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Perspective: Autonomous Laboratories and Real-Time ML Feedback Loops — A Position for Closed-Loop Discovery

Minh Tran[1*], Duc Pham[1]

Abstract

Materials discovery remains painfully slow. Traditional human-driven experimentation, followed by offline machine-learning analysis, requires weeks or months per iteration and leaves vast regions of chemical space unexplored. This position paper argues that autonomous laboratories equipped with real-time ML feedback loops represent not an incremental improvement but a necessary paradigm shift for the future of materials engineering. In these systems, robotic platforms handle synthesis and characterization while ML models continuously update and steer the next experiment, closing the discovery loop in hours rather than weeks. The current paradigm relies on human-in-the-loop decision-making, batch experimentation, and post-hoc ML training. Autonomous laboratories reverse this: robots execute synthesis and characterization tasks, a real-time ML engine analyzes streaming data, and an acquisition function immediately proposes the next candidate, all without human intervention for routine decisions. Early demonstrations have already shown accelerated discovery of battery electrolytes, perovskites, and catalysts. Real-time ML feedback loops demand online learning, rigorous uncertainty quantification, rapid acquisition functions, multi-objective optimization, constraint handling, human oversight for safety, and seamless data streaming. We articulate seven foundational principles for closed-loop discovery: integration-first design, speed as a first-class constraint, uncertainty-driven exploration, graceful degradation, data provenance, modularity, and open standards. These principles address the technical, operational, and cultural barriers that still prevent widespread adoption. While challenges remain—high initial costs, instrument integration, and long-duration experiments—the community now possesses the necessary ML maturity, robotic hardware, and orchestration tools to overcome them. This position calls for coordinated investment in shared autonomous-lab infrastructure, open standards, and training programs so that closed-loop discovery becomes the default workflow across academia and industry. Only then can materials science deliver the energy, sustainability, and electronics breakthroughs society urgently needs.

Keywords Active learning, Bayesian optimization, Closed-loop discovery, Self-driving labs, Autonomous laboratories, Real-time machine learning

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Introduction

The position

Materials discovery is too slow. The traditional paradigm—human designs experiment, runs synthesis, characterizes, analyzes, then plans next experiment—takes weeks to months. Autonomous laboratories with real-time ML feedback loops can accelerate discovery by orders of magnitude. Robots synthesize and characterize; ML models learn

continuously and decide next experiments; the loop closes in hours or days, not weeks. This position paper argues that autonomous labs are not a luxury but a necessity for the future of materials discovery. We outline principles, address challenges, and call for community investment.

The position matters now because ML models have matured, robotics has advanced, and integration is feasible. Early adopters are already demonstrating closed-loop discovery. Szymanski *et al.* [1] introduced a fully autonomous laboratory that accelerated synthesis of novel materials through integrated robotics and ML decision-making. A community survey by Hung *et al.* [2] confirmed that autonomous platforms are transitioning from proof-of-concept to practical tools. Tom *et al.* [3] provided a comprehensive review of self-driving laboratories across chemistry and materials science, documenting dozens of successful deployments. The question is no longer whether autonomous laboratories will transform materials discovery, but how rapidly the community can adopt them and what principles should guide their design [4].

This perspective is grounded in computational and data-driven materials engineering. It builds directly on demonstrated systems that combine robotic experimentation with Bayesian optimization and active learning [5, 6]. By insisting on real-time feedback rather than offline batch retraining, these platforms move beyond simple automation to true closed-loop intelligence. The result is a discovery engine that explores chemical space more efficiently, reduces human bias, and generates reproducible data at scale [7, 8].

The stakes are high. Global challenges in clean energy, sustainable catalysis, and next-generation semiconductors demand materials that do not yet exist [9, 10]. Traditional methods cannot explore the combinatorial explosion of possible compositions and processing conditions. Autonomous laboratories with real-time ML feedback loops offer a scalable solution [1, 11]. They free human researchers to focus on high-level hypothesis generation and interpretation while the robotic–ML system handles the repetitive, high-throughput workload. This division of labor is not dehumanizing; it is liberating. Scientists can pursue bolder ideas when routine experimentation is automated and accelerated.

We therefore take a clear stance: the field must prioritize closed-loop systems. Incremental improvements to traditional workflows are no longer sufficient. The community should invest in hardware–software–ML co-design, establish open standards, and create shared facilities so that every materials laboratory can eventually operate in closed-loop mode [2, 12-14].

The Current Paradigm: Why it is Too Slow

Traditional materials discovery follows a linear, human-centric loop. A researcher spends days to weeks reviewing literature, days generating a hypothesis, hours to days designing an experiment, hours to days performing synthesis, hours to days completing characterization, hours to days analyzing data, and hours to days planning the next experiment. The cycle then repeats. Total iteration time routinely reaches weeks or months.

The bottlenecks are structural. Human decision-making is inherently sequential and limited by cognitive bandwidth. Even expert researchers can evaluate only a handful of possibilities at once. Batch experimentation compounds the problem: one synthesis run is completed before the next is planned, leaving instruments idle and data unexploited. Offline ML exacerbates the delay; models are trained only after an entire campaign ends, so insights arrive too late to influence ongoing work. Data silos complete the inefficiency: synthesis logs, characterization spectra, and processing conditions reside in separate notebooks or databases, making holistic analysis difficult.

These inefficiencies carry real costs. Progress in battery electrolytes, catalysts, and semiconductors is throttled. The parameter space for even simple inorganic materials exceeds what manual exploration can cover. Valuable opportunities are missed because researchers cannot test enough candidates quickly enough. Irreproducibility remains endemic; subtle variations in human-recorded conditions or execution order are rarely captured completely.

Recent reviews of self-driving laboratories highlight exactly these limitations. Tom *et al.* [3] document how conventional workflows leave most chemical space untouched. The community survey by Hung *et al.* [2] shows that the majority of materials laboratories still rely on the same slow cycle that has persisted for decades. Even when ML is applied, it is typically retrospective—used to rationalize results after the fact rather than to drive decisions in real time [6].

The opportunity is clear: automate the entire loop. When synthesis, characterization, and decision-making run continuously under robotic and ML control, iteration time collapses from weeks to hours. Data flow becomes immediate, uncertainty is quantified on the fly, and exploration becomes systematic rather than serendipitous [5, 15]. The current paradigm is not merely slow; it is fundamentally mismatched to the scale of modern materials challenges. Autonomous laboratories with real-time ML feedback loops close that mismatch. They turn discovery into a continuous, adaptive process rather than a series of disconnected campaigns. The remainder of this paper explains how to realize that vision.

Table 1 systematically contrasts the structural limitations of traditional materials discovery with the operational advantages of closed-loop autonomous laboratories.

Table 1. Structural Comparison between Traditional Materials Discovery and Closed-Loop Autonomous Laboratories

Dimension	Traditional Paradigm	Closed-Loop Autonomous Laboratory	Analytical Implication
Decision-making	Human-driven, sequential	ML-driven, real-time	Removes cognitive bottleneck
Experimentation	Batch, discontinuous	Continuous, streaming	Maximizes instrument utilization
Learning Mode	Offline, retrospective	Online, incremental	Enables adaptive exploration
Data Flow	Fragmented, siloed	Integrated, real-time	Improves reproducibility
Iteration Speed	Weeks–months	Hours–days	Orders-of-magnitude acceleration
Exploration Strategy	Heuristic-driven	Uncertainty-driven	Systematic coverage of space
Optimization	Single-objective (often implicit)	Multi-objective (explicit Pareto)	Enables trade-off navigation
Error Handling	Manual intervention	Graceful degradation protocols	Improves system robustness
Reproducibility	Variable	High (automated logging)	Supports scientific reliability
Role of Scientist	Executor	Strategist/interpreter	Shifts cognitive labor upward

Autonomous Laboratories: What They are

An autonomous laboratory, often called a self-driving lab, is a system in which robots perform synthesis and characterization, ML models analyze results in real time, and the same models plan the next experiments—all without routine human intervention. The definition emphasizes full closed-loop operation rather than partial automation [1, 3].

The key components work together as an integrated unit. Synthesis robots include liquid handlers, robotic arms, furnaces, and sputter coaters that execute precise material preparation protocols. Characterization robots deploy instruments such

as X-ray diffractometers, scanning electron microscopes, Raman spectrometers, and conductivity probes to measure properties immediately after synthesis. The ML decision engine employs Bayesian optimization or active learning to select the next candidate based on all accumulated data [5, 6]. A real-time streaming database stores every condition and result, while control software—typically Python-based orchestration layers—coordinates the entire loop.

The closed loop operates in six clear steps: (1) the ML model suggests an experiment using the current knowledge base, (2) the robot executes synthesis, (3) the robot performs characterization, (4) data streams instantly to the ML model and database, (5) the model updates its surrogate and uncertainty estimates, and (6) the cycle repeats. Loop time is dominated by physical experiment duration (hours) rather than computation (seconds).

Early systems already demonstrate the concept. Kusne *et al.* [5] showed on-the-fly closed-loop materials discovery using Bayesian active learning. Dave *et al.* [11] deployed robotic platforms for autonomous discovery of battery electrolytes, later extending the approach to non-aqueous Li-ion systems [16]. Rooney *et al.* [7] built a self-driving laboratory specifically for adhesive materials. Additional examples include nanoparticle synthesis, metal-organic frameworks, and superconducting materials [17, 18]. These platforms remain expensive and specialized, yet they prove that closed-loop operation is technically achievable today [2].

Most current implementations are still confined to well-defined chemical spaces or single-instrument setups. Democratization requires lower-cost hardware, modular software, and community standards [12, 19]. Nevertheless, the core architecture—robotics plus real-time ML—is no longer experimental. It is ready for broader deployment. The next section details the precise ML requirements that turn a robotic platform into a true autonomous laboratory.

Figure 1 presents a hierarchical, non-cyclic architecture of the autonomous laboratory, emphasizing linear decision flow and continuous data assimilation under real-time ML control.

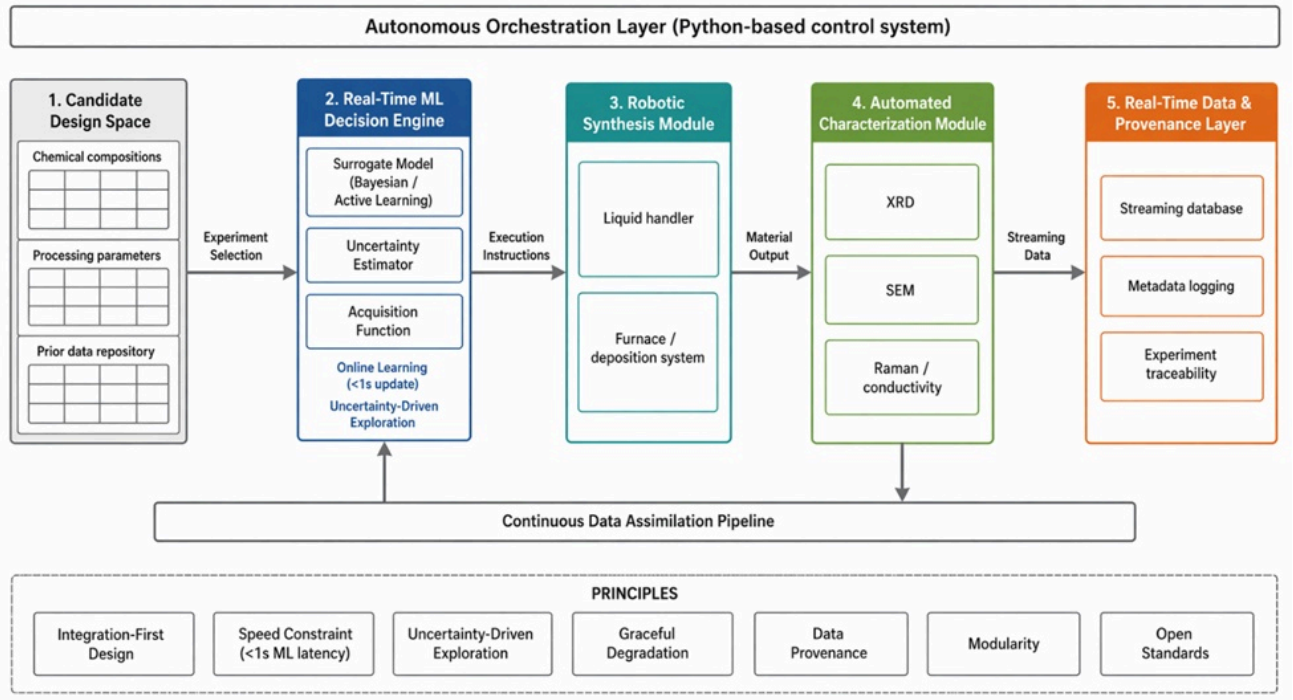

Figure 1. Hierarchical architecture of an autonomous laboratory with real-time machine learning feedback, illustrating linear decision flow, robotic execution, and continuous data assimilation without cyclical representation.

Real-Time Ml Feedback Loops: Key Requirements

Real-time ML feedback loops in autonomous materials discovery impose stringent demands that set them apart from conventional offline modeling, as the model must ingest data continuously, update its beliefs instantaneously, and recommend the next experiment within seconds [5]. Online learning therefore becomes indispensable, requiring algorithms that dynamically balance stability and plasticity to enable immediate incorporation of each new measurement while avoiding catastrophic forgetting. This imperative extends directly to uncertainty quantification, which must be both reliable and well-calibrated so that epistemic uncertainty can effectively guide exploration–exploitation trade-offs; Bayesian optimization frameworks prove particularly powerful here by maintaining posterior distributions that furnish natural uncertainty estimates to steer efficient closed-loop search [5].

Acquisition functions must in turn execute rapidly enough to fit within seconds-long decision windows, rendering computationally intensive procedures such as extensive Monte-Carlo sampling impractical and necessitating fast approximations or pre-computed surrogates [6]. Under these conditions, multi-objective optimization emerges as essential for navigating inherent trade-offs—conductivity versus stability, cost versus scalability—while dynamically maintaining the Pareto frontier in real time rather than collapsing performance into a single scalar. Constraint handling further requires adaptive mechanisms to accommodate shifting limits on temperature, precursor availability, safety thresholds, and instrument availability without disrupting the loop [20].

Human-in-the-loop oversight remains critical for safety-critical or highly anomalous situations, allowing autonomous operation on routine decisions yet seamless transfer of control when uncertainty thresholds are breached. Real-time data streaming from heterogeneous instruments—spectrometers, cameras, conductivity meters—underpins the entire architecture, demanding calibrated, timestamped feeds integrated directly into the ML pipeline [8]. When these requirements are simultaneously satisfied, as demonstrated by platforms that couple robotics with machine learning for electrolyte optimization and beyond [11, 16], the ML feedback loop can function as the intelligent core of the autonomous laboratory; the field must therefore prioritize algorithms purpose-built for streaming, multi-modal, constrained environments instead of retrofitted offline tools [21].

Table 2 consolidates the core real-time ML requirements and explicitly links them to their system-level implementations and operational consequences.

Table 2. Mapping Real-Time ML Requirements to System-Level Capabilities in Autonomous Laboratories

ML Requirement	System Implementation	Operational Role	Failure Risk if Absent
Online Learning	Incremental model updates	Enables real-time adaptation	Model staleness
Uncertainty Quantification	Bayesian posterior estimation	Guides exploration vs exploitation	Inefficient search
Fast Acquisition	Sub-second optimization routines	Maintains loop continuity	Robotic idle time
Multi-objective Optimization	Pareto frontier tracking	Balances competing properties	Suboptimal materials
Constraint Handling	Dynamic constraint encoding	Ensures feasibility & safety	Unsafe experiments
Human Oversight	Interrupt thresholds / alerts	Safety governance	Uncontrolled risk
Real-Time Data Streaming	Integrated pipelines	Enables closed-loop operation	Data latency bottlenecks
Multi-modality Integration	Unified data representations	Improves decision accuracy	Information loss

Provenance Tracking	Metadata logging systems	Ensures reproducibility	Irrecoverable experiments

Principles for Closed-Loop Discovery

Successful deployment of autonomous laboratories hinges on a coherent set of interdependent design principles that elevate closed-loop discovery from isolated demonstrations to reliable scientific infrastructure. Hardware, software, and machine learning components must be co-designed from the outset, since retrofitting ML onto legacy instruments inevitably produces brittle systems vulnerable to the first data-format mismatch [2, 12]. This integration imperative is inseparable from stringent speed requirements: the entire feedback loop must remain bounded by physical experimentation rather than computation, with ML decisions completing in under a second to prevent robotic platforms from idling [1, 7].

Under these temporal constraints, epistemic uncertainty assumes a central steering role, actively directing the acquisition function toward undersampled regions of chemical space and countering premature exploitation of known high performers [5]. The architecture must further incorporate graceful degradation, shifting seamlessly to random sampling or human-defined protocols when model uncertainty spikes or instrument faults arise, thereby avoiding complete halts [8]. Equally critical are comprehensive data provenance—capturing full synthesis conditions, characterization metadata, timestamps, and execution traces for reproducibility and meta-analysis [7, 17]—and modularity that allows swapping of synthesis modules, characterization instruments, or surrogate models without redesigning the orchestration layer [12].

Open standards for data formats, APIs, and control interfaces complete the framework, enabling interoperability and cumulative community progress rather than duplicated effort [2]. These elements reinforce one another: integration without speed yields sluggish loops, while speed absent uncertainty quantification produces inefficient search, and modularity without openness fragments the ecosystem [3, 6]. As illustrated in **Figure 1**, a central cycle connects the ML decision engine—powered by Bayesian optimization and active learning—to synthesis and characterization robots via experiment proposals, material production, and real-time data streams, with continuous internal model updating and optional human oversight paths.

Adopting this integrated approach will enable autonomous laboratories to evolve into robust, shared infrastructure capable of routine high-impact discovery [1, 22].

Objections and Responses

Despite compelling demonstrations, several persistent concerns continue to hinder broader adoption of autonomous laboratories with real-time ML feedback loops, each addressable through evidence from deployed platforms and underlying design mechanisms. Perceived high capital costs for robotics, orchestration, and characterization are indeed substantial at the outset, yet continuous operation drives amortized per-experiment costs down sharply, as Rooney *et al.* [7] showed through infrastructure payback via accelerated screening cycles unattainable by manual means; shared facilities, as Hung *et al.* [2] recommend, further democratize access through collaborative or pay-per-use models.

This economic consideration connects directly to skepticism about robotic capacity for complex synthesis. Although current systems handle well-defined workflows most effectively, rapid progress now encompasses air-sensitive solid-state battery materials [1, 23] and inert-condition nanoparticle synthesis [18], demonstrating that modular hardware paired with robust constraints allows iterative expansion from simpler starting points into more demanding chemistries.

A parallel concern regarding ML reliability dissolves under the recognition that calibrated epistemic uncertainty, rather than perfection, suffices for safe navigation; Bayesian optimization frameworks [5, 11] enable this by operating autonomously within confidence bounds and escalating to human oversight when uncertainty rises, turning each

experiment into an incremental improvement in model trustworthiness. Far from eroding scientific insight, such platforms generate denser, more consistent datasets that shift researchers from routine execution toward higher-order interpretation and hypothesis refinement [3].

Incremental pathways further ease adoption: laboratories need not implement full autonomy immediately, since connecting individual modules to Bayesian optimizers [24] delivers immediate value while building capability through modularity and open standards. These objections, though understandable, are already being systematically dismantled by functioning systems, enabling the community to advance from isolated proofs-of-concept toward robust shared infrastructure.

Relation to Other Positions

This position builds directly on several related perspectives while extending them into the physical laboratory environment.

Relation to optimization-centric workflows. Earlier calls for shifting from pure prediction to design optimization find their natural embodiment in autonomous laboratories [25, 26]. Lei *et al.* [6] demonstrated Bayesian optimization with adaptive surrogate models that move beyond retrospective analysis into active experimental steering. The closed-loop systems described here make that optimization physically executable: the surrogate does not merely recommend; the robot executes, the instrument measures, and the model updates—all in hours.

Relation to active learning. Active learning has long been advocated as a data-efficient strategy for materials discovery. Kusne *et al.* [5] and Dave *et al.* [16] showed its power in guiding robotic campaigns for battery electrolytes and closed-loop materials search. The present position extends active learning from algorithmic simulations into real-time robotic execution, where the acquisition function operates under the hard constraints of physical time, instrument availability, and safety.

Relation to reproducibility. Volk *et al.* [8] emphasized performance metrics that reveal the hidden inefficiencies of human-driven workflows. Autonomous laboratories address those inefficiencies at the root: robots follow exact digital protocols, every condition is logged automatically, and data provenance is guaranteed. Pogue *et al.* [17] highlighted how closed-loop superconducting discovery benefits from this reproducibility, turning one-off experiments into cumulative, community-accessible knowledge.

Relation to closed-loop approaches in adjacent fields. Materials science can learn from chemical engineering and synthetic biology, where autonomous platforms are already more mature. Martin *et al.* [27] outlined perspectives for self-driving labs in synthetic biology that mirror the integration and feedback principles advocated here. By adopting and adapting those lessons, materials discovery can avoid reinventing proven orchestration strategies.

Together, these related positions converge on one conclusion: closed-loop discovery is the logical next step. Autonomous laboratories with real-time ML feedback loops provide the physical and algorithmic infrastructure that turns optimization theory, active learning, and reproducibility ideals into daily laboratory reality.

Challenges and Research Priorities

Before autonomous laboratories can transition from specialized prototypes to routine tools in materials discovery, five interlocking challenges demand targeted resolution [28]. Foremost among them is seamless integration across heterogeneous instruments from different vendors, which currently produce incompatible data languages and formats; this necessitates accelerated development and community-wide adoption of open standards, extending the modular architectures already proven effective [12]. Closely linked is the demand for true real-time ML operation, where online

learning, uncertainty calibration, and sub-second acquisition functions must function reliably under continuous data streams—priorities that call for purpose-built algorithms rather than adaptations of offline methods, building directly on established Bayesian frameworks [5, 6].

This real-time imperative intensifies the need for native multi-modal fusion of synthesis logs, spectra, images, and time-series data within a unified decision engine, a capability only partially realized in current high-throughput systems and best advanced through multi-modal foundation models [22]. Equally critical for long-duration campaigns spanning days is the capacity for forward-looking planning without loop interruption, best achieved via multi-fidelity and batch active learning strategies that intelligently orchestrate parallel and sequential experiments [21]. Overarching all these technical hurdles is the embedding of robust safety and ethical mechanisms capable of enforcing verifiable constraints and preserving human authority over high-risk decisions without compromising operational speed.

Coordinated funding and open collaboration across laboratories will be essential to surmount these barriers. The resulting acceleration in discovery rates promises returns substantial enough to warrant the investment.

Recommendations for Stakeholders

Concrete actions by each stakeholder group will accelerate the transition to closed-loop discovery.

For researchers: Begin with small-scale automation of a single instrument and a simple Bayesian optimizer, as pioneered by Xie *et al.* [24] and Shimizu *et al.* [29]. Adopt open standards for data and APIs from day one. Publish both successful and failed autonomous runs so the community learns collectively.

For institutions: Invest in shared autonomous lab facilities that multiple groups can access, following the model outlined in the community survey by Hung *et al.* [2]. Develop training programs that combine robotics, ML, and materials synthesis so the next generation of scientists is fluent in closed-loop workflows.

For funders: Prioritize proposals that fund infrastructure over individual instruments. Support open-source orchestration platforms and multi-lab consortia rather than one-off demonstrations. Dedicated calls for closed-loop discovery projects, similar to those that seeded early battery electrolyte platforms [11, 16], will create critical mass.

For journals: Establish standardized reporting requirements for autonomous lab campaigns, including full provenance logs and uncertainty metrics. Encourage publication of negative results and intermediate loop states so that the field advances collectively rather than through selective success stories.

Collective adherence to these recommendations will transform autonomous laboratories from specialized prototypes into accessible infrastructure. The result will be a materials community that discovers, validates, and deploys new materials at the pace demanded by global challenges.

Conclusion

Autonomous laboratories with real-time ML feedback loops are the future of materials discovery. The current paradigm is too slow: human decision-making, batch experimentation, and offline ML keep iteration times at weeks to months. Autonomous labs change the equation—robots synthesize and characterize; ML models update continuously and decide the next experiment; the loop closes in hours.

Seven key requirements define effective real-time feedback: online learning, uncertainty quantification, fast acquisition, multi-objective optimization, constraint handling, human-in-the-loop safety, and real-time data streaming. Seven principles provide the design blueprint: integration-first, speed, uncertainty-driven exploration, graceful degradation, data provenance, modularity, and open standards. Early platforms have already validated the vision. Remaining challenges—

integration, real-time algorithms, multi-modality, long-duration scheduling, and safety—are solvable with focused community effort.

We therefore call for immediate, coordinated investment in shared autonomous-lab infrastructure, open standards, and cross-disciplinary training. Funding agencies, universities, and journals must align their priorities to make closed-loop discovery the default workflow across academia and industry. Only then can materials science deliver the breakthroughs in energy, sustainability, and electronics that society urgently requires. The technology exists. The principles are clear. The time to act is now.

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References

Szymanski NJ, Rendy B, Fei Y, Kumar RE, He T, Milsted D, et al. An autonomous laboratory for the accelerated synthesis of inorganic materials. Nature. 2023;624(7990):86-91. https://doi.org/10.1038/s41586-023-06734-w.

Hung L, Yager JA, Monteverde D, Baiocchi D, Kwon HK, Sun S, et al. Autonomous laboratories for accelerated materials discovery: A community survey and practical insights. Digit Discov. 2024;3(7):1273-9. https://doi.org/10.1039/D4DD00059E.

Tom G, Schmid SP, Baird SG, Cao Y, Darvish K, Hao H, et al. Self-driving laboratories for chemistry and materials science. Chem Rev. 2024;124(16):9633-732.
https://doi.org/10.1021/acs.chemrev.4c00055.

Lee H, Yoo HJ, Jang HS, Park B, Park YJ, Han SS. Toward self-driving laboratory 2.0 for chemistry and materials discovery. Mater Horiz. 2026;13(10):4712-39.
https://doi.org/10.1039/D5MH01984B.

Kusne AG, Yu H, Wu C, Zhang H, Hattrick-Simpers J, DeCost B, et al. On-the-fly closed-loop materials discovery via Bayesian active learning. Nat Commun. 2020;11(1):5966.
https://doi.org/10.1038/s41467-020-19597-w.

Lei B, Kirk TQ, Bhattacharya A, Pati D, Qian X, Arroyave R, et al. Bayesian optimization with adaptive surrogate models for automated experimental design. NPJ Comput Mater. 2021;7(1):194.
https://doi.org/10.1038/s41524-021-00662-x.

Rooney MB, MacLeod BP, Oldford R, Thompson ZJ, White KL, Tungjunyatham J, et al. A self-driving laboratory designed to accelerate the discovery of adhesive materials. Digit Discov. 2022;1(4):382-9.
https://doi.org/10.1039/D2DD00029F.

Volk AA, Abolhasani M. Performance metrics to unleash the power of self-driving labs in chemistry and materials science. Nat Commun. 2024;15(1):1378.
https://doi.org/10.1038/s41467-024-45569-5.

Otyepka M, Pykal M, Otyepka M. Advancing materials discovery through artificial intelligence. Appl Mater Today. 2025;47:102981.
https://doi.org/10.1016/j.apmt.2025.102981.

Gao T, Huang H, Liu Y. Machine learning-driven nanoscale synthesis for electrocatalytic performance: From data-driven methodologies to closed-loop optimization. Adv Mater. 2025:e08263.
https://doi.org/10.1002/adma.202508263.

Dave A, Mitchell J, Kandasamy K, Wang H, Burke S, Paria B, et al. Autonomous discovery of battery electrolytes with robotic experimentation and machine learning. Cell Rep Phys Sci. 2020;1(12):100264.
https://doi.org/10.1016/j.xcrp.2020.100264.

Bayley O, Savino E, Slattery A, Noël T. Autonomous chemistry: Navigating self-driving labs in chemical and material sciences. Matter. 2024;7(7):2382-98.
https://doi.org/10.1016/j.matt.2024.06.003.

Tobias AV, Wahab A. Autonomous 'self-driving' laboratories: A review of technology and policy implications. R Soc Open Sci. 2025;12(7):250646.
https://doi.org/10.1098/rsos.250646.

Joress H, Trautt Z, McDannald A, DeCost B, Kusne AG, Tavazza F. Driving U.S. innovation in materials and manufacturing using AI and autonomous labs: Building a national center and testbed for autonomous materials science. Gaithersburg (MD): National Institute of Standards and Technology; 2024. Report No.: NIST SP 1320.
https://doi.org/10.6028/NIST.SP.1320.

Liang H, Wang C, Yu H, Kirsch D, Pant R, McDannald A, et al. Real-time experiment-theory closed-loop interaction for autonomous materials science. Sci Adv. 2025;11(27):eadu7426.
https://doi.org/10.1126/sciadv.adu7426.

Dave A, Mitchell J, Burke S, Lin H, Whitacre J, Viswanathan V. Autonomous optimization of nonaqueous battery electrolytes via robotic experimentation and machine learning [Preprint]. arXiv; 2021. arXiv:2111.14786.
https://doi.org/10.48550/arXiv.2111.14786.

Pogue EA, New A, McElroy K, Le NQ, Pekala MJ, McCue I, et al. Closed-loop superconducting materials discovery. NPJ Comput Mater. 2023;9(1):181.
https://doi.org/10.1038/s41524-023-01131-3.

Park J, Kim YM, Hong S, Han B, Nam KT, Jung Y. Closed-loop optimization of nanoparticle synthesis enabled by robotics and machine learning. Matter. 2023;6(3):677-90.
https://doi.org/10.1016/j.matt.2023.01.018.

Pilon S, Savino E, Bayley OM, Vanzella M, Claros M, Siasiaridis P, et al. A flexible and affordable self-driving laboratory for automated reaction optimization. Nat Synth. 2026.
https://doi.org/10.1038/s44160-026-01053-0.

Li G, Wang Y, Kar S, Jin X. Bayesian optimization with active constraint learning for advanced manufacturing process design. IISE Trans. 2026;58(3):257-71.
https://doi.org/10.1080/24725854.2025.2475505.

Tamura C, Job HM, Chang H, Wang W, Liang Y, Sun S. Autonomous organic synthesis for redox flow batteries via flexible batch Bayesian optimization. Digit Discov. 2025;4(10):2737-51.
https://doi.org/10.1039/D5DD00017C.

Zaki M, Prinz C, Ruehle B. A self-driving lab for nano- and advanced materials synthesis. ACS Nano. 2025;19(9):9029-41.
https://doi.org/10.1021/acsnano.4c17504.

Fei Y, Rendy B, Woo J, Yang X, Li C, Zeng Y, et al. An autonomous laboratory for high-throughput air-sensitive material discovery for all-solid-state batteries. ECS Meet Abstr. 2025;MA2025-02(7):1002.
https://doi.org/10.1149/MA2025-0271002mtgabs.

Xie Y, Zhang C, Deng H, Zheng B, Su JW, Shutt K, et al. Accelerate synthesis of metal–organic frameworks by a robotic platform and Bayesian optimization. ACS Appl Mater Interfaces. 2021;13(45):53485-91.
https://doi.org/10.1021/acsami.1c16506.

Gongora AE, Xu B, Perry W, Okoye C, Riley P, Reyes KG, et al. A Bayesian experimental autonomous researcher for mechanical design. Sci Adv. 2020;6(15):eaaz1708.
https://doi.org/10.1126/sciadv.aaz1708.

Paulson JA, Tsay C. Bayesian optimization as a flexible and efficient design framework for sustainable process systems. Curr Opin Green Sustain Chem. 2025;51:100983.
https://doi.org/10.1016/j.cogsc.2024.100983.

Garcia Martin H, Radivojevic T, Zucker J, Bouchard K, Peisert S, Arnold D, et al. Perspectives for self-driving labs in synthetic biology. Curr Opin Biotechnol. 2023;79:102881.
https://doi.org/10.1016/j.copbio.2022.102881.

Cooper AI, Courtney P, Darvish K, Eckhoff M, Fakhruldeen H, Gabrielli A, et al. Accelerating discovery in natural science laboratories with AI and robotics: Perspectives and challenges. Sci Robot. 2025;10(106):eadv7932.
https://doi.org/10.1126/scirobotics.adv7932.

Shimizu R, Kobayashi S, Watanabe Y, Ando Y, Hitosugi T. Autonomous materials synthesis by machine learning and robotics. APL Mater. 2020;8(11):111110.
https://doi.org/10.1063/5.0020370.