical step but a value-laden process with systems-level consequences for the future materials landscape.

Although literature documents the rapid adoption of AI techniques in materials science, the dominant focus remains on methodological performance and empirical demonstrations rather than on the steering role of optimization objectives themselves [3, 4]. Conceptual gaps persist in understanding how alternative objective configurations generate divergent futures—such as high-performance niche materials versus broadly deployable, resilient solutions—or how feedback from discovered candidates informs objective refinement in closed optimization loops. These gaps limit the field’s ability to reason critically about the long-term implications of AI-guided materials discovery.

This manuscript addresses these gaps through a purely theoretical and conceptual analysis of objective functions in materials AI. Rather than proposing new algorithms or predictive benchmarks, it develops an original interpretive framework for understanding how optimization targets shape discovery trajectories, trade-off structures, and epistemic boundaries. The analysis proceeds by synthesizing relevant theoretical background and literature threads before articulating the proposed framework. Throughout, emphasis remains on analytical implications, interaction dynamics, and systems-level insights rather than predictive claims. By foregrounding objective functions as active shapers of scientific

futures, this work contributes a reflective perspective on how AI-driven materials science is guided—not only by data and models—but by the values embedded in what it chooses to optimize.

Theoretical Background and Literature Synthesis

Evolution of AI techniques in materials design

Artificial intelligence applications in materials science have undergone a rapid and consequential evolution, progressing from early supervised learning approaches focused on property prediction toward increasingly autonomous discovery pipelines enabled by surrogate models and generative architectures [1, 5]. Initial successes centered on learning structure–property relationships from curated datasets, demonstrating that machine learning could outperform traditional heuristics in predicting mechanical, electronic, or thermodynamic properties. More recent developments, however, have shifted emphasis from prediction alone to decision-making under uncertainty, where models actively guide exploration of vast compositional and structural spaces.

The scaling of deep learning architectures for crystal structure prediction exemplifies this transition. Large neural networks trained on extensive computational datasets have enabled accelerated identification of stable crystal configurations across diverse elemental compositions, substantially reducing reliance on exhaustive enumeration or manual intuition [1]. In parallel, Bayesian optimization has gained prominence as a principled framework for navigating expensive evaluation landscapes, particularly where first-principles calculations or experiments impose high costs [2, 6]. By coupling probabilistic surrogate models with acquisition functions that balance exploration and exploitation, Bayesian approaches enable data-efficient discovery while explicitly accounting for uncertainty.

Despite their methodological sophistication, these approaches rest on foundational assumptions regarding the smoothness, continuity, and learnability of material property landscapes. Crucially, it is the objective function that renders these assumptions operational by defining which aspects of the landscape are visible and actionable to the algorithm. Literature increasingly acknowledges that hybrid methodologies—integrating high-throughput computation, machine learning, and iterative feedback—derive much of their practical effectiveness from carefully chosen optimization targets [3]. Yet this same literature implicitly reveals that the choice of objective function exerts a directive influence, determining which regions of design space are traversed, revisited, or systematically ignored.

Role of objective functions in surrogate models and optimization

Objective functions serve as the formal interface between scientific intent and algorithmic action, translating desired material attributes into scalar or vector-valued quantities that guide search processes. Within surrogate-assisted optimization frameworks, objective functions influence both model training and acquisition strategies, shaping how uncertainty, performance estimates, and sampling priorities are balanced [2, 7]. In Bayesian optimization, for instance, commonly used objectives such as expected improvement or upper confidence bound variants encode explicit trade-offs between maximizing predicted performance and reducing epistemic uncertainty.

This formulation introduces a steering logic in which objective functions do more than rank candidate materials: they actively probe regions of the design space aligned with prioritized metrics, generating feedback that updates surrogate models and narrows subsequent exploration [6]. Over successive iterations, this feedback loop can induce path dependence, as early objective-driven decisions constrain later opportunities. From an interpretive standpoint, the optimizer’s behavior reflects not only model accuracy but also the normative assumptions embedded in the optimization.

Single-objective formulations remain prevalent due to their computational simplicity and conceptual clarity. However, by collapsing complex material desirability into a single scalar quantity, they risk convergence to local optima within rugged or multimodal landscapes. More fundamentally, they impose a unidimensional value structure that privileges certain property regimes over others. Recent syntheses highlight how techniques such as normalization, scaling, or dynamic

objective adjustment can partially mitigate these effects, yet also introduce sensitivity to hyperparameter choices and implicit weighting decisions [4]. These sensitivities underscore that objective engineering itself becomes a critical—and often under-theorized—design choice.

Multi-objective optimization and pareto frontiers in materials contexts

Multi-objective optimization frameworks address inherent conflicts among material properties by seeking Pareto-optimal sets, in which improvement in one objective necessitates a compromise in another [8, 9]. In materials science, such conflicts are ubiquitous: strength versus ductility, conductivity versus stability, performance versus cost, or functional efficiency versus environmental impact. Pareto frontiers provide a structured representation of these trade-offs, revealing not a single “best” material but a spectrum of non-dominated alternatives.

The geometry of Pareto fronts embodies rich interaction dynamics. Weighting schemes, constraint formulations, and dominance criteria directly influence frontier morphology, expanding or contracting accessible trade-off surfaces and steering optimization toward particular clusters of compromise solutions [8]. The literature demonstrates that multi-objective Bayesian optimization extends single-objective methods by maintaining diverse Pareto archives, thereby preserving exploration across non-dominated regions rather than prematurely collapsing decision-making [9, 10].

From a systems-level perspective, these processes yield insights beyond candidate selection. Iterative evaluation of Pareto fronts reveals nonlinear couplings between objectives, in which small perturbations in one metric can induce disproportionate shifts in the frontier’s shape or density. Feedback structures emerge naturally as frontier evolution informs adaptive reweighting, constraint tightening, or objective reformulation in subsequent cycles. Thus, multi-objective optimization functions not only as a technical tool but as an epistemic lens through which competing material values are surfaced and negotiated.

Generative models for inverse design and their objective dependencies

Generative modeling approaches—including variational autoencoders, generative adversarial networks, and diffusion-based models—have further transformed materials design by inverting the traditional forward mapping from structure to properties [11, 12]. Rather than evaluating candidates sampled externally, these models propose structures directly conditioned on desired attributes, offering a powerful mechanism for inverse design. In this context, objective functions operate either as conditioning signals embedded during training or as post-generation filters that rank or refine generated candidates.

Recent perspectives caution, however, that generative models do not eliminate the challenges of inverse design; instead, they relocate them to the level of objective specification [11]. The fidelity, diversity, and novelty of generated materials depend critically on how objectives are encoded and balanced within latent spaces. Interaction dynamics arise from latent representations that encode objective-driven manifolds, where tensions among reconstruction accuracy, property alignment, and diversity shape exploration behavior.

Epistemically, generative outputs reflect both the biases of training data and the normative priorities embedded in conditioning objectives. As a result, these models may reinforce dominant material paradigms while marginalizing underrepresented compositions or unconventional solutions [12]. This raises broader questions about the extent to which generative AI expands design freedom versus amplifying existing value structures embedded in data and objectives.

Challenges in incorporating sustainability and manufacturability objectives

An increasingly prominent strand of the literature seeks to integrate sustainability-related criteria—such as lifecycle carbon footprint, toxicity, or recyclability—into AI-driven optimization pipelines [13, 14]. While conceptually compelling, such integration faces persistent challenges related to data availability, metric standardization, and uncertainty

propagation. Sustainability objectives are often indirect, noisy, or context-dependent, making their translation into computable targets difficult.

Manufacturability objectives introduce additional layers of complexity. Metrics related to processability, yield, or cost frequently manifest as hard constraints that prune design spaces preemptively rather than as smooth optimization targets. The resulting trade-offs reveal powerful steering effects: prioritizing environmental or manufacturing feasibility can shift optimization toward earth-abundant elements or simpler chemistries, often at the expense of peak performance. Feedback loops emerge as candidate evaluation informs iterative refinement of objectives, progressively aligning material discovery with real-world viability rather than theoretical optima [13].

Synthesis and conceptual implications

Across these literature threads, a consistent pattern emerges: objective functions act as nexus points within AI-driven materials design. Their formulation integrates prediction accuracy, exploration breadth, constraint satisfaction, and value alignment. Systems-level behavior differs markedly depending on whether objectives are mutually reinforcing—yielding stable optimization trajectories—or strongly conflicting, producing oscillatory or unstable search dynamics.

Collectively, the literature suggests that objective functions should not be interpreted as fixed endpoints but as dynamic elements within evolving discovery systems. Through ongoing feedback, adaptation, and reinterpretation, they shape divergent materials futures—privileging certain pathways while foreclosing others. This synthesis motivates the need for a dedicated conceptual framework that foregrounds objective functions as active, value-laden drivers of materials innovation rather than passive technical components. The following section develops such a framework to systematically interpret these steering effects. The systemic roles and consequences of the components of the objective function are summarized in **Table 1**.

Table 1. Conceptual mapping of objective function components to interaction dynamics and system-level consequences in AI-driven materials optimization.

Objective component	Role in optimization	Interaction effect	System-level outcome
Performance metrics	Define optimization direction	Dominate gradients	Specialized material paradigms
Constraints	Bound feasible space	Prune exploration	Improved deployability
Weighting schemes	Balance objectives	Shape Pareto curvature	Stability vs sensitivity
Uncertainty terms	Guide exploration	Amplify feedback	Frontier volatility or robustness
Sustainability metrics	Encode societal values	Redirect steering	Resilient material futures
Iterative feedback	Update objectives	Reinforce or correct bias	Path dependence or adaptation

Proposed conceptual framework: The Objective Function Nexus (OFN)

The objective function nexus (OFN) framework introduces a novel conceptual lens for interpreting how optimization targets in AI-driven materials design actively sculpt possible materials futures. Rather than treating objective functions as static scalar quantities or fixed evaluative criteria, the OFN conceptualizes them as relational nodes within an interconnected ecosystem. Within this ecosystem, primary performance metrics, secondary constraints, weighting schemes, uncertainty quantification terms, and evaluative feedback loops interact dynamically to steer computational trajectories over time. This nexus perspective foregrounds steering logics arising from objective interdependencies, trade-offs that manifest as structured tension surfaces, and feedback mechanisms through which adjustments propagate across the system.

At its core, the OFN interprets objective specification as a process of horizon definition. Each objective configuration delineates which regions of property–composition space are rendered accessible, attractive, or actionable, while implicitly foreclosing others through prioritization and exclusion. For instance, dominance of a mechanical performance objective can contract adjacent sustainability or manufacturability branches within the nexus, generating nonlinear propagation effects. Optimized candidates emerging from such configurations reinforce specific data distributions, which in turn recalibrate surrogate models and further entrench the original priorities. In this way, objective dominance is not merely evaluative but generative, shaping both the trajectory of exploration and the informational substrate upon which future decisions are made.

Interaction dynamics within the OFN unfold through coupling coefficients, conceptualized as influence pathways that connect objectives. Alterations in a single node—such as tightening bounds on thermal stability or increasing penalty weights for toxicity—modulate gradient flows across connected objectives. These interactions yield emergent behaviors at the population level, including clustering of candidate materials around narrow optima or dispersion across broader compromise regions. Importantly, such behaviors are not reducible to any single objective but arise from the relational structure of the nexus itself.

Trade-offs within the OFN are treated as inherent structural features rather than undesirable artifacts. Pareto-like surfaces represent zones of negotiated balance among competing objectives, with their curvature reflecting relative scaling, asymmetries in weighting, and constraint stiffness. Regions of high curvature signal systemic vulnerability, where disproportionate pull from one objective can destabilize otherwise balanced configurations. Conversely, flatter regions indicate regimes of resilience, in which modest perturbations do not significantly alter optimization trajectories. The OFN thus enables interpretation of trade-offs as indicators of system health rather than mere optimization challenges.

Feedback structures play a central role in the framework. Evaluation outcomes feed back into surrogate updates, uncertainty estimates, and objective reformulations, establishing closed iterative cycles. Depending on nexus connectivity and constraint damping, these cycles may converge toward robust compromise solutions, stabilize around dominant material paradigms, or amplify drift toward increasingly specialized niches. At the systems level, the OFN reveals emergent phenomena such as self-reinforcing attractors—corresponding to entrenched material classes—or bifurcation points, where small configuration changes precipitate divergence into alternative discovery futures.

Epistemically, the OFN emphasizes that objective functions encode what is deemed measurable, optimizable, and valuable, thereby shaping the knowable subset of material possibilities. Regions lying outside quantified objectives remain epistemically opaque, not because they lack potential, but because they are rendered invisible to the optimization process. This selective visibility has profound implications for scientific discovery, as it conditions which hypotheses can be generated, tested, and validated within AI-mediated workflows.

Ethical considerations are integrated into the framework as embedded value vectors rather than external constraints. Objectives aligned with societal priorities—such as decarbonization, resource equity, or long-term resilience—reorient the nexus toward inclusive and sustainable horizons. In contrast, performance-centric formulations may marginalize such dimensions, reinforcing path dependencies that privilege short-term optimization over systemic responsibility. While **Figure 1** depicts the internal relational structure of the Objective Function Nexus, **Figure 2** illustrates how different objective configurations propagate through this nexus to steer AI-driven materials discovery toward divergent materials futures.

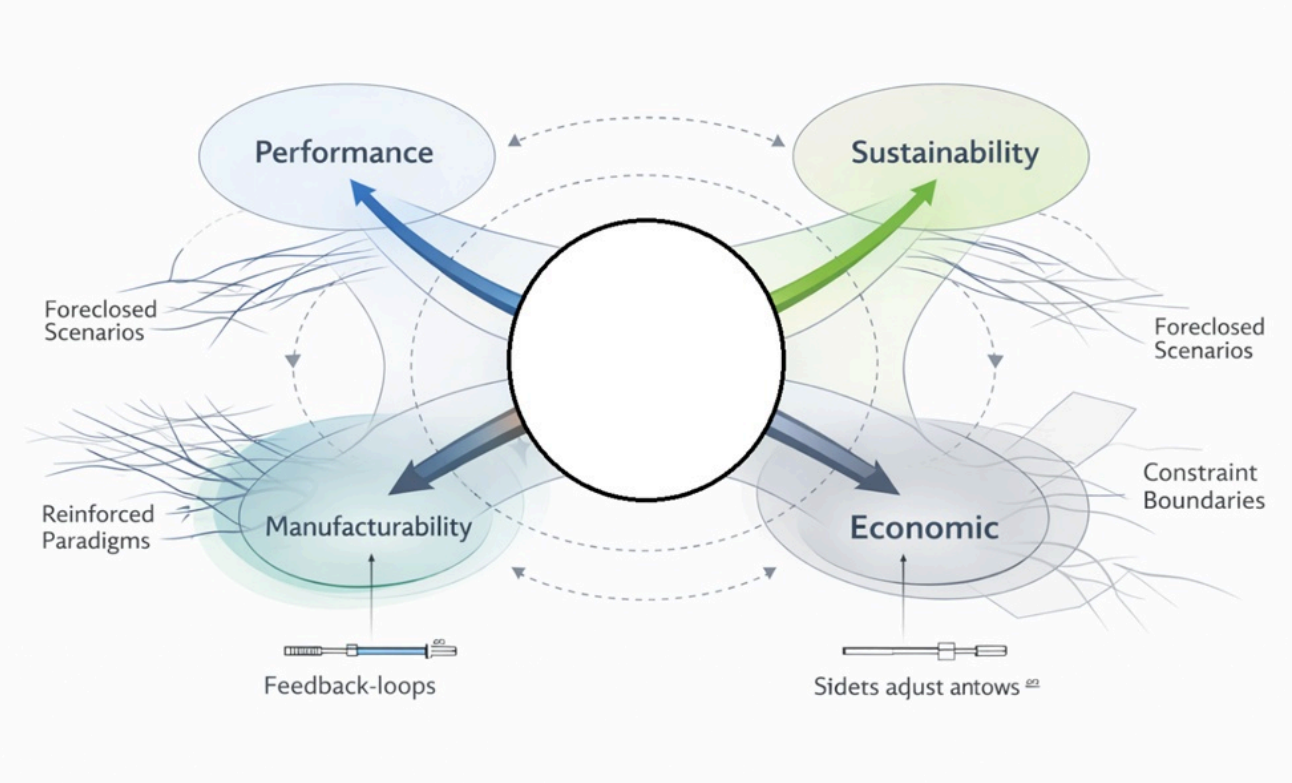

Figure 1. Objective function nexus: Radial diagram of interconnected optimization domains in materials design.

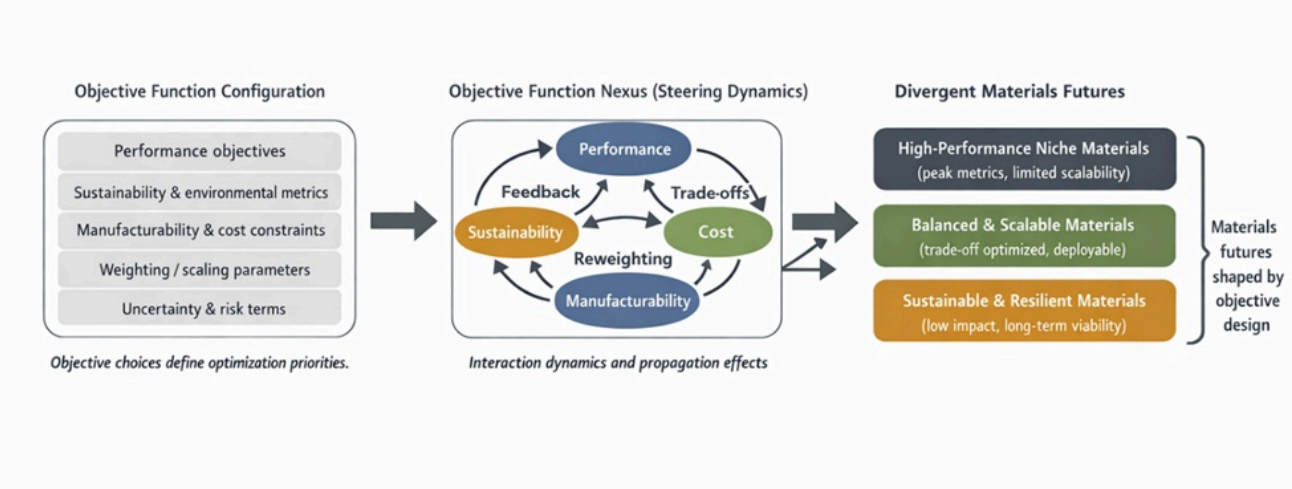

Figure 2. Objective function steering and divergent materials futures.

Analytical implications

The objective function nexus (OFN) framework illuminates the interaction dynamics in which primary performance nodes exert cascading influences across auxiliary dimensions, such as sustainability or manufacturability constraints. These interactions manifest as tension surfaces whose morphology evolves with weighting adjustments, leading to nonlinear propagation that can amplify clusters of high-performing candidates while attenuating pathways toward balanced, scalable alternatives. Systems-level insights emerge from observing how such dynamics foster self-reinforcing attractors, in which repeated evaluations consolidate data distributions that reinforce initial priorities, thereby constraining the breadth of explorable horizons across iterative cycles. Trade-offs appear not as static compromises but as structural

features that introduce damping effects or bifurcations, redirecting optimization trajectories toward specialized niches or diversified profiles depending on the relative connectivity strength among nexus elements [15, 16].

Epistemic reasoning within the OFN reveals that objective configurations define measurable subspaces, rendering certain compositional regimes opaque due to data sparsity or unquantified attributes. This opacity highlights feedback structures in which surrogate refinements preferentially populate known regimes, potentially entrenching epistemic blind spots unless deliberate constraint integrations broaden the probed manifold. Ethical considerations surface interpretively through value embeddings: objectives that embed performance primacy may orient the nexus toward resource-intensive paradigms, whereas incorporation of environmental metrics redirects steering logics toward earth-abundant compositions, albeit at the cost of reshaping accessible trade-off curvatures [17, 18].

Further interpretive layers underscore how uncertainty volumes surrounding nodes modulate exploration breadth, with high uncertainty amplifying feedback sensitivity and generating volatile frontier evolutions. Such volatility underscores systems-level vulnerabilities in which conflicting objectives induce oscillatory behavior, alternating between performance peaks and constraint-satisfying clusters. Overall, the framework positions objective functions as relational hubs that co-evolve design spaces through interdependent gradients, revealing how specification choices sculpt divergent material paradigms through ongoing adaptive tensions rather than linear convergence [19, 20].

Results and Discussion

Integrating the OFN framework with contemporary literature threads underscores the interpretive value of viewing objective functions as dynamic orchestrators within AI-driven pipelines. Surrogate and Bayesian approaches illustrate steering logics wherein acquisition strategies, informed by multi-objective fronts, propagate refinements that balance exploitation of predicted optima with uncertainty-driven diversification, yet remain tethered to the nexus's encoded priorities [21, 22]. Generative architectures extend these dynamics by conditioning latent traversals on objective-conditioned signals, producing candidate distributions whose diversity reflects underlying trade-off curvatures and interaction strengths, thereby reinforcing or challenging dominant material clusters [23, 24].

Systems-level insights from sustainability integrations highlight feedback loops wherein environmental objectives intersect with manufacturability nodes, generating pruning effects that curtail high-impact branches while fostering resilient, processable alternatives. These intersections manifest as emergent stability when objectives align reinforcingly, or as instability when conflicts dominate, prompting adaptive reweighting that gradually reshapes the optimization horizon toward viable real-world deployment [25, 26]. Epistemic and ethical dimensions integrate across threads, emphasizing that quantified value vectors inherently prioritize certain knowledges, potentially marginalizing underrepresented pathways unless iterative evaluations incorporate broader constraint sensitivities [25-28].

The framework's relational perspective complements the literature on Pareto morphologies by interpreting front evolution as nexus-mediated negotiation, in which curvature variations encode systemic trade-offs that steer futures from narrow excellence to multifaceted applicability. Interaction dynamics thus bridge methodological efficacy with broader shaping influences, revealing how objective interdependencies channel computational efforts toward horizons aligned with embedded societal or technological imperatives [29-35]. This integrative view invites continued reflective analysis of configuration sensitivities as pivotal in navigating the expansive possibilities of materials innovation ecosystems.

Conclusion

The Objective Function Nexus framework provides a conceptual lens for interpreting the directive and generative roles of optimization targets in AI-driven materials design. Through its emphasis on interconnected nodes, steering logics, interaction dynamics, and feedback structures, the OFN illuminates how objective specifications actively delineate and reshape design spaces, influencing the emergence of specialized versus balanced material paradigms. Analytical

implications and systems-level insights drawn from trade-off tensions and epistemic embeddings highlight the value-laden nature of these choices, underscoring their capacity to orient innovation trajectories toward performance-centric or sustainability-aligned futures. By fostering an interpretive understanding of nonlinear propagation and adaptive cycles, the framework provides a reflective foundation for considering the broader implications of objective function design in sculpting materials science's evolving landscape.

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References

Liang Q, Dave N, Kim J, Meredig B, Foster I. Benchmarking the performance of Bayesian optimization across multiple experimental materials science domains. npj Comput Mater. 2021;7(1):188.
https://doi.org/10.1038/s41524-021-00656-9.

Kim Y, Kim E, Antono E, Ling J, Meredig B, Wolverton C. Bayesian Optimization for Materials Design with Mixed Quantitative and Qualitative Variables. Sci Rep. 2020;10(1):6065.
https://doi.org/10.1038/s41598-020-60652-9.

Khatamsaz D, Neuberger R, Roy AM, Hossein Zadeh S, Otis R, Arróyave R. A physics informed bayesian optimization approach for material design: application to NiTi shape memory alloys. npj Comput Mater. 2023;9(1):217.

https://doi.org/10.1038/s41524-023-01173-7.

Chitturi SR, Ramdas A, Wu Y, Rohr B, Ermon S, Dionne J, et al. Targeted materials discovery using Bayesian algorithm execution. npj Comput Mater. 2024;10(1):132.
https://doi.org/10.1038/s41524-024-01326-2.

Khatamsaz D, Vela B, Singh P, Johnson DD, Allaire D, Arróyave R. Bayesian optimization with active learning of design constraints using an entropy-based approach. npj Comput Mater. 2023;9(1):46.
https://doi.org/10.1038/s41524-023-01006-7.

Menon D, Ranganathan R. A Generative Approach to Materials Discovery, Design, and Optimization. ACS Omega. 2022 Jul 24;7(30):25958-73.
https://doi.org/10.1021/acsomega.2c02494.

Chen L, Zhang W, Nie Z, Li S, Pan F. Generative models for inverse design of inorganic solid materials. J Mater Inf. 2021;1(1):4.
https://doi.org/10.20517/jmi.2021.07.

Peng B, Wei Y, Qin Y, Dai J, Li Y, Liu A, et al. Machine learning-enabled constrained multi-objective design of architected materials. npj Comput Mater. 2023;9(1):166.
https://doi.org/10.1038/s41524-023-01166-6.

Al Ani Z, Gujarathi AM, Al-Muhtaseb AH. A state of art review on applications of multi-objective evolutionary algorithms in chemicals production reactors. Artif Intell Rev. 2023;56(3):2435-96.
https://doi.org/10.1007/s10462-022-10219-z.

Takagi T, Takadama K, Sato H. Directional pareto front and its estimation to encourage multi-objective decision-making. IEEE Access. 2023;11:20619-34.
https://doi.org/10.1109/ACCESS.2023.3250238.

Zheng M, Wang Y, Teng H. A new" intersection" method for multi-objective optimization in material selection. Tehn glas. 2021;15(4):562-8.

Ma X, et al. Machine learning assisted multi-objective optimization for high-entropy alloys. J Mater Inf. 2024;4(1):108.

Hanaoka K. Bayesian optimization for goal-oriented multi-objective inverse material design. iscience. 2021 Jul 23;24(7).

Shen B, Gnanasambandam R, Wang R, Kong ZJ. Multi-task Gaussian process upper confidence bound for hyperparameter tuning and its application for simulation studies of additive manufacturing. IISE Trans. 2023;55(5):496-508.

Yue X, Kontar RA, Berahas AS, Liu Y, Johnson BN. Collaborative and distributed Bayesian optimization via consensus: Showcasing the power of collaboration for optimal design. arXiv preprint arXiv:2306.14348. 2023.

Hanaoka K. Comparison of conceptually different multi-objective Bayesian optimization methods for material design problems. Mater Today Commun. 2022;31:103440.

Li Z, Birbilis N. Multi-objective optimization-oriented generative adversarial design for multi-principal element alloys. Integr Mater Manuf Innov. 2024;13(2):435-44.

Wang S, Gao J, Yang M, Zhang G, Yin L, Tong X. OPN-Mediated Crosstalk Between Hepatocyte E4BP4 and Hepatic Stellate Cells Promotes MASH-Associated Liver Fibrosis. Adv Sci. 2024;11(47):2405678.

Wang S, Zhang J, Wang P, Law J, Calinescu R, Mihaylova L. A deep learning-enhanced Digital Twin framework for improving safety and reliability in human–robot collaborative manufacturing. Robot Comput Integr Manuf. 2024;85:102608.

Bibri SE, Huang J, Jagatheesaperumal SK, Krogstie J. The synergistic interplay of artificial intelligence and digital twin in environmentally planning sustainable smart cities: A comprehensive systematic review. Environ Sci Ecotechnol. 2024;20:100433.

Chen SC, Chen HM, Chen HK, Li CL. Multi-Objective Optimization in Industry 5.0: Human-Centric AI Integration for Sustainable and Intelligent Manufacturing. Processes. 2024;12:2723.
https://doi.org/10.3390/pr12122723..

Choi J, Kim H, Noh T, Kang YJ, Noh Y. Digital twin data-driven multi-disciplinary and multi-objective optimization framework for automatic design of negative stiffness honeycomb. Int J Precis Eng Manuf. 2023;24(8):1453-72.

Upadhyay P, Sharma T, Fatima A. Impact of AI-driven digital twins in Industry 4.0: An exploratory analysis. Int Res J Adv Eng Manag. 2024;2:1548-57.

Lind A, Elango V, Hanson L, Högberg D, Lämkull D, Mårtensson P, et al. Multi-objective optimization of an assembly layout using nature-inspired algorithms and a digital human modeling tool. IISE Trans Occup Ergon Hum Factors. 2024;12(3):175-88.

Xia C, Wang R, Jin X, Xu C, Li D, Zeng P. Deterministic network–computation–manufacturing interaction mechanism for AI-driven cyber–physical production systems. IEEE Internet Things J. 2024;11(10):18852-68.

de Souza TF, Dias Ferreira GM. Biochars as Adsorbents of Pesticides: Laboratory-Scale Performances and Real-World Contexts, Challenges, and Prospects. ACS ES&T Water. 2024;4(10):4264-82.

Lodhi SK, Gill AY, Hussain HK. Green innovations: artificial intelligence and sustainable materials in production. BULLET: Jurnal Multidisiplin Ilmu. 2024;3(4):492-507.

Foppa L, Scheffler M. Towards a Multi-Objective Optimization of Subgroups for the Discovery of Materials with Exceptional Performance. arXiv preprint arXiv:2311.10381. 2023.

Li Z, Li J, Tian J, Xia S, Li K, Li M, et al. Inverse design of cellular structures with the geometry of triply periodic minimal surfaces using generative artificial intelligence algorithms. Eng Struct. 2024;321:118988.

Cao Y, Wu G, Wang Y, Li Y, Xu H. Influence of Interfacial Tribo-Chemical and Mechanical Effect on Tribological Behaviors of TiN Film in Different Environments. Processes. 2024;12(5):923.

Jung J, Park K, Cho B, Park J, Ryu S. Optimization of injection molding process using multi-objective bayesian optimization and constrained generative inverse design networks. J Intell Manuf. 2023;34(8):3623-36.

Lee H, Yang H. Digital twinning and optimization of manufacturing process flows. J Manuf Sci Eng. 2023;145(11):111008.

Greif L, Hübschle N, Kimmig A, Kreuzwieser S, Martenne A, Ovtcharova J. Structured sampling strategies in Bayesian optimization: evaluation in mathematical and real-world scenarios. J Intell Manuf. 2025:1-31.

Gao X, Ramezanghorbani F, Isayev O, Smith JS, Roitberg AE. TorchANI: a free and open source PyTorch-based deep learning implementation of the ANI neural network potentials. J Chem Inf Model. 2020;60(7):3408-15.

Marques G, Leswing K, Robertson T, Giesen D, Halls MD, Goldberg A, et al. De Novo design of molecules with low hole reorganization energy based on a quarter-million molecule DFT screen. J Phys Chem A. 2021;125(33):7331-43.