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Accelerating materials discovery through active learning: Methods, challenges and opportunities

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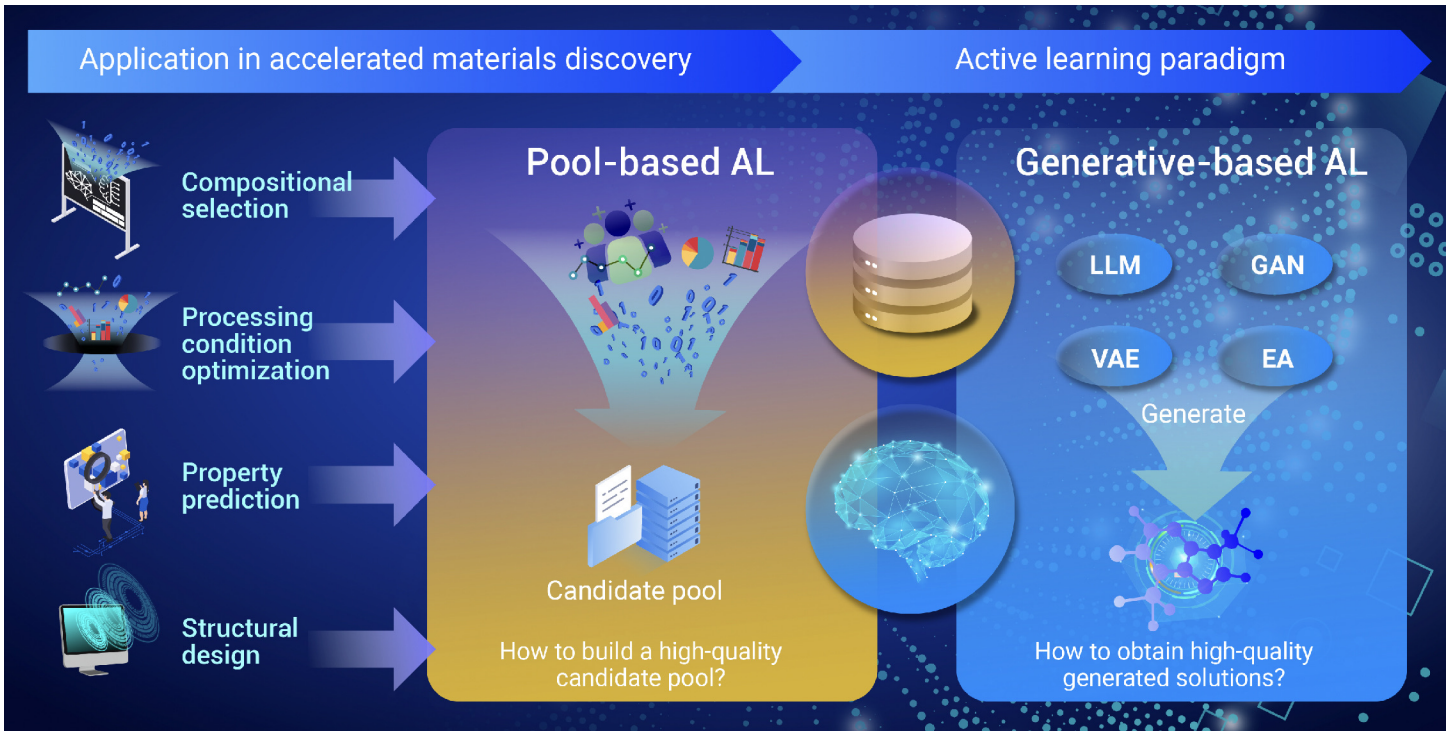
GRAPHICAL ABSTRACT



PUBLIC SUMMARY

- Active Learning (AL) selects the most informative experiments to improve models efficiently, saving cost and time.
- Under constraints, AL prioritizes knowledge gaps and reduces redundant tests, boosting exploration efficiency.
- This review offers an AL framework for interaction, integrating domain know-how and a practical roadmap.

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Accelerating materials discovery through active learning: Methods, challenges and opportunities

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The convergence of large-scale experimentation and computation has transformed materials science into a discipline where data plays a central role. However, the vast design space and high costs of experiments and simulations still slow progress. In contrast to traditional approaches, active learning (AL) identifies which experiments or simulations will provide the most valuable information. This minimizes unnecessary work and cost. By prioritizing the most informative data points, AL enables more efficient and targeted exploration, particularly when resources are limited. This approach accelerates breakthroughs in complex systems, such as superconductors, catalysts, and batteries. This review introduces a framework that categorizes AL in both experimental and computational settings. It highlights the importance of integrating domain knowledge and addresses interpretability challenges. By providing a pragmatic roadmap, it makes a strong case for adopting AL, especially to maximize impact in resource-constrained materials research.To facilitate provide additional details, we have made the supplementary materials available in the repository at https://github.com/kg4sci/awsome-AL.

INTRODUCTION

Due to recent advances in high-throughput experimentation and computational techniques materials science has entered an unprecedented era of data-driven and intelligent acceleration.[1–4] Faced with the exponential growth of chemical composition combinations, coupled with the complex interplay of multi-scale physical mechanisms, traditional experimental approaches based on empirical knowledge or blind screening are increasingly struggling to meet the demands for rapid discovery and performance optimization of novel materials. Trial-and-error experimentation often entails complex preprocessing steps, expensive reagents, and significant manpower. Furthermore, high-fidelity simulation methods like density functional theory (DFT) calculations become prohibitively time- and resource-intensive in computationally constrained environments. Against this backdrop, researchers urgently require intelligent strategies that can maximize information acquisition efficiency under limited experimental or computational budgets. In this context, Bayesian optimization and active learning (AL) have emerged as powerful tools for materials discovery. They can significantly reduce experimental costs through efficient parameter space exploration and iterative optimization, thereby achieving target properties with fewer resources and accelerating the discovery of materials with targeted properties.[5–7] AL, a methodology enabling algorithms to autonomously determine "which samples are most valuable" and prioritize their labeling, is playing an increasingly pivotal role in materials discovery and design by significantly reducing unnecessary, redundant experiments or computations.[8]

The core principle of AL is to enable the learning system to prioritize the most informative samples within the vast space of candidate elements or compounds by estimating each candidate's potential contribution to future model performance improvement. From a model training perspective, this means AL algorithms do not treat all samples equally, as in traditional random sampling. Instead, by evaluating metrics such as uncertainty, prediction variance, or model parameter changes, they selectively acquire labels only for those samples expected to most significantly reduce overall prediction error or most rapidly refine the model's decision boundaries. In materials science, where each synthesis or calculation can consume hours or even days, guidance from AL allows researchers to rapidly grasp the key performance distributions of a material system in its early stages. Subsequent experimental or computational results are then fedback to the algorithm, forming a closed-loop acceleration platform integrating experimentation and computation. This capability is particularly crucial for complex systems requiring simultaneous consideration of multiple performance metrics, such as high-temperature superconducting material design, catalyst discovery, and battery material optimization. Leveraging AL, performance landscapes that traditionally required hundreds of experiments to map can now potentially be approximated or even surpassed with results obtained from just a few dozen strategically chosen experiments.[9,10]

Existing reviews typically categorize AL for materials discovery either by optimization objective (single-objective vs. multi-objective) or by query strategy (e.g., uncertainty sampling, version space disagreement, expected-model-change, information-gain and diversity-aware methods).[6,11–15] However, such taxonomies are largely algorithm-centered and often overlook how these methods operate under the diverse experimental and computational constraints of materials research. They seldom offer an application-oriented synthesis tied to real experimental interaction and sampling scenarios, nor do they systematically assess how domain knowledge is integrated across the full AL loop. These interaction and sampling scenarios are intrinsically linked to the specific constraints of materials experimentation and computational settings. For varied scenarios, AL algorithms require tailored design and optimization to meet practical application needs, rather than being treated as a universal solution. Therefore, this review adopts a novel perspective by centering its classification on interaction and sampling scenarios. By using the pool/generative axis, existing objectives and strategies can be unified under different operational constraints, thereby enhancing the interpretability and transferability of their classification. Moreover, the point of knowledge injection becomes more concrete depending on the candidate acquisition mode—the pool-based paradigm emphasizes selection and filtering strategies, while the generative paradigm focuses on the design of generative models and prior constraints, making the process of "where to inject knowledge" more explicit and actionable. By systematically organizing AL methods according to operational contexts and highlighting both methodological advances and persistent gaps, this review aims to provide a practical roadmap for researchers implementing AL in resource-constrained materials research environments.

CONCEPTS AND WORKFLOW

AL is a paradigm within classical supervised learning framework that enables learning algorithms to actively select the most "informative" samples for label acquisition, thereby minimizing labeling costs and accelerating model convergence. Traditional supervised learning typically requires obtaining large-scale, high-quality labeled datasets during the training phase and using all of them for model training. However, in many practical scenarios, especially within materials science, the cost of acquiring sample labels through experimentation, computation, or expert evaluation is often prohibitively high. Employing random sampling or training on the entire sample set not only

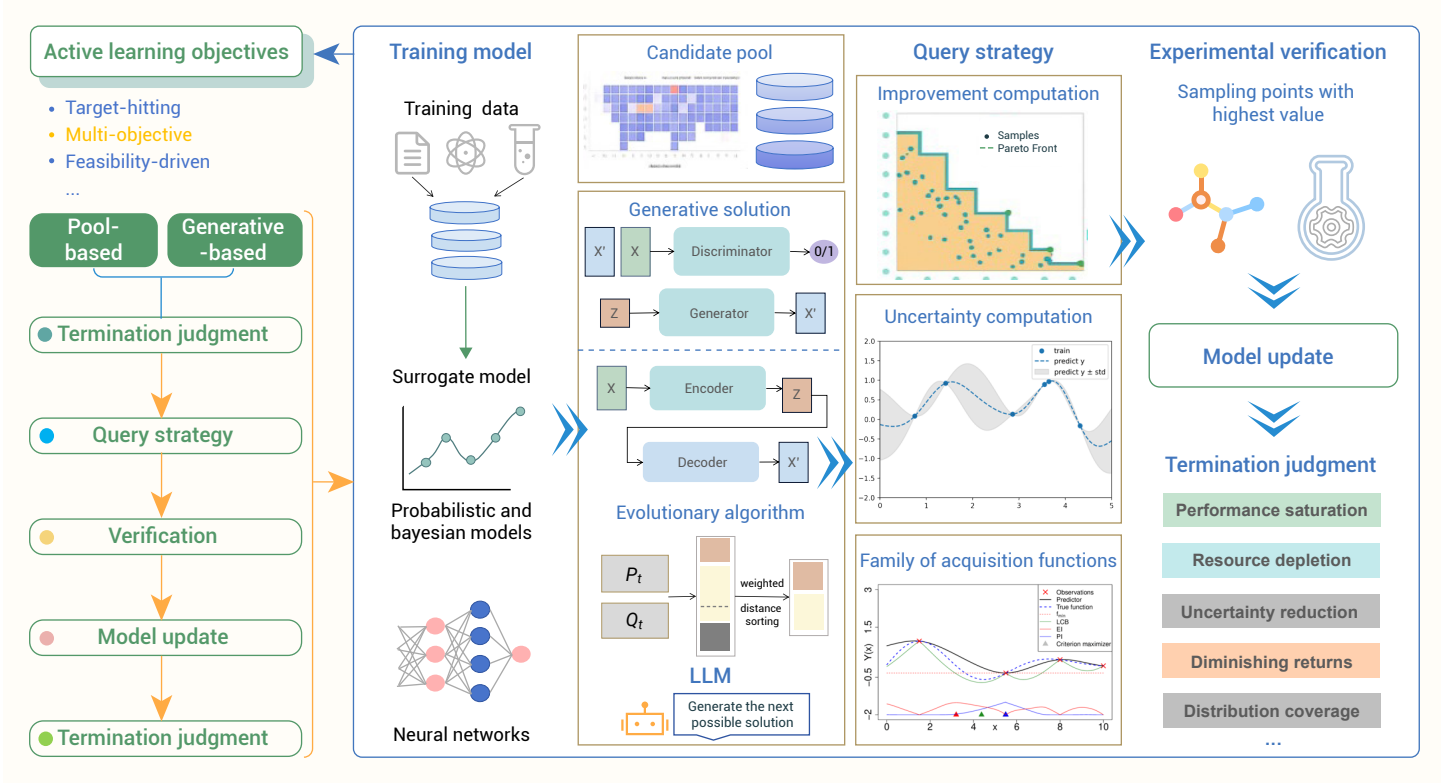

Figure 1. Schematic overview of the domain knowledge–informed materials discovery workflow, showing the integration of heterogeneous data sources, physics/chemistry-based feasibility filters, machine-learning models, and a closed-loop acquisition and validation cycle.

encounters resource bottlenecks but also risks "data wastage"—redundantly labeling samples that are easy to predict or offer minimal marginal value for model improvement. AL emerged directly from such needs. By estimating the potential contribution of each candidate sample in the unlabeled pool towards improving the current model's performance—and selectively labelling only the most informative among them—AL aims to maximize model gains with minimal labelling effort.

Conceptually, AL partitions the entire candidate space into a Labeled Set and an Unlabeled Pool. An initial model is trained on a small labeled subset and the algorithm then enters an iterative loop as illustrated in Figure 1. The cycle continues until a stopping criterion is met, such as achieving the target performance, exhausting the labeling budget, or reaching a predefined iteration threshold. The core principle lies in calculating the importance of candidate samples in each iteration round. This effectively concentrates labeling resources on the regions most valuable for model improvement, avoiding wasteful expenditure on samples that are easy to predict or informationally redundant.

From a holistic process perspective, AL comprises five aspects: Initialization, Query Strategy, Label Acquisition, Model Update, and Termination Criterion. Together, these define a general workflow that can be adapted to different research domains and practical constraints.

Methodological taxonomy

AL has developed into a broad methodological family, with numerous variants designed to reducelabeling cost and accelerate discovery. For clarity and to provide a conceptual foundation for the remainder of this review, we adopt a task-oriented classification to group AL methods by their objectives; this task axis is orthogonal to the acquisition paradigm discussed later—the former specifies what to optimize, the latter how candidates are obtained.

The first distinction is between pool-based and generative paradigms. In pool-based AL,[16,17] the learner operates over a static candidate set, ranking existing samples by informativeness or uncertainty and selectively acquiring labels. This approach is particularly relevant in materials science where large but finite libraries of known compositions or structures are available, and the goal is to prioritize which subset should be characterized or simulated. In contrast, generative ALcouples AL with generative modeling.[18–21] Instead of only selecting from a pre-defined pool, the algorithm is able to propose new candidates in an open-ended design space. These candidates may be generated through evolutionary operators, variational autoencoders, generative adversarial networks, or—more recently—large language models. The generative paradigm expands the exploration frontier and supports de novo discovery, though it requires careful feasibility filtering and validation.

A complementary axis of classification involves knowledge integration. Beyond purely data driven sampling, many AL frameworks incorporate prior knowledge into different stages of the pipeline: initializing datasets with domain heuristics, embedding physical constraints into surrogate models, modifying acquisition functions with safety rules, or designing principled stopping criteria. Such integration is particularly important in materials research, where physics-based constraints and empirical rules strongly affect experimental feasibility.

Together, these categories—pool-based versus generative, and knowledge-integrated versus purely data-driven—form the backbone of modern AL approaches. To unify these two categories, we formulate AL for materials discovery as a general iterative process that alternates between candidate acquisition and model update. The key difference between pool-based and generative paradigms lies in the definition of the candidate space. In pool-based AL, candidates are drawn from a fixed unlabeled pool, whereas in generative AL, candidates are synthesized on demand from a latent design space. This distinction can be compactly summarized as

$$\mathcal{B}_t = \begin{cases} \underset{x \in \mathcal{U} \setminus \mathcal{L}_t}{arg\max} A(x; f_{\theta_t}, P_{phys}), & (pool-based) \\ \underset{z \in \mathcal{Z}}{arg\max} A(G(z;\psi); f_{\theta_t}, P_{phys}), & (generative) \end{cases} \quad (1)$$

where $\mathcal{L}_t$ denotes the labeled set at iteration t,$\mathcal{U}$ is the unlabeled pool, f_{θ_t} is the predictive model, $A(\cdot)$ is the acquisition function, P_{phys} encodes physics- or domain-based feasibility priors, $G(z;"\psi)$ is a generator mapping latent variable z to candidate x, and $\mathcal{B}_t$ is the selected batch of candidates. After acquisition, the model is updated by

$$\theta_{t+1} = \underset{\theta}{arg\min} \mathcal{J}(\theta; \mathcal{L}_t \cup \{(x, \mathcal{O}(x)) : x \in \mathcal{B}_t\}), \quad (2)$$

where $\mathcal{O}(x)$ denotes the experimental or computational oracle providing true

labels and J(θ;·) is the training objective. In this unified framework, both pool-based and generative approaches can be viewed as optimizing an acquisition function over different candidate spaces, thereby linking the two paradigms under a common mathematical formulation. The following sections (Section 2–4) will expand on each category, illustrating representative algorithms and their applications in materials science.

Application in accelerated materials discovery

AL can be applied to various aspects of materials research, including compositional selection, structural design, processing condition optimization, and property prediction, thereby accelerating materials discovery and development.

Compositional selection. For complex multi-component systems, such as high-entropy alloys,[22,23] multinary compounds,[24] and multi-elemental catalysts,[25] AL enables the identification of optimal candidates from vast search spaces within a significantly reduced number of iterations. This approach dramatically outperforms traditional trial-and-error methods in the efficiency of discovering new materials. For example, Ma et al.[23] reported a high-entropy alloy ($Fe_{35}Ni_{29}Co_{21}Al_{12}Ta_3$) that demonstrates an unprecedented combination of simultaneously high strength and ductility, achieved through a domain knowledge-guided AL loop. The optimization process started with 140 data points in the Al-Co-Cr-Fe-Ni-Ta alloy system, using six physical features as inputs for the machine learning surrogate model. Remarkably, the desired alloy was identified within just three iterations.

Structural design. In the realm of structural design, the discovery of inorganic crystals has long been a critical topic, where high-throughput computations are often employed for the prediction and discovery of new crystal structures. Recently, graph neural networks have demonstrated remarkable capabilities in representing crystal structures and predicting their energies. As a breakthrough progress, Cubuk et al.[26] trained Graph Networks for Materials Exploration (GNoME) using large-scale AL combined with DFT calculations. The GNoME models discovered over 2.2 million stable crystal structures, increasing the known number of inorganic materials by an order of magnitude. Moreover, it was observed that the performance of GNoME models improved following a power-law relationship with the amount of available data.

Processing condition optimization. Processing condition optimization is a prototypical challenge in materials science, often labor-intensive and time-consuming. Traditionally, single variable control experiments and orthogonal experiments have been widely employed as optimization methods. However, as the number of influencing factors increases, AL demonstrates significant advantages in optimization efficiency, particularly when combined with automated experimental platforms. A notable example is the A-Lab, an autonomous laboratory developed by Ceder et al. for the solid-state synthesis of inorganic materials,[9] which integrated computations, historical knowledge, machine learning, AL, and robotics. The A-Lab employed natural language models trained on the literature to propose synthesis recipes, followed by active-learning-driven optimization. Remarkably, this platform successfully synthesized novel compounds from a set of 58 targets during 17 days of continuous operation.[41]

Property prediction. Properties are typically the primary optimization objectives in AL and are intrinsically linked to material composition, structure, and processing conditions. For instance, Raabe et al.[22] utilized AL to optimize the composition of high-entropy Invar alloys, achieving extremely low thermal expansion coefficients. Moreover, in practical applications, materials are often required to meet diverse performance criteria, which frequently involve inherent trade offs between different properties. For example, Kim et al.employed a Pareto AL framework to optimize the process parameters of Ti-6Al-4V alloys, simultaneously enhancing both strength and ductility.[27] With an initial dataset of 119 datapoints, this framework identified Ti-6Al-4V alloys exhibiting an ultimate tensile strength of 1190 MPa and a total elongation of 16.5% within just three iterations.

POOL-BASED ACTIVE LEARNING FOR MATERIALS SCIENCE

Pool-based AL, the most widely adopted paradigm in the field of materials discovery, centers on selecting the most valuable samples for labeling from a static candidate materials pool. In the pool-based AL setting, we score unlabeled candidates with an acquisition function and pick the top-ranked samples:

$$\mathcal{B}_t = \underset{x \in \mathcal{U} \setminus \mathcal{L}_t}{\mathrm{argtop}b} A(x; f_{\theta_t}) \tag{3}$$

In Eq. (3), $\mathcal{U} \setminus \mathcal{L}_t$ denotes the set of unlabeled candidates that have not yet been included in the labeled set; $A(x; f_{\theta_t})$ denotes the acquisition function that scores candidate x using the current model f_{θ_t} (examples include predictive variance, entropy, Expected Improvement (EI), or Upper Confidence Bound (UCB)); b denotes the batch size (number of samples selected per iteration); and argtop b is the operator returning the b samples with highest acquisition scores.

Facing the inherent challenge of ultra-high-dimensional combinatorial explosion within materials design spaces—such as the concentration space of multi-component alloys or combinations of molecular functional groups—this paradigm employs dynamically adaptive surrogate models to screen high-potential samples. It thereby overcomes the efficiency bottleneck of traditional grid search, serving as the core engine for high-throughput virtual screening (HTVS). The effectiveness of pool-based methods relies heavily on whether the selected model is well-suited to the current task's data structure, feature modalities, and prediction objectives. Different types of learning models exhibit significant variations in uncertainty quantification, sampling strategies, and feature representation capabilities when handling diverse materials data types. The following discussion explores several primary model types used in pool-based AL for materials discovery and their corresponding application strategies, focusing on model-task compatibility.

Probabilistic and bayesian models

Gaussian Process (GP) and Random Forest (RF) models, owing to their inherent capability for uncertainty estimation, were widely adopted in early pool-based AL applications. They are particularly well-suited for low-dimensional, structured materials composition-property prediction tasks.[28-30] GP models can directly output prediction means and variances, forming the basis for sampling strategies such as "maximum variance" or "Expected Improvement (EI)". For instance, in the task of component screening in materials, Pedersen et al. combined GP with DFT simulations, efficiently exploring the compositional space of high-entropy alloys using the EI principle, significantly reducing the number of experiments required to discover efficient oxygen reduction reaction catalysts.[31] Similarly, in the task of phase diagram construction, Kei Terayama and co-workers employed an uncertainty sampling strategy within AL to perform dense sampling around phase boundaries, thereby significantly reducing the number of required measurements.[32] Talapatra et al. integrated GP with Bayesian Model Averaging, identifying Ni-Co alloy compositions resistant to temperatures up to 1,200°C using only 10% of the experimental effort.[33] The key innovation was the development of a temperature-stability-constrained variant of the EI acquisition function, which avoided sampling in ineffective high-temperature regions and substantially improved materials design efficiency. Very recently, Niu et al. demonstrated a compelling application of GP-based Bayesian optimization for the discovery of high-performance, low-iridium oxygen evolution reaction catalysts.[34] Their study efficiently navigated a pool of 66 bimetallic oxide candidates, identifying Ir-doped TiO_2 as the most promising system, and further refined the optimal surface composition and oxygen vacancy configuration, which was subsequently validated experimentally, achieving a 23-fold enhancement in Ir mass activity compared to commercial IrO_2. Wang et al.'s work used a decision tree-based ensemble learning approach.[35] Catalysts are represented using elemental descriptors weighted by element content, aggregated into a single eigenvector by permuting invariant readouts. Extrapolated machine learning methods are used to dynamically generate and screen catalyst combinations. Farache et al. employed the RF model to leverage these descriptors for prediction and uncertainty quantification, guiding actual molecular dynamics simulations to discover multi-principal element alloys with high melting points.[36] Building on this foundation, Harwani et al. leveraged the FAIR data generated in the prior study, extended the optimization objective to include both high and low melting temperatures, and demonstrated a significantly more efficient and generalizable AL-molecular dynamics coupled workflow.[37] Nie et al. utilized a query-by-committee acquisition strategy, combining predictions for purity and catalytic activity

Table 1. Mapping of surrogate model types to primary materials task types and representative references. Entries indicate illustrative task usages observed in the literature.

Model types	Primary material task types	Representative references
Probabilistic and Bayesian Models	Composition screening; property prediction; multi-objective optimization	Composition screening: [25, 28, 29, 30, 31, 33, 36, 37, 38, 40, 41, 34]; Process condition optimization / synthesis optimization: [27]; Materials characterization: [32,54,55]
Neural Networks	High-dimensional property prediction; surrogate models for potential-energy surfaces; Crystal/molecular structure design and discovery; image/spectral characterization	Structure design and discovery: [43, 24, 26, 46, 47, 50, 52, 51, 56, 57]; Composition screening: [53,58]; Materials characterization: [59]; Scientific discovery: [44,45,60]

from XGBoost classifiers and regressors.[38] This approach successfully identified four novel oxides from a vast candidate pool within only four iterations.

Multi-objective pool-based AL simultaneously considers multiple performance metrics or prediction tasks, making it particularly suitable for materials discovery and optimization where achieving an optimal trade-off among several desired properties such as conductivity, stability, and manufacturability is essential. Studies employed GP regressors to optimize multiple objectives concurrently.[25,27,39] This overcomes the limitations of focusing on a single target, enabling the discovery of more practically valuable materials within high-dimensional design spaces. Unlike traditional methods, which typically require all target values for each sample to be known, Jablonka et al. used coregionalized GPs to model correlations between multiple targets, allowing predictions based on information from other targets, even if measurements of one target are missing.[40]

However, traditional regression models are prone to overfitting or modeling failure in high-dimensional sparse feature spaces and struggle to scale to complex modalities like graph structures or images, limiting their applicability. Recent research attempts to overcome this limitation through feature engineering and ensemble methods. For example, to address the conflict between high-dimensional features and small sample sizes, recent work employed Hierarchical Neural Networks (HNNs).[41] Genetic Algorithms were used to screen key descriptors and construct dimensionality-reduced sub-models, which were then fused using a hierarchical ensemble strategy incorporating statistical information, significantly enhancing model robustness. This method provides a new avenue for extending traditional regression models into high-dimensional materials spaces.

Neural networks

Neural networks have become a cornerstone of modern machine learning approaches to materials discovery, serving as powerful surrogate models for high-dimensional property prediction, image and spectral analysis, and, crucially, as the foundation for AL loops. One successful class of architectures comprises atom-centred multilayer perceptrons (MLPs): the Behler–Parrinello high-dimensional neural network potential (HDNNP) introduced atom-centred symmetry functions and per-atom MLPs to express total energy as a sum of local contributions, enabling molecular-dynamics-scale simulations with near-DFT accuracy at much lower cost.[42] Later transferable MLP potentials such as ANI showed these models can be trained across large organic chemical spaces to reproduce DFT energies and forces and be used within active- sampling pipelines to select new DFT points for retraining.[43] Recently, Liu et al.[44] and Bulanadi et al.[45] both applied AL approaches to the field of Autonomous Scientific Discovery. Their work utilized a Deep Kernel Learning (DKL) model, which integrates the representational power of neural networks with the uncertainty quantification of Gaussian processes, to actively explore structure–performance relationships in ferroelectric materials.

For tasks that explicitly require structural reasoning about crystals or molecules, graph neural networks (GNNs) have emerged as the model of choice because they operate directly on relational structure (atoms and bonds) via message passing and related mechanisms.[46,47] Within pool-based AL, uncertainty estimation for GNN model outputs is typically achieved via techniques like Monte Carlo Dropout (MC-Dropout) or multi-model ensembles.[48,49] The Crystal Graph Convolutional Neural Network (CGCNN) proposed by Xie et al.[50] learns global-local representations of crystal structures and has been subsequently integrated into pool-based frameworks for structural screening and property prediction. Moon et al.[24] divided 10 metals into A-site and B-site elements, constructing candidate structures according to the perovskite oxide formula, essentially an exhaustive enumeration approach. The researchers represented perovskite oxide structures as graphs, fully leveraging the properties of atomic nodes and edge connections to more intuitively reflect material structural information. In the research on atomic design of catalysts, Ge et al.[51] proposed an atomic-level catalyst design method integrating AL, Bayesian optimization, and DFT calculations. A graph convolutional neural network with dropout was employed as an approximate GP probabilistic model to predict the distributions of descriptor values based on catalyst structures. Through screening over 3,000 candidate nickel-based bimetallic catalysts, a NiIn intermetallic compound catalyst was successfully developed. Chun et al.[52] proposed to combine AL with isograph neural networks to explore the design space of single-atom catalytic sites. They designed a two-stage sampling process: the first stage uses uncertainty sampling to quickly explore unknown structures, and the second stage combines Bayesian optimization and diversity sampling to dig deep into high-potential areas. In the space of about 30,000 binary catalytic active sites, only a very small number of DFT calculations were screened to find efficient catalytic combinations with excellent performance. Xu et al.[53] used a multi-objective optimization framework—simultaneously targeting activity, cost-effectiveness, and entropic stabilization—to discover high-entropy alloy electrocatalysts with enhanced practicality in high-dimensional design spaces.

GENERATIVE ACTIVE LEARNING FOR MATERIALS SCIENCE

Generative AL expands the exploration boundaries of materials discovery by integrating candidate sample generation with uncertainty assessment. Unlike pool-based methods that rely on pre-constructed static sample libraries, the generative paradigm utilizes generative models to "instantly" construct efficient candidates within the materials design space, thereby transcending the limitations of existing samples in extremely high-dimensional combinatorial spaces. On one hand, generative models learn the latent distribution between material attributes and structures, enabling the synthesis of "novel" chemical compositions or microstructures with potential performance advantages.[61,62] On the other hand, incorporating uncertainty quantification methods into the generative loop allows for the prioritized generation and labeling of samples expected to provide the highest information gain for the surrogate model in each iteration, maximizing the utilization efficiency of experimental/computational resources. In generative AL, a generator or a search in latent/design space is used to propose candidates that maximize the acquisition score:

$$z^{(i)*} = \underset{z}{\operatorname{argmax}} A\left(G(z;\psi); f_{\theta_t}\right)(i = 1, \ldots, b) \Rightarrow \mathcal{B}_t = \left\{G\left(z^{(i)*};\psi\right)\right\}_{i=1}^{b} \quad (4)$$

In Eq. (4), $G(z;"\psi)$ denotes the generator or decoder mapping a latent/design vector z to a candidate x, with parameters "ψ (for example a VAE decoder, GAN generator, LLM sampling process, or an evolutionary operator); zdenotes the latent variable or design encoding (continuous or discrete vector); $z^{(i)*}$ denotes the i-th latent vector obtained by optimizing the acquisition function; b denotes the number of candidates to generate and select; and $A(\cdot)$ and f_{θ_t} are as defined previously. In practice, generated candidates are typically filtered for domain feasibility.

From the perspective of model-task compatibility, generative methods primarily fall into two categories: Conditional Generation and Unconditional Generation. Conditional generative models leverage existing experimental data by incorporating target performance indicators or material composition constraints at the input. The generator learns to adjust the latent space to meet these performance goals, making this approach particularly efficient for multi-objective optimization or scenarios with prior performance requirements.

Conversely, unconditional generation tends to explore broadly within the space first. Subsequent screening modules or evaluation networks then filter out unqualified samples before incorporating the remaining optimal candidates into the AL cycle. Regardless of the strategy, the key lies in the coupling between the dimensionality of the generative model's latent space representation and the modalities of material features (e.g., crystal structure, composition distribution, functional group positions). More refined multi-modal embeddings generally enhance the physical feasibility and measurability of the generated samples.

Evolutionary algorithm-based generative active learning

Evolutionary algorithms are utilized to directly evolve a batch of candidate samples within the material design space.[63] Each generation of the population generates new individuals through genetic operators such as crossover and mutation. The population is then ranked based on predefined performance metrics (e.g., mechanical strength, electrical conductivity, stability) using non-dominated sorting and crowding distance sorting. High-quality samples located on the Pareto front are selected. Unlike deep generative models, samples are not "synthesized" by a decoder from a latent space; instead, they are constructed directly within the design space via the crossover and mutation operations of genetic operators.

In the domain of Evolutionary Algorithm-Based Generative AL, several representative studies have demonstrated the power of genetic algorithms (GA) in expanding the design space beyond pre-defined candidate pools. For instance, Cluster-MLP integrates AL with GA to efficiently search for the global minimum energy configurations of pure and alloy nanoclusters, such as Pd, Cu, and Au clusters, thereby addressing both composition screening and structure discovery simultaneously.[64] In another direction, Wu et al.[65] proposed an EA-guided (Evolutionary Algorithm-guided) voxel-encoding framework for the design of hard-magnetic soft active materials, where GA was used to generate novel voxelized magnetization patterns, highlighting its role in structure design and process optimization.

These studies consistently highlight that GA, when coupled with AL, should be classified as a generative AL strategy, since new candidates are created iteratively during the evolutionary cycle.

Nevertheless, it is worth noting that in many problems,[66] GAs are used to select subsets from a fixed candidate pool. If a GA is restricted to that fixed pool and does not generate new solutions, it can be considered a form of pool-based AL.

Variational autoencoder-based generative active learning

The core value of Variational Autoencoders (VAEs) in generative AL lies in their ability to map the high-dimensional, discrete, and complex material design space into a low-dimensional, continuous, and well-structured latent space.[67-69] Firstly, the latent representations learned by the VAEs capture the nonlinear relationships between material compositions or structures, ensuring that new samples decoded through interpolation or neighborhood searches within the latent space exhibit enhanced physical plausibility and innovativeness. Secondly, the continuity and differentiability of the latent space significantly reduce the difficulty of optimization and sampling, making methods based on acquisition functions (such as Expected Improvement, EI, or uncertainty measures) more efficient in searching for new materials. Thirdly, through the probabilistic modeling of the latent distribution, VAEs inherently possess uncertainty estimation capabilities, aiding AL in more precisely identifying high-value and unexplored design regions during the exploration-exploitation trade-off. Finally, leveraging the structured properties of the latent space facilitates the incorporation of multi-objective or multi-attribute regularization, thereby better reconciling conflicts between different performance metrics while maintaining sample diversity. Rao et al.[22] utilized Wasserstein Autoencoders (WAEs) combined with Gaussian Mixture Models and Markov Chain Monte Carlo sampling to generate potential alloy compositions. WAEs learn efficient representations of alloy compositions, compressing high-dimensional data into a low-dimensional latent space conducive to large-scale search. Another typical example is the material inverse design method proposed by Xin et al.,[70] they combined VAEs and generative adversarial networks, and applied AL screening on the generated samples, successfully discovering multiple new inorganic compounds with specified bandgap ranges.

Generative adversarial network-based generative active learning

In contrast to the continuous and structured latent spaces learned by VAEs, Generative Adversarial Networks (GANs) offer a distinct generative paradigm based on adversarial training. This approach involves a generator that creates novel candidates and a discriminator that critiques them, driving the generator towards producing increasingly realistic samples. While GANs excel at generating high-diversity candidates for exploratory discovery, they typically require additional physics-based constraints or downstream filtering to ensure physical feasibility. The following studies exemplify how GAN-enhanced AL frameworks can be powerfully applied to materials discovery.

Guo et al.[71] proposed a GAN-enhanced directional constrained AL framework. By incorporating feature weight constraints into the acquisition function, this framework significantly improves the efficiency of material property optimization under small-data scenarios. Near-zero ablation rate ternary ultra-high-temperature ceramics were discovered within only two iterations. Kim et al.[72] proposed a model that continuously predicts the overpotential of new metal precursor combinations and selects points for experimental validation based on the prediction uncertainty. These experimental points are not predetermined samples from a pool but are dynamically generated by the model based on its current learned knowledge. The approach in research is primarily based on the DSTAR (DFT and Structure-free Active motif based Representation) strategy, constructing numerous active motifs by enumerating elemental combinations.[73] Although the process generated tens of thousands of candidate materials, these candidates are not a pre-existing dataset but are computationally generated. This aligns with the generative approach, as it actively explores new possibilities within the chemical space rather than selecting from a static candidate pool. Gomez et al.[74] leveraged in-house software based on the RDKit package to generate a virtual chemical library exceeding 1.6 million molecules by combining 110 donors, 105 acceptors, and 7 bridging groups. Molecules in the library underwent initial screening via quantum chemical calculations. The TD-DFT simulation results of screened molecules served as data to train a deep neural network empirical model for predicting the kTADF values of new molecules. Molecules ranked highest by the neural network predictions are then prioritized for further quantum chemical calculations and experimental validation, embodying the characteristic of AL where samples are evaluated and selected based on the model.

Notably, an important subclass of GANs—cycle-consistent architectures—enforces bidirectional consistency by learning paired forward and inverse mappings and applying a cycle consistency loss.[75] This stabilizes training in the absence of paired examples and produces models that can be used for both design-to-property and property-to-design queries, which is particularly valuable for inverse-design problems in materials and devices where paired data are scarce. Cycle-consistent variants therefore complement single-direction generative pipelines: standard GANs excel at producing highly diverse candidates, whereas cycle-consistent GANs more readily learn physically meaningful, invertible correspondences that can be embedded into closed-loop discovery workflows.[76]

Large language models-based generative active learning

Large language models (LLMs) introduce a new, pragmatic axis for generative AL in materials science by turning unstructured textual knowledge and structured databases into generative proposals, priors, and experiment strategies.[77-82] Rather than replacing established surrogate models and physics-based filters, LLMs are best understood as versatile, language-centric agents that (1) extract and formalize domain priors from literature and lab records, (2) propose candidate compositions, molecules or synthesis recipes in human-readable and machine-parsable forms, and (3) suggest next-step experimental strategies that can be scored and integrated into an existing AL loop. When carefully constrained and validated, LLMs make it possible to bootstrap discovery in knowledge-rich but label-poor settings and to accelerate the "generate →screen → validate" cycle typical of modern materials pipelines.

A practical LLM-augmented workflow layers the LLM at the generation stage and then subjects its outputs to the classical AL pipeline. In this pattern, the LLM serves as a high-recall generator that expands the search space beyond enumerated libraries, while physics and surrogate models enforce feasibility and efficiency. A concrete instance of this approach is

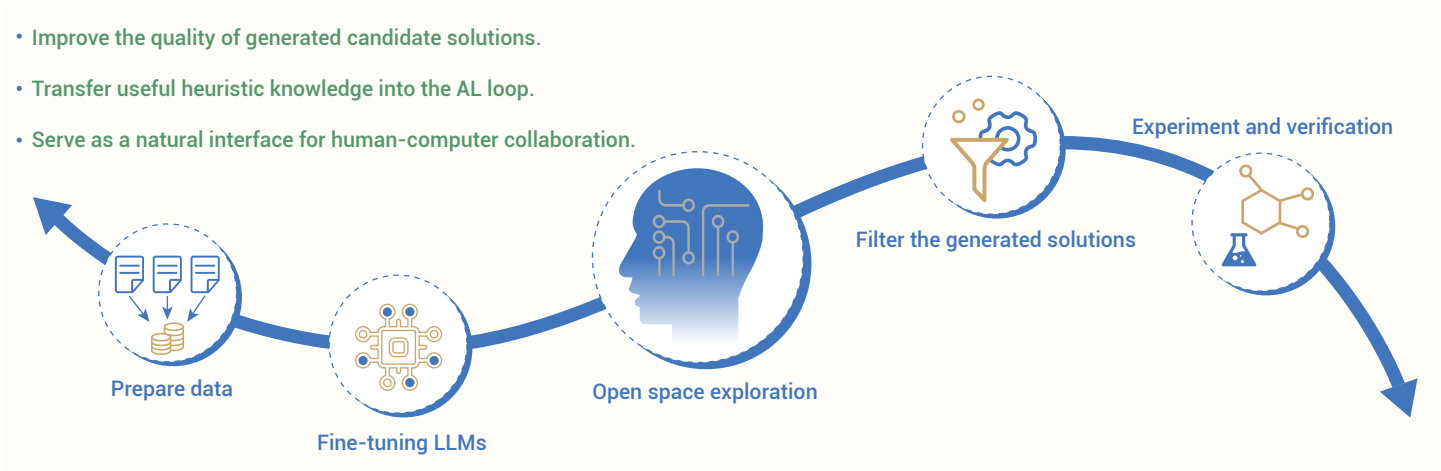

Figure 2. Schematic of the open-space exploration process for generative materials design using LLMs.

Table 2. Mapping of Generative Model Types to primary materials task typesand representative references. Entries indicate illustrative task usages observed in the literature.

Generative Model Type	Primary material task types	Representative references
Evolutionary Algorithm-Based Generative AL	Combinatorial/discrete design exploration; multi-objective optimization	Structure design and discovery:[64, 65]
VAE-Based Generative AL	Conditional/target-oriented generation; latent-space optimization; virtual library expansion	Composition screening:[22, 67, 68, 69, 70]
GAN-Based Generative AL	High-diversity candidate generation; exploratory discovery;few-shot target search	Composition screening:[70-73] Structure design and discovery:[74]
LLMs-Based AL	Textual knowledge extraction;generative proposal of compositions/structures/recipes; human-machine collaboration	Structure design and discovery:[78] Process condition optimization / synthesis optimization:[77,79,83]

described by Zhang et al.[83], where an LLM-based module generates virtual yield estimates and candidate reactions that are subsequently fed into an AL optimization loop to prioritize experiments; the study demonstrates that textual priors encoded by an LLM can act as valuable pseudo-data to overcome cold-start limitations in organic synthesis planning.

LLM integration brings three main advantages. First, LLMs can convert dispersed human knowledge into structured constraints, improving the quality of generated candidates and reducing the fraction of infeasible proposals. Second, in domains where experimental labels are scarce but textual documentation is abundant, task-specific fine-tuning of an LLM can transfer useful heuristics into the AL loop, lowering experimental cost per discovery. Third, LLMs are natural interfaces for human–machine collaboration: they can generate rationale and provenance that makes model suggestions easier for scientists to audit and act upon.

Building upon the role of LLMs as versatile, language-centric agents that can extract domain knowledge, propose candidates, and suggest experimental strategies, the integration of more general autonomous agents into AL workflows represents a promising frontier. Looking ahead, embedding autonomous agents within these closed-loop frameworks offers an additional avenue for acceleration.[84,85] In multi-agent settings, distributed intelligent agents can actively request new data, negotiate trade-offs between competing objectives, and collaboratively explore complex design spaces. Such agent-based paradigms extend the principles of active learning and may provide a scalable route toward more adaptive and resilient materials discovery systems.

FUSION STRATEGIES

Current implementations of classical Bayesian Optimization for sequential learning in materials research commonly exhibit two limitations: (1) the absence of direct mechanisms to incorporate information from prior related studies, and (2) inflexibility in adapting to researchers' qualitative feedback within the iterative loop.[86] On the one hand, machine learning models sometimes require substantial data to learn relationships already evident to domain experts. On the other hand, these shortcomings may deter materials scientists from adopting ML tools, as their domain knowledge remains underutilized in classical Bayesian Optimization iterations.

To further reduce dependency on large datasets and accelerate convergence, researchers increasingly integrate domain knowledge to constrain model kernel functions or acquisition functions. While significant progress has been made in materials science through small-data mining for identifying high-performance materials, substantial challenges persist. Notably, for many research topics, the physicochemical relationships between input features and target properties remain unclear, making it difficult to impose domain knowledge constraints within AL frameworks. Consequently, key questions emerge: how to elucidate the influence relationships between input features and performance using small datasets, and how to couple data-driven mathematical relationships between features and performance into an AL framework. Addressing these issues will facilitate the development of more efficient, cost-effective, robust, and widely applicable directionally constrained machine learning frameworks for high-performance materials exploration.

Prior knowledge-driven Initial dataset construction

AL in materials discovery often encounters the "cold start" problem, where a lack of sufficient labeled data in the initial stages results in low exploration efficiency. Traditional random sampling methods typically converge slowly and are prone to sampling low-value or non-physical regions, failing to effectively guide subsequent iterations. Incorporating domain-specific prior knowledge—such as empirical rules, thermodynamic constraints, or structural features—can significantly alleviate this issue by precisely anchoring initial sampling points or constraining the search space, thereby improving the quality of the starting dataset. For example, candidate samples can be filtered based on physical or chemical rules—such as requirements for material stability, stoichiometric constraints, or reaction condition limitations—enabling the construction of a more representative and credible initial dataset. This provides a robust foundation for iterative optimization in AL.

For instance, in ultra-high-temperature ceramic design, researchers pre-screened candidate compositions satisfying "eutectic point temperature >

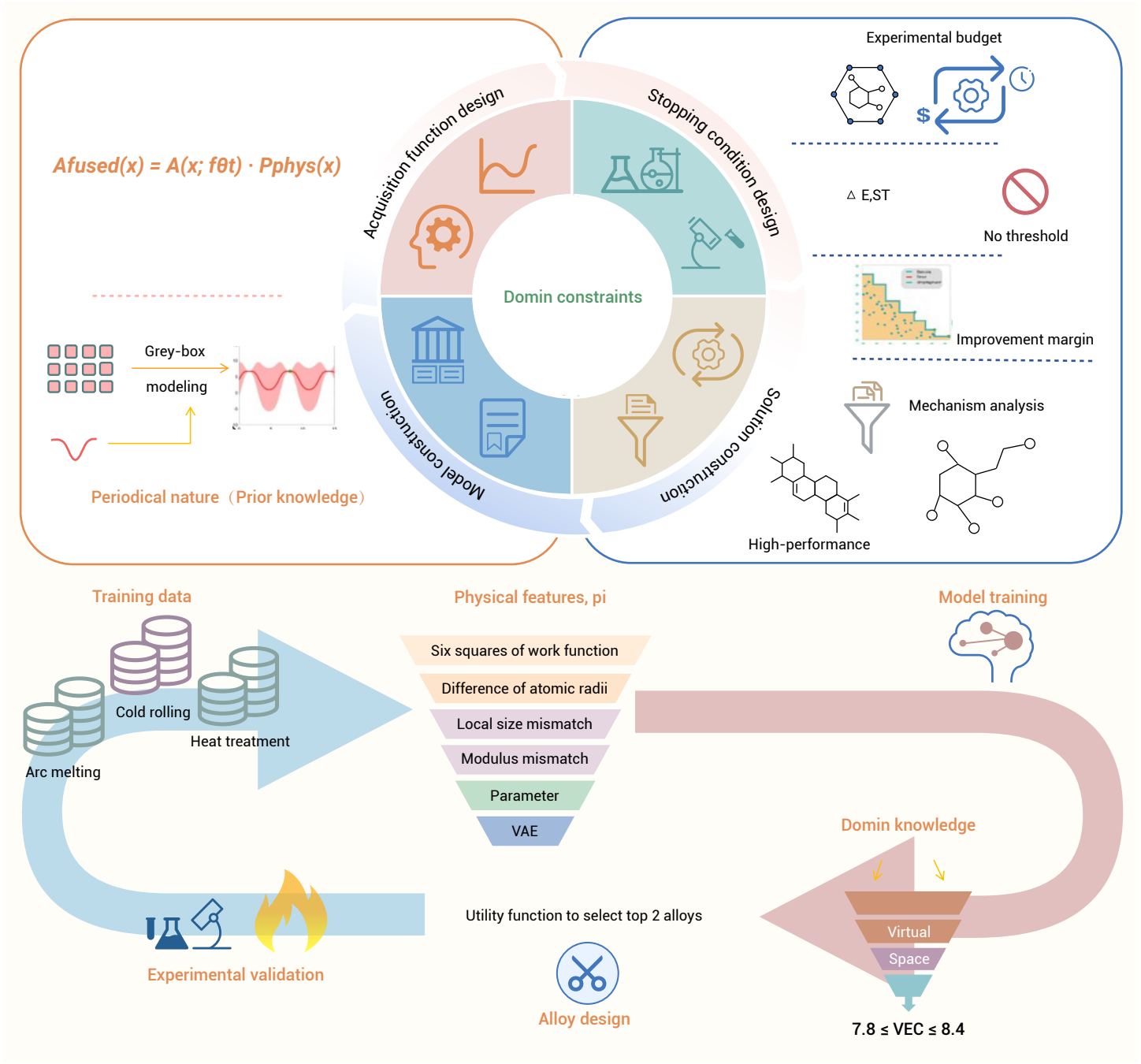

Figure 3. The domain knowledge–informed AL loop A concrete case study—a domain knowledge–based machine learning model for the discovery of ultra-strong and ductile FeNiCoAlTa high-entropy alloys (HEAs). (Reproduced with permission.[23] Copyright 2025, Nature Publishing Group.)

3000 K" and "thermal expansion coefficient mismatch rate < 5%" based on ablation mechanism analysis (oxidation layer kinetic models) and known high-melting-point component databases (e.g., HfB-ZrC systems).[71] This strategy constructed a seed set containing only 30 samples, enabling the discovery of breakthrough materials with linear ablation rates below 10 m/s in the first experimental round. In organic synthesis, the Chemma model proposed by Zhang et al.[83] leverages pre-trained chemical knowledge to generate virtual yield predictions across the reaction space, providing initial "pseudo-data" for subsequent AL workflows and mitigating the blindness of starting from scratch. Such knowledge-guided approaches essentially transform domain cognition into spatial filters, establishing high-quality starting points for subsequent iterations.

Prior knowledge-embedded model construction and training

The rationality of surrogate models directly influences the decision quality of AL. Incorporating prior scientific knowledge into the design framework reduces their dependency on statistical information. As information within the box becomes partially observable, black-box optimization transitions into gray-box optimization. Successful studies on gray-box modeling for optimizing chemical processes and describing biological phenomena are well-documented.[87-91] In materials science, although studied systems may be too complex for explicit simulation, it remains feasible to establish reliable assumptions about underlying physical or chemical principles that bind isolated queries to specific design spaces. Encoding material rules into models significantly enhances generalization capabilities under small-sample conditions.

Some of the present authors have already demonstrated the utility of augmenting GP models by physics-informed prior means in the context of accelerated alloy modeling and discovery.[92] In this context, Khatamsaz et al.[93] developed a physics-informed Bayesian optimization framework with parametric constraints, demonstrating improved efficiency in materials design, particularly for NiTi shape memory alloys. By embedding physical knowledge

into GP kernels, their approach achieves faster convergence to optimal solutions, explores broader design spaces, and reduces data dependency compared to traditional black-box optimization methods. Similarly, Moon et al.[24] enhanced model interpretability by hard-coding structure-property correlation rules derived from XRD data. Experimental validation showed that correctly ordered XRD features increased model accuracy from 0.75 to 0.882. Beyond the aforementioned examples, Physics-Informed Neural Networks (PINNs) embed physical laws directly into their architecture or loss functions, thereby enabling physically consistent predictions even in data-sparse regions and significantly enhancing the model's generalization capability and interpretability.[94,95] Within an active learning framework, PINNs can serve as powerful, physics-constrained surrogate models.

In addition to integrating physical knowledge into surrogate models, a complementary strategy is to embed it directly into the architecture and training objectives of generative models themselves. Such "knowledge-embedded generative models" aim to ensure the rationality of generated candidate materials from the outset, thereby reducing reliance on cumbersome post-processing filters. For instance, models such as G-SchNet96 progressively construct 3D molecular structures by utilizing auxiliary tokens to guide the generation process, thereby enhancing the quality of the generated outcomes; whereas the Crystal Diffusion Variational Autoencoder (CDVAE)[97] leverages the symmetry invariance of materials to generate crystal structures that are more feasible in terms of energy. Furthermore, thermodynamically-inspired diffusion models offer another physics-aware generative pathway.[98] This class of models inherently biases the sampling toward physically plausible states when generating material microstructures, molecular configurations, and others, enabling effective exploration within the latent space to propose novel candidate materials that possess target properties while conforming to physical laws. By internalizing domain knowledge into the generative mechanism, these models can navigate the vast and complex materials design space more efficiently, directly proposing candidates that are both novel and highly feasible. Employing similar models in active learning will significantly enhance the overall efficiency of the generative AL cycle.

Knowledge-enhanced acquisition function design

As the decision engine of AL, the integration of prior knowledge with acquisition functions critically determines exploration effectiveness.[99] Current mainstream methods achieve knowledge guidance by modifying acquisition function expressions.[100] To enable rapid optimization, Sun et al.[101] incorporated phase stability constraints from DFT calculations as probabilistic constraints during experimental acceleration of perovskite optimization, avoiding compositions prone to phase segregation. Liu et al.[102] employed dual probabilistic constraints to quantify "safety boundaries" for thin-film formation quality and device performance. By multiplying these probabilistic constraints with the original UCB acquisition function based on model-predicted probabilities, they achieved "soft filtering" that ensures experimental success rates without excessively suppressing exploration of unknown high-performance regions. Rupnow et al.[10] constructed a candidate set of experimental conditions within a predefined parameter space comprising seven variables. To accommodate the high-throughput, parallelized experimental environment, the authors designed a cyclic, multi-mode acquisition function. This design was implemented to address the issue of the robotic system repeatedly requesting identical experimental conditions in a parallel setting. One of the acquisition strategies—the space-filling point—operates independently of the surrogate model's quality. It is a distance-based, robust exploration strategy that ensures continued exploration even during early stages with inaccurate model predictions or in unexplored regions of the parameter space. Kusne et al. used a graph-based method to estimate per-sample phase probabilities$P(x)$. They combine $P(x)$with a performance surrogate $F(x)$ into an acquisition function g(F, P) that trades-off minimizing phase uncertainty and a GP-UCB–style performance/uncertainty objective, thereby prioritizing phase boundaries and high-uncertainty regions to accelerate materials discovery.[103] In the polarization-dynamics sampling task on $PbTiO_3$ films, Vasudevan et al. retained and tuned classic acquisition functions such as EI/PI/CB, added a short-term memory term to avoid repeated sampling at adjacent locations, and incorporated high-resolution PFM images as priors—either raw pixels or CNN-extracted features—into the surrogate and acquisition pipeline, enabling more efficient localization of high electromechanical-response regions while greatly reducing sampling points and measurement time.[54]

When optimization objectives require approaching specific target values rather than extremum points, acquisition functions can be fundamentally redesigned. Recent work introduced the Expected Absolute Improvement (EAI) function for the special case where linear ablation rate (LR) must approach zero.[71] This function quantifies the "proximity to zero" concept using absolute distance as the optimization target, explicitly accounting for bidirectional deviations. Through symbolic regression, the researchers derived weight expressions quantifying feature impacts on LR and embedded them into the EAI acquisition function, enabling explicit representation of differential feature contributions toward target performance. Tian et al. also designed a target-oriented Bayesian optimization method, t-EGO, to rapidly identify promising candidates with given target properties. This method incorporates the absolute difference between the predicted property value and the target-specific value into the EI criterion, allowing candidate properties to approach the target value from either above or below. As a result, it can potentially reduce the number of iterations required to identify target-specific properties.[104]

These studies identified optimal solutions with exceptionally low pool sampling rates, highlighting the significant advantage of prior-knowledge-integrated AL in pool-based optimization scenarios. The fused acquisition function can be expressed as:

$$A_{\text{fused}}(x) = A(x; f_{\theta_t}) \cdot P_{\text{phys}}(x) \tag{5}$$

In Eq. (5), $A_{\text{fused}}(x)$ denotes the fused acquisition score used for selection when domain knowledge is available; $P_{\text{phys}}(x)$ denotes a physics- or domain-derived feasibility score for candidate x, typically normalized to [0, 1] (it may also be a hard mask taking values in {0, 1}); the term $A(x; f_{\theta_t})$ is the model-driven acquisition as above. Alternative fusion schemes include a weighted sum $"\alpha A + (1-"\alpha) P_{\text{phys}}$, constrained optimization, or probabilistic filtering depending on the application. A practical $P_{\text{phys}}(x)$ should be a calibrated probability that a candidate x is physically plausible and experimentally synthesizable. Common, complementary sources are:

Analytic rules / masks. Fast, deterministic filters based on stoichiometry, valence/charge balance, simple thermodynamic bounds or known infeasible regions. Use these as hard masks or to set $P_{\text{phys}}(x) = 0$ for obviously impossible candidates.

Learned classifiers. Train a probabilistic classifier on labeled feasible/infeasible examples derived from DFT or experimental records; calibrate outputs so the predicted probability is meaningful for decision-making.

Fast physics proxies / multi-fidelity estimators. Use inexpensive approximate models to produce a continuous feasibility score. Combine multi-fidelity sources using hierarchical or Bayesian fusion (cheap proxies guide screening; expensive oracles validate a small set).

Knowledge-guided stopping condition design

Determining when to stop AL remains a critical and difficult decision, especially in resource-constrained environments like materials discovery.[105] Recent work has introduced knowledge-guided stopping criteria that bring domain knowledge, model stability, and task costs into the stopping decision. One widely used approach monitors how consistent the model's predictions are on an unlabeled pool across successive iterations and stops when this consistency reaches a predefined level.[106] Another approach estimates the expected change in the model or its generalization error that would result from labeling the remaining samples and stops when that change is below a theoretical or statistical threshold.[107] Recent research emphasizes cost-aware stopping criteria that explicitly balance accuracy gains against annotation expenses. Pullar et al. introduce a comprehensive cost framework where the optimal stopping point minimizes the following combined cost:[108]

$$C(a, j, l, m, n) = (1-a)mn + jl$$

where a represents accuracy, j the number of labels used, l the cost per label, m the cost per misclassification, and n the expected number of predictions over the model's lifetime. Their large-scale comparison of 13 stopping criteria

across nine datasets reveals that different criteria excel under varying cost conditions: Stabilizing Predictions performs optimally under balanced cost scenarios, while Classification Change dominates when labels are relatively cheap compared to misclassification costs. In materials discovery applications, this translates to setting stopping conditions that reflect both experimental budgets and project objectives.

Furthermore, for applied screening and streaming tasks, conservative statistical procedures have been developed that are simple to implement, reduce the risk of missing rare candidates, and still yield substantial resource savings.[109,110]

DISCUSSION

The effective implementation of active learning requires prudent choices at two levels: the learning paradigm and the surrogate model. The decision between a pool-based and a generative paradigm is primarily dictated by the nature of the search space. A pool-based approach is the apt choice when the goal is to efficiently screen a fixed, finite candidate library. In contrast, a generative paradigm becomes essential for de novo discovery, where the goal is to explore an open-ended design space that cannot be pre-enumerated. Concurrently, the selection of a surrogate model should be guided by the data modality and the need for uncertainty quantification. Simpler, well-calibrated models (e.g., Gaussian Processes) are highly sample-efficient for problems with structured, low-dimensional features, while more complex architectures (e.g., graph or deep neural networks) are necessary for handling high-dimensional or unstructured data (e.g., crystal graphs, spectra), albeit with a higher data cost for reliable uncertainty estimation.

Building on these methodological foundations, AL has already demonstrated considerable promise in materials discovery, with encouraging progress reported across diverse applications. Yet, translating these successes into broader practice remains difficult, as the inherent complexity of material systems—characterized by intricate couplings among composition, structure, processing parameters, and functional properties—continues to pose significant challenges. This diversity gives rise to a number of general obstacles:

Scarcity of high-quality datasets and benchmarks

Experimental and high-fidelity computational data in materials science are often costly and time-consuming to acquire, leading to severely limited sample sizes available for training. Furthermore, variability in experimental conditions, instrument sensitivity, and batch effects frequently introduce distributional biases, which undermine the generalization capability and predictive reliability of models. Future efforts should prioritize the development of standardized, open-data platforms and benchmark suites that encompass diverse material classes and properties. Community-wide initiatives for data sharing, along with advances in automated and reproducible data capture, will help mitigate data scarcity and bias. Additionally, self-supervised and transfer learning techniques offer promising pathways to leverage unlabeled data and pre-trained models, reducing dependence on large curated datasets.

Curse of dimensionality in high-dimensional feature space

Material properties are influenced by a multitude of factors including chemical composition, structure, and synthesis conditions. These contribute to an exceedingly high-dimensional design space within which high-performing materials are often sparse. In practice, materials problems often feature specific structural complexities such as hierarchical multiscale organization, strong symmetry/periodicity constraints, and localized discrete features that induce locally correlated but globally sparse manifolds and modal mismatches across spectra, images and simulation outputs. This sparsity undermines sampling efficiency for conventional AL and slows convergence. Future research should focus on developing dimension-reduction techniques and feature learning methods tailored to materials science, such as physics-informed embeddings and symmetry-aware representations.[111-114] In particular, methods that can learn from unpaired or unmatched datasets have shown promise for translating between simulation/proxy outputs and experimental measurements, thereby increasing effective supervision in sparse materials design spaces.[115] Incorporating hierarchical and multi-fidelity modeling approaches can also help navigate complex spaces more efficiently by leveraging cheaper computational or experimental proxies.[116]

Incorporation of physicochemical constraints

The processes of material generation and selection must adhere to fundamental physical and chemical principles—such as thermodynamic stability, synthesizability, and stoichiometric constraints. Without explicit mechanisms to incorporate such domain knowledge, AL algorithms may propose candidate materials that are either infeasible to synthesize or physically implausible, thereby reducing the practicality of experimental validation. A key future direction is the deeper integration of physics-based models and rule-based filters into the AL loop, for instance through hybrid gray-box modeling or constraint-aware acquisition functions. Developing generative models that inherently respect thermodynamic and compositional rules will also be critical to ensure that proposed candidates are both novel and feasible.

Data bias, interpretability and trust in generative active learning

Generative AL can substantially enlarge chemical and materials search spaces, but its practical utility hinges on addressing key failure modes: unconstrained generators often propose synthetically infeasible candidates; training-set bias and cold starts skew outputs; and limited provenance and poorly calibrated uncertainty hinder expert triage and waste costly high-fidelity evaluations. We therefore recommend an integrated validation and engineering strategy: embed domain knowledge as hard or probabilistic constraints during generation; apply multi-fidelity filtering that moves candidates from fast heuristics to surrogate models and reserves DFT/experiment for only the highest-confidence hits; mitigate bias with data augmentation, transfer learning and curated seed sets; and report provenance together with calibrated uncertainties and standardized metrics, including negative results to strengthen community benchmarks.

Automation and closed-loop integration

While coupling AL with automated experimental platforms holds great potential for accelerating materials development, the implementation of end-to-end closed-loop workflows presents substantial engineering hurdles.[117] The specific challenges are that there's no unified data format or logging standard; data transfer must be fast enough to support real-time decision making; models need to learn on the fly and be able to update or roll back when problems are detected; and there must be common interfaces, standardized calibration procedures, and safety protections to seamlessly connect diverse robots and instruments. Future work should emphasize the development of modular, interoperable software and hardware standards to facilitate seamless integration between simulation, machine learning, and robotic experimentation.[118] Advances in real-time data assimilation and adaptive control algorithms will further enhance the robustness and autonomy of self-driving laboratories.

Despite these challenges, continued advances in artificial intelligence, multiscale modeling, and automated experimentation are expected to enable more efficient and reliable search and design strategies within complex material systems. Further application of AL will likely play a pivotal role in driving innovation in critical fields such as energy storage, catalysis, and structural materials.

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AUTHOR CONTRIBUTIONS

All authors contributed to the manuscript and approved the final version.

DECLARATION OF INTERESTS

Yi Du is an Academic Editor of The Innovation Informatics and was blinded from reviewing or making final decisions on the manuscript. Peer review was handled independently of this member and their research group. The other authors declare no conflicts of interest.

DATA AND CODE AVAILABILITY

The data that support the findings of this study are openly available at https://github.com/kg4sci/awsome-AL.

SUPPLEMENTAL INFORMATION

It can be found online at https://doi.org/10.59717/j.xinn-inform.2025.100013