



Perspective

AI/ML-Driven Design and Optimisation of Quantum Dots: A Perspective Toward Intelligent Materials Discovery

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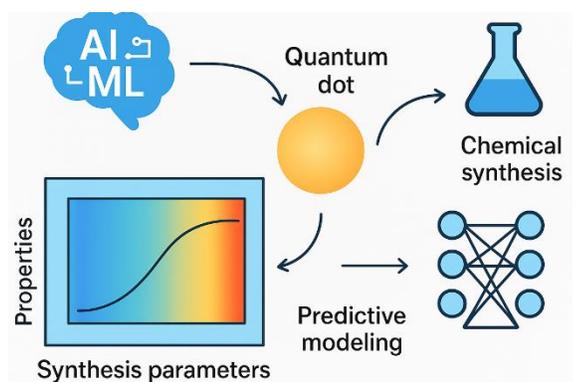
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ABSTRACT

Quantum dots (QDs), nanoscale semiconductors with size-dependent and tunable optoelectronic properties, are central to next-generation technologies spanning displays, photovoltaics, bioimaging, and quantum information systems. However, their synthesis and optimisation remain challenging due to the intricate interplay of reaction parameters and nonlinear physicochemical interactions. The integration of artificial intelligence (AI) and machine learning (ML) is redefining this landscape, enabling predictive design, autonomous synthesis control, and accelerated discovery across the QD domain. This Perspective highlights the conceptual advances and methodological innovations driving AI/ML-assisted QD research, emphasising achievements in data-driven modelling, synthesis optimisation, and materials informatics. Persistent challenges, including data scarcity, model transparency, and limited generalizability, are critically examined, alongside emerging strategies toward physics-informed and autonomous discovery frameworks. We propose that the convergence of intelligent algorithms and human expertise will catalyse a paradigm shift from empirical experimentation toward rational, self-evolving materials design in quantum dot science.

Keywords: Artificial intelligence (AI); Autonomous synthesis; Data-driven modelling; Intelligent materials discovery; Machine learning (ML); Materials informatics; Optoelectronic properties; Physics-informed learning; Predictive design; Quantum dots (QDs); Synthesis optimization.



1. Introduction

Quantum dots (QDs) represent one of the most profound advancements in nanomaterials science since the discovery of fullerenes and carbon nanotubes [1],[2],[3],[4],[5]. Their exceptional optical tunability, stemming from quantum confinement effects, enables precise control over absorption and emission spectra through manipulation of particle size, shape, and composition. This unique property has revolutionised technologies such as quantum dot light-emitting diodes (QLEDs), high-efficiency solar

cells, and nanoscale biosensing systems [6],[7],[8]. However, despite their immense potential, achieving consistent, high-quality QDs remains a scientific and engineering challenge. Their optical and electronic behaviour is governed by a complex interplay of synthesis variables, including precursor ratios, ligand chemistry, solvent polarity, temperature, and nucleation kinetics. Small perturbations in any of these parameters can result in significant variations in size distribution, defect density, and surface passivation, ultimately influencing emission efficiency, stability, and colour purity.



Traditional synthesis strategies have largely relied on chemical intuition, empirical optimisation, and iterative experimentation. While these methods have yielded critical insights, they are inherently limited in scope and efficiency [9],[10]. The multidimensional parameter space governing QD synthesis is vast and nonlinear, making exhaustive exploration through manual experimentation infeasible. Moreover, the lack of standardised protocols and reproducibility between laboratories hinders the translation of empirical results into predictive design rules. This bottleneck has motivated the scientific community to explore artificial intelligence (AI) and machine learning (ML) as transformative approaches for accelerating QD discovery. By analysing large experimental and computational datasets, AI/ML algorithms can identify hidden correlations, construct predictive models for synthesis–structure–property relationships, and autonomously guide optimisation toward desired optoelectronic outcomes.

The integration of AI/ML into QD research marks a paradigm shift from descriptive to predictive materials science [11],[12]. Supervised learning has been employed to forecast band gaps, emission wavelengths, and quantum yields, while unsupervised models have been used to classify synthesis regimes and identify latent material families. Reinforcement learning and Bayesian optimisation techniques enable adaptive experimentation, allowing algorithms to iteratively refine synthesis parameters in real time. These advances have laid the foundation for autonomous laboratories and self-driving experimental platforms that combine robotic synthesis with AI-driven decision-making. Such systems can perform hundreds of synthesis and characterisation cycles with minimal human input, optimising nanomaterial properties far more efficiently than traditional methods. This convergence of automation, computation, and data science is redefining the pace and precision of nanomaterials research.

Nonetheless, several critical challenges persist in realising the full promise of AI/ML-driven QD design. Data scarcity and inconsistency remain major obstacles, as most published datasets are fragmented, unstandardized, and lack essential metadata describing reaction dynamics or surface chemistry. Additionally, the “black box” nature of deep learning models limits interpretability, hindering the extraction of mechanistic insights crucial for scientific understanding. To address these issues, emerging frameworks such as physics-informed machine learning and hybrid AI–quantum mechanical modelling are being developed to merge predictive accuracy with physical transparency. As the field progresses, a synergistic integration of computational intelligence, experimental automation, and human expertise is expected to define the next frontier of QD science, transitioning from empirical discovery toward intelligent, self-evolving materials engineering.

Herein, the study is designed to explore and critically analyse the transformative integration of AI and ML in the rational design, synthesis, and optimisation of QDs. The primary objective is to elucidate how data-driven methodologies can unravel the complex, nonlinear relationships linking synthesis parameters, structural attributes, and optoelectronic performance. This work aims to assess recent advances in predictive modelling, autonomous experimentation, and materials informatics that collectively redefine the landscape of QD research. Furthermore, the study seeks to identify existing challenges, such as data scarcity, model interpretability, and limited cross-domain generalisation that impede widespread adoption of AI/ML frameworks. Ultimately, the study is structured to propose a forward-looking vision wherein physics-informed, human-guided machine learning enables intelligent, autonomous, and sustainable discovery pathways for next-generation quantum dot materials.

2. AI/ML Integration in Quantum Dot Science

The integration of AI/ML into QD research marks a transformative step toward intelligent materials design. By leveraging data-driven algorithms capable of capturing complex, nonlinear relationships between synthesis parameters and material properties, AI/ML approaches overcome the inefficiencies of traditional trial-and-error experimentation. These techniques enable predictive modelling, rapid optimisation, and even autonomous discovery of QDs with tailored optoelectronic characteristics. Through supervised learning, reinforcement learning, and Bayesian optimisation, AI can not only forecast outcomes such as emission wavelength or quantum yield but also guide experimental systems toward optimal synthesis conditions in real time. As a result, the convergence of AI/ML with nanochemistry is accelerating the transition from empirical exploration to intelligent, closed-loop materials engineering, heralding a new era of automated, data-informed innovation in quantum dot science.

The Rationale for AI/ML in Materials Design: The discovery and optimisation of advanced materials are increasingly driven by data-intensive methodologies that transcend conventional experimental paradigms [13]. In traditional synthesis workflows, even modest variations in precursor ratios, ligand chemistry, or temperature profiles can necessitate hundreds of iterative experiments. For QDs, whose properties depend on a highly multidimensional and nonlinear parameter space, such trial-and-error approaches are inherently inefficient and often fail to capture the intricate correlations governing material behaviour. AI/ML introduce a fundamentally different design philosophy, one that leverages computational intelligence to uncover hidden patterns within complex datasets. Algorithms such as random forests, gradient-boosted decision trees, support vector machines (SVMs), and deep neural networks have demonstrated the capacity to learn nonlinear relationships between synthesis parameters (e.g., precursor identity, solvent polarity, ligand functionality) and resultant material properties (e.g., bandgap, emission wavelength, quantum yield, or carrier lifetime). Once trained, these models can rapidly predict QD properties for untested combinations of variables, dramatically reducing the experimental burden. Moreover, when integrated with Bayesian optimisation or reinforcement learning frameworks, AI systems can autonomously explore and refine synthesis pathways through iterative, closed-loop feedback cycles, thereby transforming materials discovery into a self-optimising process.

Data Generation and Representation: Data serves as the cornerstone of all AI/ML-driven materials research [14]. In the context of quantum dot science, data sources are diverse, encompassing experimental measurements, computational simulations, and process-level metadata. Experimental datasets typically include optical absorption and emission spectra, X-ray diffraction (XRD) patterns, transmission electron microscopy (TEM) images, and photoluminescence lifetimes, while computational data may derive from density functional theory (DFT) calculations or molecular dynamics simulations [15]. Process data such as temperature profiles, solvent polarity, and precursor concentrations to further enrich the dataset, providing contextual insight into reaction dynamics. Transforming these heterogeneous data streams into machine-readable formats requires robust feature engineering. Ligand-related descriptors, for instance, can encode steric and electronic effects, while reaction conditions may be normalised or represented through thermodynamic parameters. More recently, representation learning approaches, such as graph neural networks (GNNs), have gained traction for their ability to capture atomic connectivity and electronic structure directly from raw data, reducing reliance on manual feature construction. Despite these advances, data scarcity and inconsistency remain pervasive challenges. The majority of QD-related datasets are small, fragmented, and non-standardised, which undermines the generalizability and transferability of trained



models. Establishing community-wide data standards and open repositories is, therefore, a crucial prerequisite for the maturation of AI/ML-enabled QD research.

Predictive Modelling of Quantum Dot Properties: Machine learning models have achieved considerable success in predicting and optimising quantum dot properties by correlating synthesis parameters with optoelectronic performance [16]. For example, random forest models have been employed to predict the emission wavelength and quantum yield of CdSe and InP QDs, yielding mean absolute errors below 10 nm. Bayesian optimisation frameworks have efficiently identified optimal precursor ratios and reaction temperatures for PbS and CsPbBr₃ QDs, enhancing particle monodispersity and photoluminescence quantum yield (PLQY). Deep neural networks trained on spectroscopic data have accurately classified QD compositions, defect states, and emission behaviours, providing rapid, data-driven insight into synthesis outcomes. Such predictive frameworks have demonstrated an order-of-magnitude reduction in experimental iterations compared with conventional manual optimisation. Importantly, these approaches shift the paradigm from empirical trial-and-error to hypothesis-free exploration, where relationships between structure and function emerge through statistical inference rather than deterministic modelling. This transition signifies the growing maturity of data-centric materials science, one where discovery is increasingly guided by algorithmic reasoning rather than intuition alone.

Autonomous and Closed-Loop Systems: The integration of AI/ML with robotic and microfluidic experimental platforms represents a defining frontier in quantum dot research. Automated synthesis systems equipped with precise control over flow rates, injection timing, and temperature gradients can execute hundreds of reactions per day, generating consistent and high-resolution datasets [11]. When combined with real-time spectroscopic monitoring, ML algorithms can dynamically adjust reaction parameters to steer synthesis toward pre-defined performance objectives such as emission wavelength, colour purity, or PLQY. Pioneering demonstrations of such self-driving laboratories have successfully achieved autonomous optimisation of perovskite and CdSe QD syntheses. In these systems, reinforcement learning algorithms continuously refine synthesis conditions based on reward functions tied to optical performance metrics, enabling adaptive improvement across successive experiments. This closed-loop paradigm transcends traditional human-in-the-loop workflows. AI not only interprets experimental data but also generates hypotheses, tests them autonomously, and refines its predictive understanding through iterative learning. As this integration matures, autonomous materials discovery is poised to become a cornerstone of next-generation nanoscience, where intelligent systems accelerate innovation through continuous, data-driven experimentation.

3. Critical Analysis of Current Limitations

Despite significant progress, the integration of AI/ML in QD research continues to face systemic barriers that constrain predictive reliability, interpretability, and scalability. While data-centric approaches have accelerated the pace of discovery, fundamental challenges persist in data quality, model transparency, transferability, and reproducibility. A critical evaluation of these issues is essential to guide the next phase of AI/ML-driven QD innovation, as shown in Figure 1.

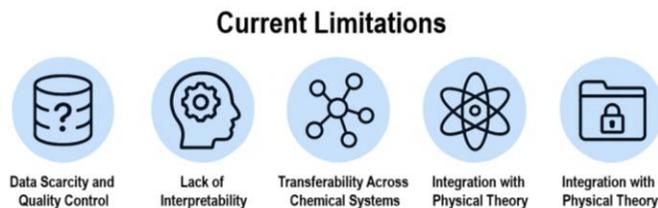


Figure 1: Limitations in AI/ML-Driven Design and Optimisation of Quantum Dots.

3.1. Data Scarcity and Quality Control

Reliable and generalizable ML models require large, diverse, and high-fidelity datasets, yet the datasets currently available in QD research are often limited, fragmented, and poorly standardised. Most published datasets contain fewer than a few hundred samples, insufficient for robust statistical learning. Compounding this issue, experimental protocols vary considerably across laboratories, with inconsistencies in reporting key variables such as ligand purity, precursor concentration, ramp rates, and solvent composition. These variations hinder model transferability and cross-study validation.

An additional challenge arises from publication bias: the literature overwhelmingly emphasises successful syntheses while omitting failed or inconclusive experiments. Such selective reporting produces data imbalance, leading ML models to overfit and capture coincidental correlations rather than causal mechanisms. The absence of “negative” examples ultimately compromises predictive robustness. To address these deficiencies, the research community must prioritise data standardisation and transparency, implementing machine-readable metadata formats, uniform experimental documentation, and open-access repositories. Establishing such infrastructure will enable reproducible, transferable, and statistically meaningful AI/ML applications in QD science.

3.2. Lack of Interpretability

Although deep learning architectures and ensemble models have achieved high predictive accuracy in QD research, they often function as **black boxes**, offering limited mechanistic insight into the underlying physicochemical processes. This opacity conflicts with the foundational scientific goal of understanding *why* specific synthesis parameters yield certain outcomes. The inability to trace predictions back to chemical intuition restricts trust and hinders the broader adoption of AI-driven insights in experimental practice. To mitigate this challenge, interpretable AI frameworks are increasingly being introduced. Techniques such as SHAP (Shapley Additive Explanations), LIME (Local Interpretable Model-Agnostic Explanations) and attention-based neural networks can quantify feature importance and provide local explanations for model outputs. These methods facilitate partial mechanistic understanding by revealing which synthesis variables, such as ligand type or temperature, most strongly influence emission wavelength or quantum yield. Nonetheless, achieving true mechanistic interpretability, where predictive models yield chemically meaningful explanations aligned with reaction kinetics or thermodynamics, remains a critical and unresolved frontier.

3.3. Transferability Across Chemical Systems

Another fundamental limitation lies in the restricted transferability of ML models across different QD compositions and chemical systems. Models trained on one material family (e.g., CdSe QDs) often fail to generalise to others (e.g., perovskite, carbon, or III–V semiconductor QDs) due to intrinsic differences in bonding, crystal structure, and defect chemistry. Consequently, feature–property relationships are frequently system-specific, and retraining is required for each new QD class. This lack of cross-domain



adaptability limits AI's ability to accelerate the discovery of entirely new materials.

Emerging solutions include transfer learning, wherein knowledge gained from one system is adapted to another through re-training on smaller datasets, and multi-fidelity modelling, which integrates experimental and simulated data at varying levels of accuracy. Furthermore, hybrid AI-physics approaches that couple ML models with quantum mechanical or thermodynamic constraints show great promise. By grounding predictions in physical theory, such frameworks can enhance both generalisation and scientific interpretability, moving the field closer to universal predictive models for QD behaviour.

3.4. Integration with Physical Theory

Purely data-driven methodologies, while powerful, can occasionally produce predictions that defy fundamental chemical or physical principles. To ensure physical plausibility, researchers are increasingly incorporating domain knowledge directly into ML architectures through physics-informed machine learning (PIML). These models embed constraints such as conservation laws, thermodynamic boundaries, and quantum-mechanical relationships into the training process. The result is a synthesis of empirical learning and theoretical understanding that enhances both predictive accuracy and scientific validity. By uniting data-centric and physics-based reasoning, PIML represents a critical step toward bridging the long-standing divide between empirical modelling and first-principles theory in QD science.

3.5. Reproducibility and Transparency

Reproducibility remains a cornerstone of scientific credibility, yet it continues to be a major concern in AI/ML-based QD research. Many studies fail to provide comprehensive documentation of model architectures, hyperparameter configurations, training datasets, or pre-processing protocols, making independent replication difficult. Moreover, the lack of open-source access to data and code limits transparency and hinders collective progress.

To foster a culture of reproducibility and openness, the QD community must align with the FAIR data principles, ensuring that datasets and models are *Findable, Accessible, Interoperable, and Reusable*. Publicly available repositories, standardised benchmarking datasets, and shared codebases will be essential to validate AI/ML findings and build cumulative knowledge. Only through transparent, reproducible research practices can AI truly mature from a computational tool into a reliable scientific partner in the discovery and design of next-generation quantum dot materials.

4. The Emerging Landscape and Future Outlook

The future of AI/ML-driven quantum dots research lies in the establishment of standardised, open, and interoperable data ecosystems that promote reproducibility and cross-disciplinary collaboration. Building comprehensive databases that include both successful and failed syntheses, complete with detailed metadata and standardised descriptors, will enable statistically robust model training and benchmarking. Leveraging natural language processing (NLP) for automated data extraction from the scientific literature can further expand datasets and minimise manual curation. Concurrently, the integration of physics-informed and explainable AI architectures represents a transformative step toward interpretable and physically grounded predictions. Physics-informed neural networks (PINNs), graph neural networks (GNNs), and hybrid ML-DFT models can incorporate fundamental laws of chemistry and thermodynamics, ensuring both accuracy and chemical plausibility. Explainable AI frameworks will further elucidate the governing parameters that influence QD synthesis and perfor-

mance, allowing researchers to move from empirical prediction toward mechanistic understanding.

In parallel, the rise of autonomous and self-learning laboratories promises to redefine materials discovery by coupling robotic synthesis, in situ characterisation, and reinforcement learning into closed-loop experimental systems capable of continuous self-improvement. These platforms can explore vast chemical spaces, iteratively refine synthesis conditions, and dramatically accelerate optimisation, transforming months of manual experimentation into days. Furthermore, sustainability will emerge as a guiding principle, as AI enables multi-objective optimisation to balance optoelectronic performance with environmental responsibility, identifying lead-free or cadmium-free alternatives. The integration of QD-level predictive models with device-level simulations spanning QLEDs, photovoltaics, and sensors will bridge the gap between nanoscale design and macroscopic performance, ushering in an era of intelligent, sustainable, and fully automated quantum dot engineering.

4. Conclusion

The integration of artificial intelligence and machine learning with quantum-dot science has progressed from proof-of-concept regressions to autonomous, closed-loop platforms that can optimize emission colour within a single daylight cycle. Nonetheless, the field remains in an adolescent state: models are accurate yet fragile, datasets are growing yet biased, and synthesis successes are reported while thousands of unwritten failures accumulate in laboratory notebooks. Realizing the full potential of AI-driven quantum-dot discovery will require community adoption of standardized, FAIR experimental logs that record not only the triumphant synthesis but also the silent, informative failures; interpretable algorithms that map latent variables to chemically meaningful descriptors such as ligand steric constants or surface reaction enthalpies; and physics-informed architectures that embed thermodynamic conservation laws and quantum-mechanical boundary conditions directly into the loss function. When these elements converge, the next decade could witness self-driving laboratories that explore lead-free, earth-abundant compositions while simultaneously optimizing device-level efficiency, colour purity and environmental sustainability. Such autonomous systems will not replace human creativity they will amplify it, freeing researchers to pose bolder questions about quantum confinement, energy transfer and emergent nanoscale phenomena. The future of quantum dots, therefore, lies at the nexus of human curiosity and machine persistence, where intelligent algorithms become the invisible yet indispensable reagents of every successful synthesis.

Declaration

Competing Interests: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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