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Toward Autonomous Materials Intelligence: A Human–AI–Physics Framework for Discovering, Optimizing, and Validating Next-Generation Materials

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Abstract

The discovery of next-generation materials remains a slow, iterative, and resource-intensive process. Conventional approaches rely on sequential cycles of hypothesis generation, synthesis, characterization, and interpretation. Although this process has produced transformative materials, its pace is increasingly misaligned with urgent technological needs in energy, sustainability, electronics, and advanced manufacturing. Recent advances in artificial intelligence, robotics, high-throughput experimentation, and computational physics have created new opportunities to accelerate materials discovery. Self-driving laboratories and closed-loop experimentation systems can now propose experiments, execute them, learn from results, and refine subsequent decisions. These developments suggest the emergence of autonomous materials intelligence as a new paradigm for scientific discovery. However, current approaches often treat artificial intelligence, physics-based simulation, and human expertise as separate instruments rather than as mutually reinforcing partners. AI models may generate predictions without sufficient physical grounding, simulations may remain disconnected from experimental feedback, and human judgment may enter only after automated decisions have already been made. This fragmentation limits the development of truly autonomous and scientifically trustworthy materials discovery systems. This conceptual framework article develops a Human–AI–Physics framework for autonomous materials intelligence. The framework positions human expertise, AI algorithms, and physics-based models as co-equal pillars in a self-driving discovery pipeline. It explains how these pillars interact across discovery, optimization, and validation cycles. The article synthesizes 26 peer-reviewed publications published between 2017 and 2024 across autonomous experimentation, materials informatics, active learning, generative models, graph neural networks, physics-informed machine learning, and self-driving laboratories. The synthesis is not presented as a review or meta-analysis. Instead, it is used to construct a systems-oriented conceptual architecture for integrating human judgment, machine learning, and physical laws. The proposed framework defines autonomous materials intelligence as an iterative workflow in which AI proposes, physics constrains, humans guide, and experiments validate. By linking these functions into a closed-loop system, the framework offers a blueprint for discovering, optimizing, and validating next-generation materials with greater speed, interpretability, and scientific rigor.

Keywords Conceptual framework, Materials discovery, Autonomous materials intelligence, Human–AI–physics framework, Optimization, Validation

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Introduction

Materials discovery has historically depended on cycles of expert intuition, trial-and-error experimentation, and computational screening, but these cycles remain slow relative to the scale of modern technological demand. Machine learning has begun to reshape this process by enabling property prediction, materials screening, and pattern recognition across large datasets, as shown in early materials informatics work by Liu and colleagues [1]. The broader promise of machine learning for molecular and materials science is that algorithms can search design spaces that are too large for purely human exploration [2]. Yet speed alone does not solve the deeper problem of how automated suggestions become scientifically meaningful materials knowledge.

The rise of self-driving laboratories has transformed this challenge from one of prediction to one of autonomous action. Closed-loop systems can now combine robotic synthesis, real-time characterization, and machine learning decision-making, as demonstrated in autonomous thin-film discovery and Bayesian active-learning workflows [3, 4]. Mobile robotic chemists further show that experimental platforms can physically navigate chemical search spaces with minimal direct intervention [5]. These systems mark a shift from computational acceleration toward embodied materials intelligence.

Despite this progress, autonomous materials discovery remains conceptually fragmented. Active-learning systems may optimize experiments efficiently, but they do not always clarify the role of human scientific judgment in defining meaningful objectives [6]. Physics-informed machine learning can embed physical structure into models, but it is often developed separately from robotic experimentation and laboratory feedback [7, 8]. As a result, current systems risk becoming powerful but partial solutions rather than integrated discovery frameworks.

This article addresses that gap by proposing a Human–AI–Physics framework for autonomous materials intelligence. The framework treats human experts as goal-setters and interpreters, AI systems as adaptive explorers of materials space, and physics-based models as constraint engines that preserve scientific plausibility. It builds on the convergence of high-performance computing, artificial intelligence, and robotics described by Pyzer-Knapp and colleagues [9]. The purpose is to articulate a conceptual architecture for self-driving materials discovery that is autonomous without being detached from human reasoning or physical law.

Literature Gap

The first major gap is the separation between AI-driven materials discovery and autonomous experimentation. Machine learning frameworks for materials design have advanced rapidly, including graph networks for molecules and crystals and deep learning architectures for ordered and disordered materials [10, 11]. At the same time, self-driving laboratories have developed as experimental platforms capable of closed-loop synthesis and characterization [12, 13]. However, the literature often treats predictive modeling and autonomous execution as adjacent capabilities rather than as components of one unified intelligence system.

The second gap concerns the incomplete integration of physics into AI-guided autonomy. Physics-informed neural networks and broader physics-informed machine learning approaches demonstrate how governing equations, conservation principles, and physical constraints can improve generalizability and interpretability [7, 8]. In materials science, universal interatomic potentials and charge-informed neural network potentials show how learned models can approximate physically meaningful atomic interactions across broad chemical spaces [14, 15]. Yet these physics-aware advances are not always embedded into self-driving laboratory workflows where experimental data continuously revise both AI and physics models.

The third gap concerns the under-specified role of the human scientist. Community perspectives on autonomous experimentation emphasize infrastructure, data standards, and coordination across laboratories, but the conceptual position of human oversight within the loop remains unevenly defined [16]. Accounts of self-driving laboratories in chemistry further identify the need for meaningful human choices in problem framing, safety, interpretation, and scientific validation [17]. **Table 1** maps the existing research silos and the integration gaps that the framework addresses.

Table 1. Current Research Silos and Integration Gaps in Autonomous Materials Discovery

Research silo	Representative contribution	Dominant strength	Inte addr fran
AI-driven materials prediction	Machine learning, graph networks, and deep learning models predict properties and screen large candidate spaces [2, 10, 18].	Rapid exploration of high-dimensional chemical and structural spaces.	Pre re stron to p con expe feasi hu de sc obj
Autonomous experimentation	Self-driving laboratories combine robotic synthesis, characterization, and adaptive decision-making [3, 5, 12].	Closed-loop experimental execution with reduced manual intervention.	Lab aut re de inte with inf mod h ove
Active learning and Bayesian optimization	Adaptive sampling selects informative experiments under uncertainty [4, 6].	Efficient navigation of experimental search spaces.	Opti must to d g val stand inter ph mecl
Physics-informed modeling	Physical laws and mechanistic constraints are embedded into machine learning systems [7, 8].	Improved interpretability, generalizability, and scientific plausibility.	Physi mod to (in auto wo rathe is comp t
Generative materials design	Generative and inverse-design methods propose candidate structures with target properties [19, 20].	Creation of novel candidate materials beyond known databases.	Ge can m filte ph prior hum va exper
Human scientific expertise	Experts define goals, curate data, interpret outcomes, and judge plausibility [16, 17].	Contextual reasoning, safety awareness, and theory-building.	Hum m ex forn v auto decis rath trea ex supe

Framework Logic

The Human–AI–Physics framework begins from the premise that autonomous materials intelligence is not simply automation applied to materials science. Rather, it is a coordinated intelligence architecture in which each pillar compensates for the limitations of the others. AI extends search capacity across vast materials spaces, physics preserves consistency with known laws, and humans define the scientific and technological meaning of the search. This logic draws from the broader movement toward autonomous experimentation systems that combine data, instruments, and decision algorithms into adaptive discovery platforms [16].

Human intuition enters the framework as a source of purpose, constraint, and interpretation. Experts translate societal and technological needs into materials objectives, such as stability, catalytic activity, conductivity, manufacturability, or sustainability. They also decide which trade-offs matter when competing properties cannot all be maximized simultaneously. This role is consistent with the view that self-driving laboratories require careful problem formulation and scientific oversight, not just automation [17].

AI functions as the exploratory and inferential engine of the framework. It learns structure-property relationships, proposes candidates, estimates uncertainty, and chooses experiments likely to be informative or performanceenhancing. Active learning is especially important because it allows systems to sample materials space adaptively rather than exhaustively [6]. Generative models and inverse-design methods extend this capability by proposing novel solid-state materials and crystal structures that may not exist in current databases [19, 20].

Physics-based models function as the framework's constraint and explanation layer. They prevent AI-generated candidates from drifting into unphysical regions of the design space and help connect statistical predictions to mechanisms. Physics-informed machine learning provides a conceptual foundation for this role because it embeds governing equations and physical priors into learning systems [8]. In autonomous materials intelligence, physics is therefore not a post hoc explanation but a continuous participant in candidate generation, screening, optimization, and validation.

Human–AI–Physics Integration

The integration of human, AI, and physics elements requires more than placing separate tools in sequence. In the proposed framework, integration means that each decision point is jointly shaped by human goals, AI inference, and physics constraints. For example, an AI model may recommend a synthesis condition, but that recommendation is filtered by physical feasibility and interpreted against expert expectations. This approach builds on self-driving laboratory concepts in which AI decision-making is coupled to experimental execution but extends them by assigning explicit roles to human and physics-based reasoning [12, 21].

Physics-informed AI is the first integration mechanism. Instead of relying only on correlations in materials datasets, AI models can incorporate conservation laws, thermodynamic plausibility, atomistic interaction patterns, and mechanistic constraints. Universal graph deep learning interatomic potentials and charge-informed atomistic models illustrate how learned representations can encode physically meaningful relationships across chemical systems [14, 15]. Such models are crucial when autonomous systems extrapolate beyond known materials, where purely data-driven predictions may be unreliable.

Human-guided AI is the second integration mechanism. Experts influence model development by curating datasets, defining target properties, selecting descriptors, interpreting uncertainty, and identifying implausible recommendations. The importance of flexible automation in materials discovery shows that effective autonomy often depends on adaptable workflows rather than rigid replacement of human judgment [22]. Human participation therefore shifts from manual execution toward strategic supervision, interpretation, and theory formation.

Experimentally grounded feedback is the third integration mechanism. Autonomous laboratories produce new measurements that update AI models, recalibrate physics-based simulations, and revise human hypotheses. Closed-loop discovery systems using Bayesian active learning already demonstrate how experimental feedback can guide materials exploration in real time [4]. Within the proposed framework, this feedback is expanded into a triadic learning cycle in which every experiment teaches the algorithm, tests the physics, and informs the scientist.

Figure 1 presents the integrated Human–AI–Physics architecture that connects expert judgment, adaptive AI exploration, physics-based constraints, and experimental feedback into one autonomous materials intelligence system.

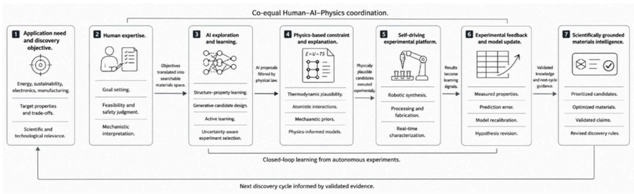

Figure 1. Human–AI–Physics Architecture for Autonomous Materials Intelligence

Discovery Module

The Discovery Module is the entry point of the Human–AI–Physics framework because it translates broad materials objectives into candidate materials spaces. In this module, human experts define the target function, such as catalytic activity, charge transport, mechanical resilience, synthesis feasibility, or environmental stability. AI models then explore chemical, compositional, and structural possibilities that would be infeasible to enumerate manually, a capability anticipated in machine-learning approaches to materials discovery and design [1, 23]. Physics-based models constrain this exploration by rejecting candidates that violate known thermodynamic, structural, or mechanistic principles.

Generative and inverse-design models are central to discovery because they enable autonomous systems to propose materials rather than merely rank known options. Generative adversarial networks for crystal structure prediction demonstrate how AI can construct candidate structures in a data-driven manner while searching beyond existing experimental records [19]. Continuous representations for solid-state materials similarly support inverse design by connecting desired properties to candidate structures in latent materials spaces [20]. In the framework, these generative outputs are treated as hypotheses that require physical screening and human interpretation before synthesis.

Discovery also depends on representation learning because autonomous systems must encode materials in ways that preserve chemically and physically meaningful relationships. Graph networks provide a flexible framework for molecules and crystals by representing atoms and bonds as structured relational data [10]. Multi-fidelity learning further allows models to combine data from different levels of accuracy, such as approximate simulations and higher-fidelity calculations, to improve materials prediction under data scarcity [11]. These capabilities allow the Discovery Module to search broadly while still learning from uneven and heterogeneous materials datasets.

Human judgment remains essential in the Discovery Module because novelty alone is not a sufficient discovery criterion. Experts determine whether a proposed material is scientifically interesting, experimentally plausible, safe to synthesize, and relevant to the intended application. Recent large-scale deep learning approaches show that AI can accelerate the identification of promising inorganic materials, but expert framing remains necessary to decide which candidates matter and why [18]. Thus, discovery in the framework is not a fully automated act of generation but a guided expansion of the materials imagination.

Optimization Module

The Optimization Module converts promising candidates into improved materials by iteratively refining composition, processing, structure, and performance. It relies on Bayesian optimization and active learning to choose experiments that balance exploitation of known high-performing regions with exploration of uncertain regions. Closed-loop Bayesian active learning has already shown that materials systems can be optimized on the fly through adaptive sampling [4]. In the proposed framework, optimization is the module where AI most visibly acts as an experimental strategist.

Optimization requires models that can reason under uncertainty because experimental campaigns are costly and incomplete. Active learning in materials science emphasizes the value of uncertainty-aware sampling for targeted design, especially when the number of possible experiments is far larger than the number that can realistically be performed [6]. Human experts use this uncertainty information to decide whether the system should pursue performance gains, mechanistic clarification, robustness, or risk reduction. Physics-based models then help distinguish uncertainty caused by sparse data from uncertainty caused by genuine physical complexity.

Autonomous laboratories make optimization operational by linking model recommendations directly to synthesis and characterization. Self-driving thin-film discovery demonstrates how an autonomous platform can select experiments, fabricate samples, measure outcomes, and update decisions within a closed loop [3]. Mobile robotic chemistry extends this logic by showing that robotic systems can physically perform experimental searches in complex chemical spaces [5]. The Optimization Module generalizes these examples into a framework component that continuously adjusts materials variables in response to measured performance.

Physics-informed surrogate models are especially valuable in optimization because they can accelerate convergence while preserving interpretability. Machine learning models for solid-state materials have increasingly incorporated structural, compositional, and physical information to improve predictive reliability [24]. Interatomic potentials learned across the periodic table further suggest that AI models can approximate atomistic behavior at scales useful for screening and refinement [14]. In the framework, optimization succeeds when AI efficiently improves performance, physics keeps the search plausible, and humans judge whether the resulting trade-offs are acceptable.

Validation Module

The Validation Module determines whether discovered and optimized materials are scientifically credible, reproducible, and application-relevant. It transforms candidate performance from a model prediction or local experimental success into a validated materials claim. Autonomous experimentation systems can generate dense feedback streams, but validation requires interpreting those streams against uncertainty, physical expectations, and experimental limitations [16]. Therefore, validation is not a final checkpoint but a recurring epistemic function within the closed loop.

Uncertainty quantification is central to validation because autonomous systems must know when their predictions are reliable and when they are extrapolating beyond evidence. Physics-informed machine learning provides one route to validation by constraining learned predictions with physical laws and mechanistic structure [8]. Charge-informed neural network potentials similarly show how learned models can encode physically relevant information that improves atomistic modeling across diverse systems [15]. In the Validation Module, uncertainty estimates guide whether a candidate should be accepted, retested, reformulated, or rejected.

Experimental feedback is the mechanism through which validation updates the entire framework. When characterization results differ from predictions, the discrepancy can reveal missing physics, biased training data, measurement artifacts, or overlooked synthesis variables. Self-driving laboratory roadmaps emphasize that autonomous systems must treat failed or surprising experiments as valuable information rather than mere errors [21, 25]. **Table 2** presents the integrated Human–AI–Physics framework and its core operational modules.

Table 2. Integrated Human–AI–Physics Framework for Autonomous Materials Intelligence: Discovery, Optimization, and Validation Modules

Operational module	**Human role**	**AI role**	**Physics ro**
Discovery	Defines target properties, application context, feasibility boundaries, and scientific priorities.	Generates candidate compositions, structures, and design hypotheses from large materials spaces.	Screens candidates thermodynar structural, a mechanisti plausibility
Optimization	Evaluates trade-offs, adjusts objectives, and interprets performance pathways.	Uses Bayesian optimization, active learning, and surrogate modeling to select informative experiments.	Constrain search trajectorie through physical law atomistic models, ar mechanisti assumption
Validation	Judges scientific credibility, reproducibility, safety, and application relevance.	Quantifies uncertainty, detects anomalies, and identifies cases requiring retesting or recalibration.	Tests wheth prediction remain consistent w known physi principles a mechanisti explanatior
Autonomous workflow integration	Reframes goals as knowledge accumulates and determines when autonomy requires intervention.	Coordinates module transitions and learns from cumulative closed-loop data.	Maintains continuity between prediction mechanism and experiment reality.

Validation also protects autonomous systems from false confidence. A model may predict high performance because it has learned a statistical shortcut, while an experiment may appear successful because of uncontrolled processing variation. Autonomous synthesis of novel materials illustrates the promise of integrated robotic experimentation, but also underscores the need for validation standards that connect synthesis outcomes to reliable claims [26]. The Validation Module therefore ensures that autonomy accelerates discovery without weakening scientific rigor.

Autonomous Workflow

The autonomous workflow links Discovery, Optimization, and Validation into a continuous cycle rather than a linear pipeline. Discovery produces candidate materials, optimization improves them through adaptive experimentation, and validation determines whether the resulting claims are reliable enough to inform the next cycle. This workflow reflects the broader vision of materials acceleration platforms, where computation, robotics, and data-driven decision-making converge to reduce discovery time [13]. In the Human–AI–Physics framework, the loop becomes intelligent because each cycle updates not only a dataset but also the relationship among human goals, AI models, and physical understanding.

At the beginning of each cycle, human experts translate an application need into operational objectives. AI systems then convert those objectives into candidate structures, synthesis conditions, or experimental strategies. Physics-based models evaluate whether the proposed paths are plausible before the autonomous laboratory commits resources. This logic extends the self-driving laboratory model by making human direction and physical constraint explicit components of every decision rather than external additions [12, 17].

During the experimental phase, robotic platforms synthesize, process, and characterize materials while AI systems monitor incoming results. Flexible automation is important because materials workflows vary across thin films, powders, catalysts, batteries, alloys, and molecular systems [22]. High-performance computing and robotics can further expand the scale of this loop by allowing simulation, prediction, and experimentation to operate in parallel [9]. The workflow therefore requires not only algorithms but also modular infrastructure that can adapt to different classes of materials problems.

After validation, the system returns to discovery with better models and sharper human understanding. Unexpected results may open new hypotheses, while failed candidates may improve uncertainty estimates and reveal constraints that were absent from the initial model. Autonomous experimentation systems are most powerful when they treat every cycle as both a performance search and a knowledge-building process [16]. The workflow therefore becomes progressively more capable as AI learns from data, physics models are recalibrated, and humans refine the scientific questions.

Figure 2 illustrates how autonomous materials intelligence progresses through Discovery, Optimization, and Validation modules while continuously converting experimental outcomes into updated AI models, recalibrated physics assumptions, and refined human hypotheses.

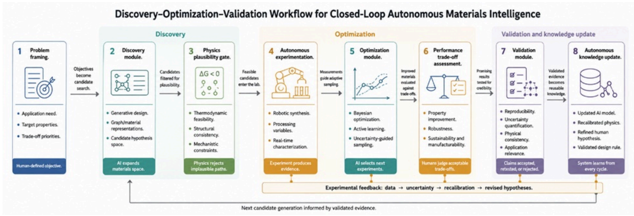

Figure 2. Discovery–Optimization–Validation Workflow for Closed-Loop Autonomous Materials Intelligence

Implications

The first implication is that autonomous materials intelligence can accelerate functional materials development without reducing discovery to algorithmic search. Large-scale AI models and graph-based materials representations already indicate that candidate identification can be expanded dramatically across chemical and structural spaces [10, 18]. When linked to autonomous experimentation and validation, this capability can compress the time between hypothesis and tested material. The framework suggests that acceleration will be greatest when AI generation, physics-based filtering, and experimental feedback are designed as one system.

The second implication concerns the changing role of human scientists. In self-driving laboratories, humans are less likely to act primarily as manual experimenters and more likely to act as designers of objectives, interpreters of anomalies, auditors of uncertainty, and builders of theory. Perspectives on autonomous chemical experimentation emphasize that human judgment remains essential for framing meaningful problems and evaluating whether autonomous results are scientifically useful [17]. The Human–AI–Physics framework therefore does not remove the scientist from discovery but relocates expertise to higher-level reasoning and governance.

The third implication is infrastructural. Realizing autonomous materials intelligence requires interoperable data systems, flexible robotic platforms, uncertainty-aware AI models, physics-informed simulations, and validation protocols that can be shared across laboratories. Community perspectives and recent Chemical Reviews synthesis both show that self-driving laboratories require coordinated standards, modularity, and integration across instruments, algorithms, and scientific communities [16, 25]. The framework provides a conceptual basis for that integration by defining what each component must contribute to discovery, optimization, and validation.

Conclusion

This article has proposed a Human–AI–Physics framework for autonomous materials intelligence. The framework defines materials discovery as a closed-loop process in which human expertise, artificial intelligence, and physics-based modeling operate as co-equal partners. It positions discovery, optimization, and validation as interdependent modules rather than separate stages.

The framework's central contribution is its integrative logic. AI proposes and learns, physics constrains and explains, humans guide and interpret, and experiments validate and recalibrate. Together, these functions provide a blueprint for self-driving laboratories that are not merely automated but scientifically grounded.

The immediate path forward is to build platforms that embody this integration in practice. Such platforms should combine generative design, active learning, physics-informed modeling, robotic experimentation, uncertainty quantification, and human oversight in one adaptive workflow. By doing so, autonomous materials intelligence can accelerate the discovery, optimization, and validation of next-generation materials while preserving the rigor and creativity of scientific inquiry.

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