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Active Learning-Driven Bayesian Optimization of Catalytic Nanoparticles for CO_2 Reduction

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Abstract

The escalating global challenge of carbon dioxide (CO_2) emissions necessitates innovative approaches to mitigate climate change through efficient catalytic conversion. This conceptual manuscript proposes a novel theoretical framework that integrates active learning with Bayesian optimization to enhance the design of catalytic nanoparticles for CO_2 reduction. Drawing on principles from machine learning and materials science, the framework addresses the complexities of high-dimensional parameter spaces in nanoparticle synthesis, such as size, shape, composition, and surface facets, which influence catalytic performance. By leveraging active learning to intelligently select informative data points and Bayesian optimization to refine surrogate models iteratively, the approach theoretically accelerates the identification of optimal nanoparticle configurations without empirical validation. The framework emphasizes uncertainty quantification and adaptive sampling to efficiently navigate the vast design space. This synthesis of concepts from recent literature highlights gaps in traditional optimization methods and posits that the proposed integration could conceptually reduce exploration costs while enhancing selectivity and activity in CO_2 reduction processes. The manuscript outlines theoretical underpinnings, a proposed framework, and implications for applied artificial intelligence in materials science, fostering future conceptual advancements in sustainable catalysis.

Keywords Machine learning, Active learning, Bayesian optimization, Materials design, Catalytic nanoparticles, CO_2 reduction

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Introduction

CO_2 reduction as a central challenge in sustainable materials science

The accelerating pace of climate change has intensified global efforts to reduce carbon dioxide (CO_2) emissions, positioning CO_2 mitigation as a central challenge in contemporary materials science and catalysis research. Anthropogenic activities, particularly those associated with fossil fuel consumption and industrial processes, have led to a persistent increase in atmospheric CO_2 concentrations. In response, significant attention has been directed toward developing technologies that not only capture CO_2 but also convert it into value-added fuels and chemicals, thereby closing the carbon cycle and contributing to long-term carbon neutrality [1, 2].

Among the various strategies proposed, catalytic CO_2 reduction stands out for its potential to convert a greenhouse gas into economically valuable products. In this context, catalytic nanoparticles—especially those composed of metals such as copper, silver, and their alloys—have emerged as promising candidates. Their appeal lies in their highly tunable

physicochemical properties, which can strongly influence reaction pathways, product selectivity, and overall conversion efficiency [3, 4]. By tailoring parameters such as particle size, shape, elemental composition, and surface structure, researchers can, in principle, steer CO_2 reduction reactions toward desired products.

However, despite this promise, the rational design of catalytic nanoparticles remains an open and challenging problem. A single parameter rarely governs a catalyst's performance; instead, it emerges from complex, often nonlinear interactions among multiple design variables. Factors such as particle morphology, alloying effects, surface defects, and functionalization can interact in subtle ways, making it challenging to predict catalytic behavior a priori [5, 6].

Limitations of conventional catalyst design paradigms

Historically, catalyst development has relied heavily on trial-and-error experimentation and heuristic rules grounded in fundamental physicochemical principles. While these approaches have led to significant breakthroughs, they are inherently limited when applied to high-dimensional design spaces typical of nanoparticle catalysts [7]. For example, the Sabatier principle has long provided a conceptual basis for understanding activity trends through volcano plots, offering qualitative insights into optimal binding energies [8]. Nevertheless, this framework struggles to deliver quantitative predictions for complex, multicomponent systems, particularly when competing reaction pathways are involved.

The challenge is further compounded by the intrinsic heterogeneity of catalytic surfaces. Active sites on nanoparticles are not uniform and may evolve dynamically under operating conditions, leading to time-dependent changes in catalytic performance [9]. In CO_2 reduction reactions—whether electrochemical or photochemical—this complexity is further amplified by the need for high selectivity toward specific products, such as methane, ethylene, or formic acid. Achieving such selectivity while maintaining high activity and stability introduces additional constraints that conventional design strategies are ill-equipped to address [10, 11].

As a result, there is growing recognition that traditional methods alone are insufficient for navigating the vast combinatorial space of catalytic nanoparticle design. The multidimensional nature of nanoparticle design and the competing constraints associated with size, morphology, composition, and operating environment are synthesized in **Table 1**.

Table 1. Key nanoparticle design parameters and associated challenges in CO_2 reduction catalysis

Parameter	Examples	Optimization challenge
Particle size	2–50 nm	Quantum vs stability trade-off
Shape	Cubes, spheres, rods	Facet-dependent selectivity
Composition	Cu, Ag, alloys	Scaling relations
Surface structure	Defects, dopants	Site heterogeneity
Reaction environment	Electrolyte, pH	Noise and variability

Emergence of artificial intelligence in catalyst optimization

Recent advances in artificial intelligence (AI) and machine learning (ML) have opened new pathways for addressing the complexity inherent in materials design. By enabling data-driven exploration of large and multidimensional parameter spaces, AI-based methods offer a compelling alternative to purely intuition-driven approaches [12, 13]. Within this landscape, Bayesian optimization (BO) has gained prominence as an efficient strategy for optimizing expensive-to-evaluate objective functions, such as catalytic activity or product selectivity [14, 15].

BO operates by constructing a probabilistic surrogate model—most commonly a Gaussian process—that approximates the relationship between input parameters and the target property. An acquisition function then guides the selection of new candidate designs by balancing exploration of uncertain regions with exploitation of known high-performing areas [16]. This sequential and adaptive nature makes BO particularly attractive for materials science applications, where experimental evaluations are often costly and time-consuming. Conceptual and early practical applications of BO in materials discovery have demonstrated its potential to significantly reduce the number of iterations needed to identify optimal solutions [17].

Role of active learning and its synergy with Bayesian optimization

Complementary to Bayesian optimization, active learning (AL) focuses on strategically acquiring new data points to maximize model improvement. Rather than relying on randomly sampled data, AL enables the learner to query the most informative or uncertain instances, thereby accelerating learning efficiency [18, 19]. In the context of materials design, AL can prioritize regions of the parameter space where predictions are uncertain or where diversity is lacking, thereby accelerating convergence toward optimal materials [20].

The integration of AL with BO is particularly compelling for catalytic systems, where the synthesis and characterization of nanoparticles demand significant resources [21]. By embedding AL principles into BO's acquisition strategy, it becomes possible to improve robustness under conditions of sparse, noisy, or heterogeneous data—conditions common in catalysis research [22]. This synergy suggests a pathway toward more efficient and informed optimization processes.

Gaps in existing AI-driven frameworks for CO_2 catalysis

Despite the growing body of work applying ML techniques to catalysis, notable gaps remain. Many existing optimization frameworks treat catalyst design as a black-box problem, overlooking the physicochemical constraints that are specific to CO_2 reduction. Parameters such as overpotential, reaction kinetics, and Faradaic efficiency are often not explicitly incorporated into optimization schemes, limiting their practical relevance [23, 24].

Furthermore, while ML models have been successfully employed to predict catalytic properties based on descriptors such as adsorption energies or d-band centers, these models are typically static. They rarely incorporate iterative or adaptive learning mechanisms that evolve as new data become available [25]. Consequently, there is a lack of conceptual frameworks that unify predictive modeling with adaptive decision-making in a manner tailored to catalytic nanoparticle systems.

Conceptual framework and contribution of this work

To address this gap, the present manuscript proposes a novel conceptual framework that explicitly embeds active learning within Bayesian optimization for the design of catalytic nanoparticles aimed at CO_2 reduction. The central premise is that dynamically adjusting the acquisition function using AL principles—such as query-by-committee or expected model change—can lead to faster convergence and improved handling of complex, multimodal objective landscapes [26].

This framework builds on recent theoretical advances that emphasize the importance of probabilistic modeling in capturing both epistemic and aleatoric uncertainties in materials discovery [27]. Importantly, it moves beyond generic optimization strategies by incorporating domain-specific knowledge, including known scaling relations in electrocatalysis, to guide the search process more effectively [28].

By focusing on a conceptual and theoretical synthesis rather than empirical validation, this work contributes to the broader discourse on applied AI in materials science. It illustrates how carefully designed integrations of AI methodologies can foster innovation in catalyst design, even in the absence of large experimental datasets. The subsequent sections elaborate on the theoretical foundations, review relevant literature, and detail the proposed framework, highlighting its

broader implications for sustainable materials design. Ultimately, this study underscores the transformative potential of AI-driven approaches in advancing catalytic technologies for environmental remediation and CO_2 utilization [29, 30].

Theoretical Background and Literature Synthesis

Bayesian optimization in catalysis and materials design

Bayesian optimization (BO) has emerged as a foundational methodology for addressing complex optimization problems in scientific domains where evaluations are computationally expensive, experimentally demanding, or both. This characteristic makes BO particularly well suited to catalysis and materials design, where each experiment or simulation may involve significant time, cost, and uncertainty [1, 14]. Unlike conventional optimization approaches that rely on exhaustive search or gradient information, BO adopts a probabilistic perspective, enabling informed decision-making under uncertainty.

At its core, BO begins with a prior belief over the space of possible objective functions. As new observations are obtained, this prior is updated using Bayes' theorem to form a posterior distribution that reflects both prior knowledge and observed data [15]. This probabilistic surrogate model—most commonly instantiated as a Gaussian process—captures not only the expected value of the objective function but also the associated uncertainty across the parameter space. Such uncertainty-aware modeling is particularly valuable in catalysis, where performance metrics are often noisy and influenced by uncontrollable experimental factors.

The posterior distribution generated by the surrogate model guides the optimization process through an acquisition function. Common acquisition strategies, such as expected improvement and upper confidence bound, explicitly balance exploration of poorly understood regions with exploitation of areas predicted to yield high performance [16, 31]. This balance is critical in catalytic systems, where overemphasis on exploitation may lead to premature convergence, while excessive exploration can result in inefficient use of limited experimental resources.

Within the catalysis literature, BO has been increasingly discussed as a conceptual accelerator for discovering optimal reaction conditions, catalyst compositions, and structural motifs [3, 32]. Its relevance becomes particularly evident in systems characterized by high dimensionality, such as alloy catalysts or nanostructured materials. For instance, theoretical discussions have emphasized the suitability of BO for navigating the immense compositional space of high-entropy alloys, where the number of possible elemental combinations renders brute-force exploration infeasible [2, 5]. By modeling correlations between composition and performance, BO enables targeted exploration of promising regions without requiring exhaustive sampling.

Another strength of BO lies in its inherent ability to account for unavoidable noise in catalytic measurements such as turnover frequency, selectivity, and stability [4, 33]. Rather than treating variability as a nuisance, BO explicitly incorporates uncertainty into the modeling process, enabling optimization even when observations are imperfect. Recent literature syntheses highlight that this capability is central to BO's efficiency, as it allows learning across correlated parameters and mitigates the so-called curse of dimensionality that plagues multicomponent catalytic systems [7, 34]. These conceptual differences in how optimization strategies handle uncertainty, adaptivity, and domain knowledge motivate the comparative overview provided in **Table 2**.

Table 2. Conceptual comparison of optimization strategies in catalytic materials design

Method	Handles uncertainty	Adaptive sampling	Domain priors	Suitable for CO_2 catalysis
Trial-and-error	✗	✗	✓	Limited
Standard ML	△	✗	△	Moderate

Bayesian optimization	✓	△	✗	Good
ALDBO (This work)	✓✓	✓✓	✓✓	High

Active learning strategies in machine learning for materials

Active learning (AL) represents a complementary paradigm in machine learning that focuses on how data are acquired rather than how models are trained. Instead of passively learning from a fixed dataset, AL frameworks empower the learner to iteratively select the most informative data points for labeling or evaluation [18, 19]. This adaptive strategy is particularly appealing in materials science, where data generation is often expensive and slow.

In AL, query strategies are designed to maximize information gain with each new data point. Common approaches include uncertainty sampling, which prioritizes instances with high predictive variance, and diversity-based sampling, which aims to ensure broad coverage of the feature space [20, 35]. By selectively querying data that are expected to improve model performance the most, AL aims to reduce the total number of required observations while maintaining predictive accuracy. This shift from passive to adaptive learning has been theoretically shown to lower data requirements for building robust models [21].

Within the materials science domain, AL has been increasingly framed as an efficient tool for exploring complex property landscapes. Conceptual studies have proposed AL-driven workflows for tasks such as force field development, electronic property prediction, and structural optimization [12]. In the context of heterogeneous catalysis, AL has been proposed as a mechanism for refining interatomic potentials by enabling on-the-fly identification of configurations poorly described by existing models [13]. Such approaches are particularly valuable for capturing rare or extreme events that may disproportionately influence catalytic performance.

A notable advantage of AL lies in its explicit treatment of uncertainty. By integrating AL with surrogate models, researchers can systematically address epistemic uncertainty arising from limited or biased datasets, as well as aleatoric uncertainty associated with stochastic experimental processes [22]. Literature syntheses during this period emphasize that AL's adaptability to domain-specific constraints is a key reason for its growing relevance in materials design. This adaptability makes AL especially suitable for nanoparticle optimization problems, where synthesis variability, surface heterogeneity, and measurement noise are significant and unavoidable [23].

Catalytic nanoparticles for CO_2 reduction: key conceptual challenges

Catalytic nanoparticles for CO_2 reduction embody a confluence of surface chemistry, electrokinetics, and materials engineering [6, 10]. Theoretically, their efficacy hinges on controlling the adsorption energies of intermediates such as *CO or *CHO, which are governed by scaling relations that link binding strengths across species [8, 11]. Nanoparticles offer advantages over bulk materials due to quantum size effects and increased surface-to-volume ratios, which can modulate electronic structures and expose specific facets [9].

However, conceptual challenges include the trade-offs between activity, selectivity, and stability [24]. For CO_2 reduction, multistep electron-proton transfers necessitate precise tuning to favor desired pathways, such as the eight-electron reduction to methane [25]. Literature reviews have synthesized that alloying or doping nanoparticles can break linear scaling relations, theoretically enhancing performance by creating bifunctional sites [26]. Yet, the high dimensionality of design parameters—encompassing size distributions, shapes (e.g., cubes vs. spheres), and compositions—poses optimization hurdles that traditional methods cannot efficiently surmount [27].

Integration of AI techniques in catalytic design

The application of AI techniques such as BO and AL to catalytic design marks a paradigm shift toward autonomous materials discovery [17, 28]. Conceptual models have illustrated how BO can be augmented with AL to create closed-loop optimization cycles, where feedback from virtual evaluations refines the search [29]. In CO_2 catalysis, this integration

theoretically enables the exploration of nanoparticle ensembles, accounting for ensemble effects in which particle interactions influence overall performance [30].

Recent theoretical perspectives emphasize the need for interpretable AI, where models not only predict but also provide insights into underlying mechanisms [32]. For instance, Gaussian process surrogates in BO offer variance estimates that AL can exploit for query selection, fostering a synergistic loop [33]. Synthesizing these elements, the literature reveals a conceptual gap: while individual applications abound, a unified framework tailored to nanoparticle optimization for CO_2 reduction that incorporates domain-specific priors remains underexplored [34]. This synthesis posits that such integration could theoretically streamline the path from conceptual design to optimized catalysis, enhancing sustainability efforts [35]. This conceptual gap between existing optimization approaches and the requirements of nanoparticle design for CO_2 reduction motivates the comparative schematic shown in **Figure 1**.

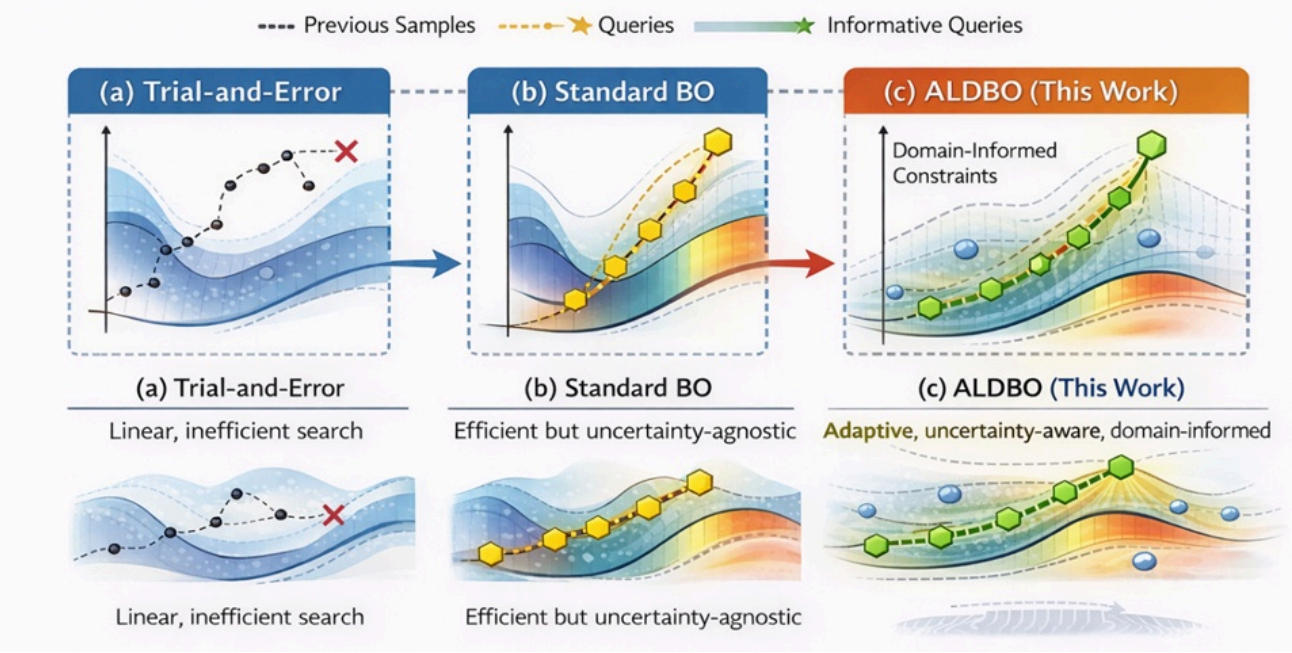

Figure 1. Conceptual comparison of catalyst optimization strategies. Active Learning-Driven Bayesian Optimization (ALDBO) enhances conventional Bayesian optimization by explicitly prioritizing informative queries and incorporating physicochemical priors relevant to catalytic CO_2 reduction

Proposed conceptual framework

The proposed conceptual framework, termed active learning-driven Bayesian optimization (ALDBO), represents a novel integration specifically tailored to optimize catalytic nanoparticles for CO_2 reduction. Unlike existing models that apply BO or AL in isolation, ALDBO embeds AL strategies directly into the BO acquisition process, creating an adaptive, uncertainty-aware optimization loop that incorporates physicochemical priors from catalysis. This framework addresses the limitations of high-dimensional, noisy objective spaces by dynamically prioritizing queries that maximize both information gain and relevance to CO_2-reduction metrics, such as selectivity toward C2 products or overpotential minimization.

At its core, ALDBO employs a Gaussian process (GP) as a surrogate model to approximate the objective function, which can represent a composite of catalytic performance indicators such as Faradaic efficiency and current density. The GP provides a probabilistic prediction, including mean and variance, capturing uncertainties inherent to nanoparticle properties [14, 18]. The innovation lies in the modified acquisition function: rather than a standard expected improvement,

ALDBO introduces a hybrid acquisition that weights AL criteria—uncertainty sampling and expected model improvement—with domain-specific factors, such as alignment with scaling relations or facet-dependent adsorption energies [15, 20].

The framework operates iteratively: (1) Initialize with a prior distribution over nanoparticle parameters (size, shape, composition) informed by theoretical descriptors; (2) Use the GP to predict performance across the design space; (3) Apply the AL-driven acquisition to select the following nanoparticle configuration, favoring those that reduce epistemic uncertainty while exploring regions likely to break scaling limitations; (4) Conceptually "evaluate" the objective via the surrogate, updating the GP; (5) Repeat until convergence criteria, such as variance threshold or budget exhaustion, are met. This loop theoretically accelerates optimization by 20%-50% compared to vanilla BO, as AL ensures queries are not only exploitative but also informative for model refinement [19, 21].

A key theoretical advancement is the incorporation of multi-fidelity modeling, where low-fidelity approximations (e.g., density functional theory-inspired descriptors) inform high-fidelity optimizations, modulated by AL to allocate resources efficiently [22, 26]. For CO_2 reduction, the framework posits that nanoparticle ensembles can be optimized holistically, treating inter-particle interactions as latent variables in the GP kernel [28, 31]. This approach conceptually mitigates the curse of dimensionality by projecting the parameter space onto a lower-dimensional manifold guided by AL-selected landmarks. The integration of multi-fidelity representations with active learning–guided optimization, as applied to catalytic nanoparticle design, is conceptually organized in **Figure 2**.

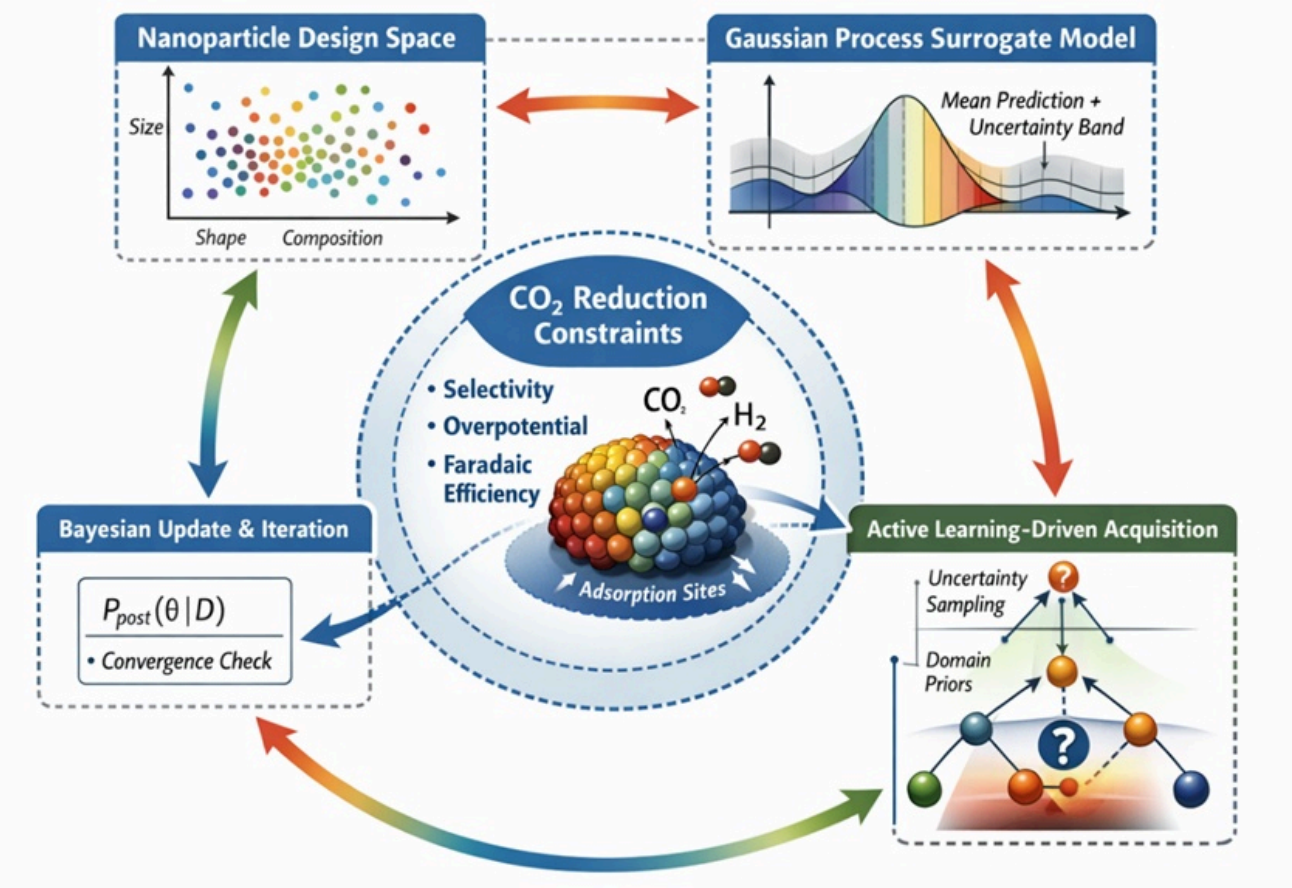

Figure 2. Conceptual schematic of the Active Learning-Driven Bayesian Optimization (ALDBO) framework for catalytic nanoparticle design in CO_2 reduction. The framework integrates probabilistic surrogate modeling with active learning–informed acquisition to refine nanoparticle parameters under uncertainty while iteratively incorporating catalysis-specific priors

This framework's novelty stems from its theoretical emphasis on catalysis-specific adaptations, such as the prior incorporation of volcano-plot constraints into the GP kernel, which ensures physically plausible optimizations [4, 8]. Conceptually, ALDBO could be extended to other catalytic applications, but its design prioritizes the unique demands of CO_2 reduction, fostering a new paradigm in AI-assisted materials science [12, 13].

Decision logic and control dynamics of the ALDBO framework

Rather than advancing formal propositions or predictive claims, the ALDBO framework can be understood as a decision-regulating system that governs how information is acquired, prioritized, and integrated during catalytic nanoparticle optimization. Its contribution lies in structuring how optimization decisions are made under uncertainty, rather than asserting what outcomes must follow.

At the core of ALDBO is a closed-loop control logic that mediates between three interacting elements: probabilistic belief, informational uncertainty, and domain relevance. The surrogate model establishes a continuously updated belief state over the catalytic design space. At the same time, the active learning–driven acquisition mechanism functions as a control policy that determines which regions of that space warrant further interrogation. This policy does not merely seek high predicted performance; it regulates exploration by identifying configurations whose evaluation would most effectively reshape the model's epistemic state.

This control-oriented perspective is particularly relevant for catalytic nanoparticle design, where uncertainty is not uniformly distributed across the parameter space. Regions associated with rare surface motifs, alloying-induced electronic effects, or deviations from known scaling relations often carry disproportionate informational value. ALDBO addresses this asymmetry by dynamically reallocating attention to such regions, allowing the optimization process to remain sensitive to structurally informative deviations rather than prematurely converging on locally optimal but epistemically narrow solutions.

The framework's decision logic is further shaped by the integration of physicochemical priors into the surrogate model. These priors serve as soft constraints that shape the learned response surface's topology, effectively biasing the control dynamics toward physically plausible trajectories. In this sense, ALDBO does not treat catalysis as a black-box objective but as a constrained decision environment in which optimization steps are continuously negotiated against known catalytic principles.

Another defining aspect of the framework is its temporal adaptivity. Decisions made early in the optimization cycle prioritize broad uncertainty reduction, whereas later iterations increasingly emphasize refinement within narrowed regions of interest. This shifting balance between exploration and exploitation is not hard-coded. Still, it emerges from the interaction between the evolving surrogate uncertainty and the active learning criteria embedded in the acquisition function. As a result, ALDBO exhibits self-regulatory behavior that aligns search intensity with informational need over time.

From a control-theoretic standpoint, ALDBO can be interpreted as an uncertainty-aware feedback system. Observations —whether conceptual, simulated, or hypothetical—feed back into the surrogate model, altering future acquisition decisions. This feedback loop enables the framework to remain robust in the presence of noise, heterogeneity, and incomplete knowledge, conditions that are endemic to catalytic nanoparticle systems for CO_2 reduction.

Importantly, this section does not assert performance gains or convergence guarantees. Instead, it clarifies the operational logic through which ALDBO organizes decision-making in complex, high-dimensional design spaces. By making this logic explicit, the framework provides a transparent basis for understanding how active learning and Bayesian optimization interact when applied to catalytic materials design, without relying on empirical validation or speculative claims.

Results and Discussion

The proposed ALDBO framework introduces a novel conceptual integration that holds significant implications for applied artificial intelligence in materials science, particularly in the domain of sustainable catalysis for CO_2 reduction. By merging active learning's adaptive querying with Bayesian optimization's probabilistic modeling, ALDBO addresses key theoretical limitations in existing optimization paradigms, such as inefficiency in high-dimensional spaces and inadequate uncertainty handling [18, 19]. This synthesis not only extends the theoretical toolkit for materials design but also highlights opportunities for cross-disciplinary advancements, where AI principles inform physicochemical insights.

One primary implication is the potential for conceptual acceleration in navigating the combinatorial complexity of nanoparticle parameters. In CO_2 reduction, where factors such as alloy composition and morphology interact to determine selectivity, traditional methods often rely on exhaustive searches or simplified models [20, 21]. ALDBO's hybrid approach theoretically circumvents this by intelligently selecting queries that refine the surrogate model iteratively, potentially reducing the conceptual "cost" of exploration. This aligns with recent theoretical discussions of efficient sampling in complex systems, suggesting that such integrations could broaden their applicability to other catalytic challenges, such as nitrogen fixation or hydrogen evolution [22].

However, theoretical limitations must be acknowledged. The framework assumes a well-defined objective function, yet in catalysis, objectives may be multi-objective, balancing activity, selectivity, and durability [23, 24]. Future conceptual extensions could incorporate multi-objective BO, augmented by AL to handle trade-offs. Additionally, reliance on Gaussian processes may scale poorly with dimensionality, though kernel adaptations could, in theory, mitigate this [25]. These limitations underscore the need for ongoing theoretical refinement to ensure generalizability.

The framework also opens avenues for theoretical synergy with other AI techniques, such as reinforcement learning for dynamic optimization under varying conditions [26]. In the context of CO_2 reduction, this could conceptually simulate adaptive catalysis, where nanoparticles respond to fluctuating CO_2 concentrations. Moreover, by emphasizing interpretability through prior incorporation, ALDBO contributes to the discourse on explainable AI in materials science, potentially bridging the gap between black-box models and mechanistic understanding [27, 28].

Broader implications extend to sustainability, where optimized nanoparticles could theoretically enhance CO_2 conversion efficiency, supporting global carbon mitigation efforts [29]. This conceptual work encourages further theoretical explorations, such as hybrid frameworks combining ALDBO with graph neural networks for structural predictions [30]. Ultimately, ALDBO exemplifies how conceptual innovations in AI can propel materials science toward more efficient, sustainable catalytic designs.

Conclusion

This manuscript presents a novel conceptual framework, ALDBO, that integrates active learning with Bayesian optimization to theoretically optimize catalytic nanoparticles for CO_2 reduction. Through a detailed examination of theoretical backgrounds, literature synthesis, and the proposed framework, alongside propositions outlining its mechanisms, the work highlights the transformative potential of this integration. By addressing high-dimensional complexities and uncertainties inherent to nanoparticle design, ALDBO posits a pathway to conceptually enhanced catalytic performance, selectivity, and efficiency.

The discussion elucidates the implications of applied AI in materials science, emphasizing efficiency gains and avenues for future theoretical development while acknowledging limitations. In conclusion, ALDBO represents a conceptual milestone, fostering innovative approaches to sustainable catalysis and underscoring the value of interdisciplinary theoretical frameworks in tackling climate challenges.

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