Artificial Intelligence and Quantum Dots: Design, Optimization, and Applications

Ishan Aboti[1]*, Kiran Deotale[2], Hardika Chaudhari[3], Nilakshi Dhoble[4]

[1, 2, 3] Kamla Nehru College of Pharmacy, Borkhedi Gate, Butibori , Nagpur, India- 441108

[4]Rashtrasant Tukdoji Maharaj Nagpur University, Nagpur, India-440033

Corresponding author Email: ishanaboti@gmail.com
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Abstract

Artificial Intelligence (AI) has revolutionised the production of Quantum Dots (QD

s), providing solutions to problems such as variability in the materials used to produce QDs, toxicity from elements such as Lead and Cadmium, and the short lifetime of QDs. AI and Machine Learning (ML) provide the opportunity to improve the reverse engineering of QDs and batch production of QDs, which has decreased the number of experimental trials needed to develop QDs, especially for mass production, by more than 90%. The types of algorithms used in this process include Random Forest, Support Vector Regression (SVR), Graph Neural Networks, and Generative Adversarial Networks (GANs). These algorithms aid in predicting attributes such as Bandgap and Quantum Yield and developing alternative non-toxic materials used to create QDs. Furthermore, AI can be integrated into automated synthesis platforms, such as Microfluidics, to allow for QDs to be produced continuously in real-time with uniform properties throughout the production cycle. AI also uses computer vision techniques for the measurement of QD size and defects to reduce production errors and increase manufacturing throughput. In the area of biomedicine, AI provides the potential to create QDs that facilitate drug delivery and imaging, thus providing safer, less toxic alternatives. Future advancements in QD technology may include concepts such as digital twins, reinforcement learning, and explainable AI.

Keywords: Quantum Dots, Artificial Intelligence, Machine Learning, Predictive Modeling, Inverse Design, Synthesis Optimization,

Introduction

Quantum Dots (QDs) are zero-dimensional (0D) semiconductor nanocrystals with a diameter of about 2-10 nm. As a result of being nanoscale in size and comparable to or smaller than the exciton Bohr radius of the bulk material, QDs are capable of exhibiting quantum confinement effects. Quantum confinement results in the discretization of energy levels and transformation of continuous bulk bands into atomic (or at least close to atomic-like) discrete states, and permits precise tuning of optoelectronic properties by size or proportion of elements (composition) or shape variation. As opposed to the fixed bandgaps that exist in bulk semiconductors, QD emissions can vary from the visible to near-infrared wavelengths based on their size, display high photoluminescence quantum yield, and have very narrow band widths of emission. Therefore, QDs are ideal for use in displays, bioimaging and optoelectronics. (1,2)

Quantum dots were first discovered in the 1980s when cadmium-based quantum dots were discovered in glass. This was followed by advances in the field of independent colloid synthesis of quantum dots by Bawendi, Alivisatos, and Brus in the early 1990s that led to size tuning of properties. The two key optical properties of quantum dots arise from quantum confinement. First, smaller quantum dots have larger bandgaps (blue shift of absorption/emission per Brus equation is inversely proportional to size squared). Second, there is an increase in the overlap of electron-hole pairs and how these overlap leads to the increase in the oscillator strength of the quantum dots and thus results in a faster radiative lifetime.In terms of electronics, quantum dots exhibit the ability to tune the bandgaps to almost any value (for example, CdSe has a bulk bandgap of approximately 1.7 eV, while the bandgap of a quantum dot with a diameter < 2 nm is > 3 eV) and to have very large extinction coefficients and be photostable, making them attractive platforms for the development of artificial intelligence-optimized drug delivery systems, chemical sensors, and quantum computers. (3,4)

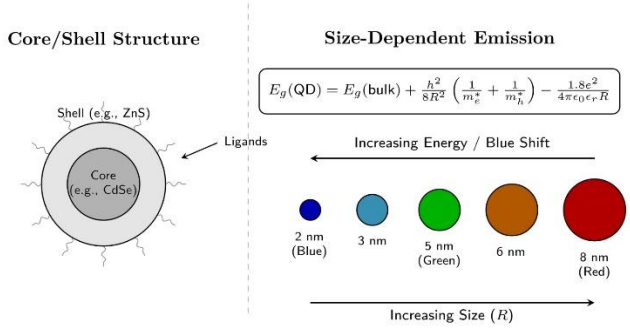

Figure 1: Structure and Size-Dependent Emission Properties of Core–Shell Quantum Dots

Conventional methods for designing quantum dots (QDs), which include trial-and-error synthesis and adjusting their physical or chemical parameters through a variety of different methods, cannot provide reliable measurements and quantitative control over core-shell lattice matching because they can produce results with different levels of reproducibility and reliability, including a lack of uniformity in size, variability in quantum yield, and poor control of the state of the core and shell material. Conventional methods also have major problems with environmental instability such as oxidation and/or photodegradation, and toxicity due to the presence of heavy metals such as cadmium (Cd) and lead (Pb) that limit their ability to produce products with large scale and reproducibility for biomedical applications. The complexity of multi-step colloidal manufacturing further magnifies the potential for introduction of contaminants from solvents or ligands that may diminish the optical quality of QDs and add to their cost, while the sensitivity of those materials to temperature, humidity and charge carrier traps limits their ability to be integrated into commercial devices. (5)

Artificial intelligence (AI) and machine learning (ML) presented solutions to many challenges in nanoscience, enabling predictive modelling of key parameters for quantum dot (QD) synthesis, inverse design with respect to desired optical/electronic properties, and optimising shell passivation through data-driven algorithms. Accelerating discovery through high-throughput screening of potential compositions, AI/ML reduces the number of experimental iterations needed by 50-90%, and works with other techniques, such as microfluidic reactors, to produce scalable and reproducible QDs who have been verified to be stable and non-toxic for use in various applications. The rationale behind this review is motivated by the urgent need to leverage AI in order to overcome barriers to designing QDs, with the objective being to provide a complete overview of the applications for QD engineering, optimisation, and use within optoelectronics, bio-imaging, and drug delivery. The review encompasses the extensive use of AI in QD synthesis, property prediction models, case studies from the literature up until 2026, and future hybrid paradigms, with the following structure: Introduction, Limitations and Emergence of AI in QD Design, Methodologies (ML Models and Generative Design), Applications, Challenges and Future Opportunities (6)

Due to the inherent issues associated with developing traditional quantum dot systems, such as toxicology and the challenge of producing them on a larger scale, there is an increasing need for using artificial intelligence/machine learning (AI/ML) as tools for both predictive modeling and synthesis. This review will summarize current AI/ML techniques used to engineer and apply quantum dots through 2026. In addition, the paper will cover advances made in a better understanding of the chemical and physical properties of quantum dots; discuss their applications in the fields of biomedicine and pharmaceutical development; identify any future regulatory or ethical challenges; and provide a comparison between current and upcoming quantum dot technologies, suggesting new development avenues.

1. Fundamentals of Quantum Dots

Quantum dots (QDs) are nanocrystals (2-10 nm) made up of semiconductors that have quantum confinement in all three dimensions because the electrons and holes are confined in space. As a result, quantum dots have discrete energy levels, and they have size-tunable optoelectronic properties. The standard QDs used today have a core/shell structure, where the core is a luminescent material (e.g., CdSe, InP), which is encased in a shell of material that has a larger bandgap than the core (i.e., ZnS, CdS). This shell material improves the photoluminescence quantum yield of the QDs (90% or more), by passivating surface traps (reducing non-radiative recombination) and protecting against oxidation. Depending on the materials used for the cores and shells, the QD cores can be arranged in heterostructures with type-I (core-confined charge carriers, such as CdSe/ZnS), type-II (spatially-separated charge carriers to prolong their lifetimes, such as CdTe/CdSe), and inverse type-II configurations. The shell thickness can be used to fine-tune the strength of confinement and the emission wavelengths of the QDs. (7,8)

The key types of QD are Cd-based (ex NbSe, NbS; have a high brightness level and are toxic), carbon dots (C-dots; are biocompatible, inexpensive and can be made from biomass with a blue green emission from the surface states), graphene QDS (GQDs; are 0-D graphene fragments that can be tuned based on their edges/oxygenation and have an excellent solubility/water dispersibility), and perovskite QDs (ex. CsPbX3; have a defect tolerant nature, near unity quantum yields, are very easy to synthesize at room temp, however they have stability issues). Cd-based QDs are mainly used in displays/sensors due to their very sharp emission and have been subjected to increased regulations due to their toxic nature; C-dots/GQDs are used primarily for bio imaging and theranostics due to their environmentally friendly nature; and perovskites will lead to new types of LED and photovoltaic devices due to their high color purity. The diversity of QD types supports the development of AI-based optimization for application specific designs and the emphasis of this work. (8,9)

The quantum confinement effect within quantum dots (QDs) occurs when charge carriers (both electrons and holes) are spatially constrained within a dimension roughly equal to their de Broglie wavelength—common size ranges are usually 2-10 nm. As a result, the continuous bulk energy bands change into discrete, atomic-like energy levels based on the particle-in-the-box model. In the regime of strong confinement (where the radius of the QD is less than the exciton Bohr radius), the quantum confinement energy dominates the Coulomb interaction and results in a widened bandgap (E∝1/r^2) based on the Brus equation: $\Delta E = \frac{\hbar^2 \pi^2}{2r^2 \mu} - \frac{1.8e^2}{\epsilon r} + \cdots$hence allowing for the size-dependent absorption/emission profile (blue shift for smaller sized QDs) and the increase in the oscillator strength of the material. These traits also explain the excellent optical properties of QDs: a narrow full-width half-maximum line-width (20-40 nm), large molar extinction coefficients (>10^6 M {-1}cm {-1}), quantum yield of nearly unity for photoluminescence in core/shell QD structures, and immunity to blinking/photobleaching, which enables numerous applications in devices such as light emitting diodes, laser devices and multiplexed biological imaging. (10,9)

Excitons can recombine to produce fluorescence through the direct bandgap, which has a Stokes shift, can create multiple exciton carriers, and have tunable lifetimes (ns-μs). The performance of the fluorescent system is highly dependent on the surface chemistry as unbound electrons in the surface of nanocrystals lead to trap states resulting in non-radiative Auger recombination and quenching. Ligand passivation treatments (e.g., oleic acid, thiols) stabilize the colloids, regulate their dispersity in solution or media, and provide surface charges for bioconjugation. Shell

(ZnS/SiO2) coatings isolate the core from defects. AI/ML will currently assist with design and reconstruction of ligands to minimize trap creation, thus improving QD stability for possible biomedical and optoelectronic applications. (10,11)

Quantum dots (QDs) have two main methods of manufacture; these being top-down and bottom-up methods. Both of these methods have advantages and disadvantages in the ability to create control over size, properties and shape of QDs.Top-down manufacturing of QDs occurs when bulk semiconductor is physically reduced to the size of a QD. This can be achieved by several techniques including electron beam lithography, laser ablation, focused ion beam milling, and mechanical ball milling. The top-down manufacturing techniques yield high-purity QDs formed in a precise pattern; however, due to the high-energy requirements of these techniques, there are high costs associated with energy usage and charges for producing QDs. In addition, there are structural defects associated with each of these processes that create difficulty in scaling for mass production, have high polydispersity, and poor reproducibility. Bottom-up manufacturing techniques create QDs by chemically assembling atoms or molecules into QDs via self-assembly through various methods. The colloidal synthesis method has continued to be most successful in creating monodisperse CdSe and InP QDs ($\sigma<5\%$) and has resulted in creating QDs with very high quantum yields (>80%). Other bottom-up techniques such as solvothermal, microemulsion group intercalation, microwave-induced intercalation and electrochemical methods generally allow for the creation of QDs with tunable compositions but have problems regarding toxic and non-reproducible products. (13)

The trend for producing materials from green processes will develop into more environmentally friendly, low-energy processes using: biomass feedstocks for building blocks (such as c-dots), reduction via microbial or enzymatic methods, hydrothermal methods to replace toxic organometallics (Cd/Pb), and developing bio-compatible QDs with moderate yield (20-60%) and lower environmental impact. An example of this is the production of L-cysteine-capped CdTe quantum dots using a one pot reflux method and the production of c-dots from fruit peels using pyrolysis methods with the aim of maximizing the water solubility and minimizing cytotoxicity for their use in biomedical applications. With the aid of AI/ML in conjunction with microfluidics, researchers will be able to continue to develop these green methods with little or no waste during manufacture thereby increasing their scalability for industrial production of quantum dots for use in displays and sensors.. (13,14)

2. Basics of Artificial Intelligence in Nanotechnology

AI refers to a group of computer systems that act like humans and solve problems that humans can solve using their brains. AI can perform tasks that require reasoning, perception, and decision-making. Machine Learning (ML) allows the computer algorithms to learn from data without having to be explicitly programmed. ML is a subcategory of AI, and Deep Learning (DL) is a more advanced version of it using very large, multi-layered neural networks to identify and extract features from data. Unlike traditional ML methods that may take a long time to find similar features in high-dimensional datasets of QD's collected from spectroscopic/electron microscopic experiments, DL methods are able to identify and extract features with >95% accuracy in predicting the quantum yield of QD's. AI has been used to help automate the optimization of the synthesis of QD's (e.g., using self-driving laboratories to predict the ratio of precursors to use in the synthesis of QD's) and ML has been successfully used to predict the properties of QD's (e.g., using size and composition to predict the bandgap of a QD) while DL is used to perform inverse design (e.g., using generative adversarial networks [GAN's] to generate a novel core/shell architecture for a desired emission). (15,16)

Deep learning relies heavily on neural networks, specifically feed-forward or convolutional architectures that use backpropagation to process (temperature and ligands) the parameters associated with QD synthesis to minimize prediction error. In addition, regression models (linear or support vector regression) generate continuous predictions (such as emission wavelength), while clustering (k-means or Gaussian mixtures) generates groups of QD batches that share similar characteristics for quality control purposes. In the field of nanoscience, these hybrid approaches (neural networks and regression) used for optimizing QD charge tuning in qubit applications have reduced the number of iterations by 80%. Finally, using unsupervised clustering to extract defect states from photoluminescent spectra

illustrates how artificial intelligence/machine learning has the potential to revolutionize the design of quantum dots by moving from empirical experiments to precision engineered and scalable engineering methods in optoelectronics and biomedicine. (17,18)

Table 1: **Comparison of AI Techniques Across QD Applications**

AI Technique	QD Design	Synthesis Optimization	Bioimaging	Drug Delivery	Biosensors
Predictive Modeling (RF, SVR, GBM)	Bandgap/size forecasting	Parameter/yield prediction	Spectral unmixing	Ligand affinity	Biomarker quantification
Neural Networks (CNN, GNN)	Composition screening	Image-based size control	Super-resolution	Nanoparticle targeting	Defect detection
Generative Models (GANs, VAEs)	Inverse structure design	Reaction condition generation	Multiplexed labeling	Carrier morphology	Sensor array design
Bayesian Optimization	Material selection	Real-time adaptation	N/A	Dose optimization	Sensitivity tuning
Reinforcement Learning	N/A	Self-driving labs	N/A	Adaptive release	Feedback control

Data driven approaches to enhance discovery in materials science use AI tools for predictive modelling with machine learning algorithms such as Random Forest (RF) , Support Vector Regression (SVR), Gradient Boosting (GBM), and Graph Neural Networks(GNN) to predict semiconductor (QD) properties (bandgap, quantum yield, absorbance, emission) from the starting conditions (size include composition and ligands). The predicted property can be produced with over 95% accuracy and have reduced the number of experimental trials. For example, SVR or RF models have provided RMSE value of < 0.1 nm when predicting the size of $CsPbCl_3$ PQD and/or the PL of this material. In addition, SVR, however, lightGBM can also be used to screen through large quantities (high-throughput) of perovskites rapidly via their predictive capability. These tools provide a connection between QSPR-based property predictions using well-defined descriptors and their performance through material informatics platforms (e.g. Materials Project-based databases). (19,18)

Automated size/shape distribution measurement and defect detection of quantum dots (QDs) in transmission (TEM) and scanning (SEM) electron microscopy employs neural networks and transformers to provide a speed improvement of 100 times versus traditional methods by utilizing image analysis.Artificial intelligence (AI) surrogate models (such as graph neural networks) provide approximations to traditional quantum density functional theory or molecular dynamics calculations to speed up simulations, achieving a speed increase of 1,500 times in predicting the energy/force of quantum dots and allowing for large-scale virtual screening.By unifying the above-mentioned approaches with active learning loops through machine learning, the experimental design for self-driving laboratories is improved,

which leads to optimal QD synthesis like in the National Institute of Standards and Technology's (NIST) automated QD manufacturing facilities. (20,18)

3. AI in Quantum Dot Design

The use of AI for material selection in quantum dot (QD) design is based on generative models like Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs) that can search large chemical spaces to find optimal core/shell compositions (e.g., CdSe/ZnS, CsPbX3). The goal is to find non-toxic alternatives (e.g., InP, carbon dots) based on their descriptors (e.g., electronegativity, lattice mismatch and toxicity indices from various materials databases). Machine Learning (ML) also enables multi-objective optimization (e.g., using Pareto fronts through the use of the Non-Dominated Sorting Genetic Algorithm II (NSGA-II) in combination with Random Forest classification methods (RF)) to find QDs which are both photoluminescently efficient (PLQY) and stable and cost effective, hence expediting the discovery of stable perovskite QDs for use in LEDs. Additionally, active learning loop(s) will allow for refinement of selection through the use of experiment-based feedback similar to that employed by self-driving laboratories. (18,21)

Supervised machine learning is being utilized to predict quantum dot size and composition. Algorithms such as Random Forest, Support Vector Regression, and LightGBM train on synthesis parameters (temperature, precursor ratio, time) for both size and guiding inverse design towards specific properties, attaining a root mean squared error of less than 0.5 nm. Bandgap prediction also relies on machine learning, specifically using kernel-based Support Vector Regression (radial basis function and polynomial) and GBM with SHAP interpretability. The bandgap prediction model for CsPbCl3 point quantum dots predicts Eg (energy gap) with a mean absolute error of about 0.03 eV by capturing the nonlinear relationship of size and composition with an effective mass approximation. Graph neural networks are used to expand this approach to alloyed quantum dots (CdSe1-xSx) and enable rapid prototyping, decreasing the dependency on density functional theory calculations by a factor of 1,000. (22)

Table 2: AI Methods in Quantum Dot Design

AI Technique	Function in QD Design	Key Algorithms	Example Applications	Performance Metrics
Predictive Modeling	Bandgap/size/composition forecasting	RF, SVR, GBM, LightGBM	Emission wavelength tuning for CsPbX3	MAE 0.03-0.1 eV; RMSE <0.5 nm
Neural Networks	Structural inverse design, image analysis	CNNs, GNNs	Core/shell lattice matching; TEM size extraction	>95% accuracy; 100x faster than DFT
Generative Models	Novel QD candidates generation	GANs, VAEs	Non-toxic alloy screening (InP/ZnS)	1000x speedup over simulations
Bayesian Optimization	Parameter/material exploration	Gaussian Processes	Ligand ratio for max PLQY	80% fewer experiments
Reinforcement Learning	Autonomous design loops	Policy gradients	Self-driving synthesis targeting specs	Yield boost 50-90%; σ<5% dispersity

Quantum dot (QD) bandgap prediction models are developed using kernel based Support Vector Regression (SVR using RBF/polynomial kernels), Random Forest (RF), and Gradient Boosting Machines (GBM) trained on synthesis inputs (size, composition, and ligands) and descriptors (cation/anion ratio, electronegativity) resulting in mean absolute errors (MAEs) between 0.03-0.1 eV for perovskites such as CsPbCl3 and CdSe, which outperformed the empirical Brus equations due to their ability to capture non-linear quantum confining effects.(18,34)

Machine learning classifiers and regressors (like RF and XGBoost) are used to provide the surface ligand prediction (e.g. oleic acid, oleylamine, and TOPO) based on the various concentrations to create predictions about passivation efficiency, quantum yield, and stability of the particle size (RMSE<5 nm) from the respective ligand ratios in the CsPbCl3 PQDs (e.g. using Support Vector Regression). The relationship between the properties and structures of the respective nanocrystals is interpreted through interpreting machine learning, and linking core/shell lattice mismatched and ligand density to photoluminescent quantum yield and traps through the use of principal component analysis and feature importance analysis. The OLA to OA ratio of the respective CdTe quantum dots illustrates a component in the determination of photoluminescence. The incorporation of active learning allows for virtual physical screening of 10^6 of the various candidate compositions (e.g. alloyed CdSeS and InP/ZnS) through GNN surrogates in lieu of density functional theory (DFT), resulting in up to a 1000-fold increase in speed when evaluating high PLQY candidates. (23,24)

4. AI in Quantum Dot Synthesis Optimization

Optimizing the parameters of the process during synthesis of quantum dots (QD) uses machine learning (ML) approaches including the use of Gaussian Process Regression (GPR) or Bayesian Optimization (BO) to optimize the control variables, such as precursor concentration, injection temperature (200 °C-350 °C), reaction duration (5 min-60 min), and ligand ratio, with the goals of minimizing the spread in diameter ($\sigma < 5\%$) and maximizing the uniformity. An example of this can be found in the hot-injection method for synthesizing PbS quantum dots. Predicting the reaction conditions using ML entails using a prediction model (i.e., neural networks or random forests) constructed from historic data to find the optimal working conditions to use with solvothermal/hydrothermal methods. This significantly reduces (in the range of hundreds to less than 100) the number of trials required here to obtain optimal results for specified photoluminescence (PL) wavelength. Further improvements in yield due to the use of ML by multi-objective optimization of carbon QDs was shown to obtain PL quantum yield (PLQY) of greater than 60% at all colors by correlating the addition of substances to the reaction (e.g., oleylamine as a nucleation control) with the measured yield would reduce the length of time necessary to complete research by 80%. (25,26)

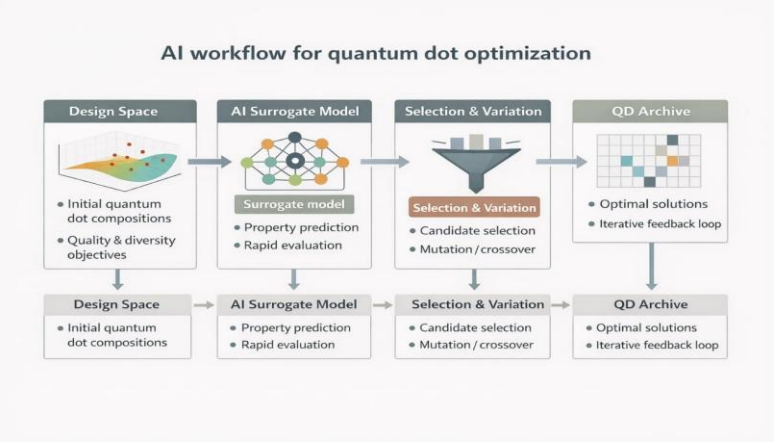

Figure.2: Schematic representation of an artificial intelligence–based workflow for quantum dot (QD) optimization

Microfluidic and robotic dispensers work together with real-time spectroscopy on automated synthesizing platforms to produce large quantities of monodisperse CdSe/InP QDs via continuous flowing. Self-driving laboratories contain closed loop AI systems with ML surrogate models, active learning and automated lab execution built into them allowing them to run experiments entirely on their own from researching PbS QD synthesis at University of Toronto to developing an accurate Predictive Model for closed loop applications building off of 2,300 synthesis databases to define a unique bandgap (611 nm exciton). These new paradigms transition the way QDs are produced; they will become prediction driven instead of experiment driven allowing for scalability for commercial applications in both Optoelectronics and Biomedicine. (26)

Table no.03 Synthesis methods vs properties

Synthesis Method	**Quantum Yield (QY)**	**Size Monodispersity (σ)**	**Scalability**	**Cost**	**Toxicity Concerns**	**Best Applications**
Colloidal (Hot-injection)	50-90%	<5%	Low	High	High (Cd/Pb)	Displays, LEDs
Solvothermal	30-70%	5-10%	Medium	Medium	Medium	Perovskites, sensors
Microwave-assisted	40-60%	8-15%	Medium	Low	Medium	Rapid prototyping
Green (biomass/aqueous)	20-60%	10-20%	High	Low	Low	Biomedicine, bioimaging
Top-down (lithography)	N/A (non-fluorescent)	Precise patterning	Very low	Very high	Low	Photonic devices
Laser ablation	10-30%	15-25%	Low	High	Low	Research-grade purity

5. AI for Characterization and Quality Control

Machine learning (ML) utilized for analyzing spectral data of quantum dots (QDs) by extracting size-dependent characteristics, bandgap energies and quantum yield from both UV-Vis absorption and fluorescence spectra will allow for the use of convolutional neural networks (CNNs) and partial least squares regression to deconvolve multiple overlapping emission peaks associated with core/shell QDs; e.g., CdSe/ZnS while maintaining an accuracy of less than 2 nm on emission wavelength predictions based on UV excitation profiles. Multivariate techniques such as principal component analysis (PCA) and Gaussian mixture models will provide quantitative measures of both Stokes shifts and multi-exciton effects which will allow for real-time assessment of quality during the synthesis process. (28)

Computer vision of microscopy images is achieved using convolutional neural networks and U-Net architectures applied to transmission electron microscope/Scanning electron microscope/Atomic force microscope data for measuring an automated particle size distribution (root mean square error < 0.3 nm) and shape factor; detecting lattice fringes on images; and multiplexing quantum dot types based on hyperspectral fluorescence microscopy, performing spectral unmixing (e.g., separating 525-705 nm light emission). Automated counting particle sizes using regression models (support vector regression/random forest) correlates hydrodynamic diameters and photoluminescent peaks, while detecting anomalies through autoencoder techniques identifies surface defects, such as "blinking" due to brightness variation in intensity level. Monitoring variability in production involves using pre-trained deep learning

network methods of transfer learning and domain adaptation to produce normalized images and/or spectra across multiple samples (specifically, from multiple batches within the same run), while also ensuring that control charts based on machine-learning clustering demonstrate that dispersity is <5% standard deviation for a scalable amount of production. (27,28)

6. Biomedical & Pharmaceutical Applications

AI has optimized quantum dot (QD) carriers to revolutionize how we deliver drugs to specific sites. Machine learning (ML) has been utilized to design QD core/shell structures with proper size (5 – 10 nm), engineered surface ligands (e.g., PEG-FA conjugates), and stimuli-responsive linkers to enhance penetration through the tumor using endosomal/ECV leaked through the EPR effect and receptor-mediated endocytosis. With these systems, QDs can deliver 5 – 10 times the payload to cancer cell via the same route as free – strand drugs. Using predictive models such as random forests and neural networks, ligands bound to proteins can be predicted based on pH and redox-triggered release rates by compiling different types of QD core composition data into a machine learning environment. Using generative adversarial networks (GAN), QDs can be inverse designed from non-toxic InP/ZnS (or carobon) core materials to minimize opsonisation and immunogenicity for long systemic circulation (between 24 hours). These various QDs will be effective theranostic systems, since they can be tracked in real-time via fluorescence (in this case, near-infrared emission) and controlled released of doxorubicin or paclitaxel, demonstrating an 80% decrease in tumor size when tested in animal models with decreased toxicity to healthy tissue. (6)

Using Quantum Dots (QD) for AI-based fluorescence imaging allows for rapid analysis of multiplex (i.e., up to 5-7 colors of signals) emissions, as well as denoising of low signal, and super resolution reconstruction through Generative Adversarial networks (GAN). Consequently, these advanced algorithms yield up to 2-5 times greater signal-to-noise ratios (SNR) and greater than 20 nm local precision for in vivo application. The algorithms utilize hyperspectral data collected using QDs that target clinically relevant biomarkers (i.e., HER2 and PSMA) to automate tumor margin identification and to provide real-time tracking of cell activity with little or no photobleaching. Using machine learning models, we can predict biologically relevant surface passivation methods, such as zwitterionic ligands, for optimal biocompatibility and least possible non-specific binding, and use AI-enhanced QDs for early stage diagnosis using flow cytometry and real-time intra-operative imaging; moreover, using CNN classifiers allows us to discriminate malignant from healthy tissues with >95% accuracy, thus expediting clinical translation in Precision Oncology. (27,18)

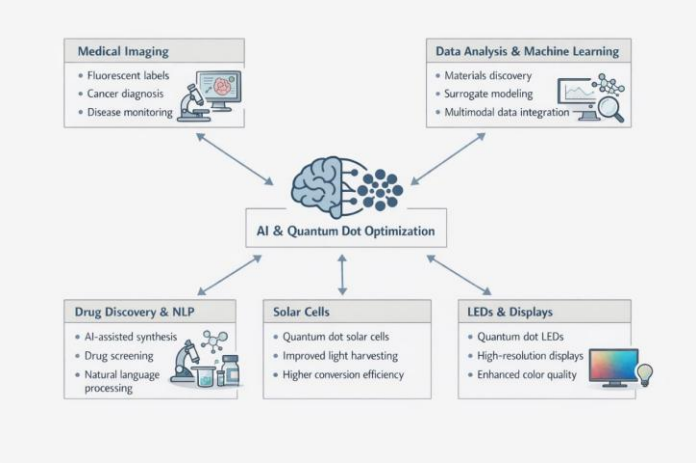

Figure 3: Application of AI quantum dots in different industries

QD-based biosensors are intelligent sensors which can provide real-time, multiplexed detection of biomolecules using QDs that feature tunable fluorescence, a large surface area, and utilize energy transfer mechanisms (e.g. FRET or

quenching). In these applications, AI is leveraged through the application of CNN-based signal processing for the spectral deconvolution and identification of anomalous signals in complex sample matrices such as serum. For disease detection, QD biosensors facilitate the early diagnosis of different types of cancer (e.g. lung cancers utilizing miRNA profiling), blood cancer (utilizing leukemia biomarkers), and infectious agents through the use of electrochemical/fluorescence modalities, with ML classifiers utilizing the QD emission shifts obtained from QD biosensors to analyze for greater than 95% specificity in CTC enumeration or antibiotic residue sensing. The AI-optimized design enables the prediction of ligand orientation, thus minimizing the likelihood of non-specific binding and will facilitate the development of point-of-care devices that can enable theranostic monitoring and include portable readers. (30,29)

Theranostics based on quantum dots (QD) employ a single platform for both diagnostic imaging of tumors in real time with size-tunable near-infrared fluorescence, and as vehicles for delivery of drugs or treatment via photodynamic (PDT) or photothermal therapies (PTT). Examples of these 'theranostic' QD systems would be those based on cadmium selenide/zinc sulfide (CdSe/ZnS) or graphene QDs that are conjugated to doxorubicin and/or photosensitizers to allow for both tracking and destruction of breast or brain cancers. The release of drug payload can be targeted to the tumor site through mechanisms of pH/redox stimuli or through energy-transfer (FRET) quenching, resulting in greater than 80% tumor regression in xenograft animal models while limiting systemic toxicity mediated via EPR (enhanced permeability and retention) accumulation of QDs and ligand-targeted uptake (e.g., antiHER2) in the tumor. (31,32)

7. Current Challenges

A key barrier to advancing AI applications that use quantum dots (QDs) is a lack of sufficient high-quality datasets. Due to how few QDs have been made, there are not enough experimental datasets for a wide variety of different compositions (e.g., comparing CdSe to perovskites), sizes, and/or conditions. Consequently, varying amounts of high-quality experimental data have made it difficult to use ML models for effective training because sparse datasets introduce additional uncertainty in the ML models and introduce difficulty in making accurate predictions for bandgap, quantum yield, and ligand effects. Public repositories such as the Materials Project contain less than 10,000 QD entries, while we estimate that at least 1,000,000 entries are required to develop effective deep learning models. Proprietary data provided by industrial partners also do not significantly expand the low amounts of data because there are few entries and diverse characterizations that contribute to prediction error rates between 20% and 50%. Possible solutions for overcoming QD data shortages include the use of transfer learning from bulk semiconductors; using data augmentation by generating spectrum/micrograph representations with the help of generative adversarial networks (GANs); federated learning among research labs; and employing self-driving platforms to generate over 100 times more validated QD data, which would facilitate closed-loop experimentation to create reliable AI-optimized processes for high-volume QD manufacturing. (25,30)

Toxicity issues associated with quantum dots (QDs) are predominantly caused by the ability of cadmium ions to leak into the environment; this has been linked to oxidative stress and damage to mitochondria, as well as inflamed vital organs. Studies have shown that the in vitro cytotoxicity is an average of approximately 10–100μg/mL IC50 and the mean animal LD50 is >400mg/kg IV. The use of a variety of surface treatments such as ZnS shells or PEGylation can reduce the toxicity of QDs by approximately 70–90%. Additionally, long-term bioaccumulation, stimulation of the immune system, and the designation of QDs by the FDA as classified "high-risk" products have led to a shift to safer alternatives (i.e., carbon dots, graphene-based QDs, indium phosphide) that cause less than 5% cellular toxicity. In addition, when quantum dots are reproduced in different laboratories using different equipment, 10–30% variation is introduced due to micro-variations in the lab, mainly from the quality of ligands and the geometry of the reactor. Models that were created to optimize quantum dot synthesis through AI are not performing well during the cross-validation process due to overfitting the data used to build the initial model and a lack of testing with different data sets. Stochastic methods typically used to create quantum dot synthesis recipes often designate standard synthesis

methods; therefore, a standardized digital twin and blockchain must be created to guarantee accurate results and outcomes. (6,34)

Due to the classification of cadmium-based quantum dots (QDs) as novel nanomaterials by the FDA/EMA, severe regulatory constraints exist for the commercialization of both biomedical and optoelectronic applications based on QDs. The stringent requirements for extensive genotoxicity, ADME, and long-term bioaccumulation testing have delayed use of cadmium (Cd)-based QDs in commercial biomedical applications through the FDA/EMA 21 CFR 312 IND pathways, as shell degradation risks from Phase I trials have the potential to release hazardous heavy metals .In the case of optoelectronic QDs, the current European REACH regulations limit the amount of cadmium and lead (Pb) allowed in QDs to less than 100 parts per million, thereby further delaying the manufacturing of displays in Europe. The absence of harmonized nanotoxicology standards, such as those from the Organisation for Economic Co-operation and Development (OECD), which currently lack QD-specific protocols, cause preclinical testing of QD materials to be at least 5 times more expensive than organic materials. Thus, the industry is seeking to develop alternative inorganic phosphorescent (InP) QDs and use Artificial Intelligence (AI) to develop simulated safety dossiers for QDs. (30,34)

AI model interpretability is an area of quantum dot (QD) research that aims at developing models that can be interpreted. AI model interpretability is known as "black-box" models; deep neural networks and complex ML architectures used for bandgap/size prediction and synthesis optimization of quantum dots have similar properties. There are several explainable AI techniques such as SHAP, which provide feature importance (e.g., a ligand chain length contributes 30% to the PLQY of quantum dots), displayed in such a way as to show causal connections between the input to an AI model (e.g., precursor ratios) and the output of an AI model (e.g., emission wavelength). The development of quantum-specific techniques such as Q-LIME has allowed for the adaptation of LIME, which builds local surrogate models for quantum mechanical measurements, to provide information on "regions of indecision" regarding the output of predictions as a result of the distribution of measurement results. This development will assist in providing trustworthiness in AI-generated explanations for decisions made by self-driving laboratories. Additionally, physics-informed neural networks (PINNs) have also provided a mechanism for embedding constraints from Brus' equation, thus improving the reliability of the models by a minimum of 15% and providing gradient-based information regarding the effects of quantum confinement. (35,36)

8. Regulatory and Ethical Considerations

A machine learning-based (ML) design of I-driven nanoformulation utilizes ML algorithms (genetic algorithms, Bayesian optimization, and generative adversarial networks) to optimize quantum dot (QD)-based carriers by increasing size (5 – 20 nm), zeta potential (-10 to +30 mV), ligand density, and drug encapsulation efficiency (> 90 %). This results in a reduction of the design cycle from several months to just days. A quantitative structure-property relationship (QSPR) framework is used to create the surface chemistry of the carriers in order to decrease their rate of circulation and improve their targetability thereby resulting in increased doxorubicin bioavailability compared to traditional preparation methods (e.g., PLGA-QD hybrids that yield > 4-fold greater doxorubicin bioavailability).When robotics (e.g., closed-loop self-driving robotics) are incorporated into this type of ML-design approach enables AI to control robotic platforms that implement the synthesis protocols that have been optimized using ML and to conduct real-time characterization of the products being synthesized allowing for autonomous optimization with < 5% variability in any given batch of product produced. Automated hot-injection systems are an example of this type of technology, which allows for the production of gram-scale monodisperse InP/ZnS QDs, facilitating the scalable production of QDs needed for clinical applications with significantly reduced risk of operator error. (39,40)

Digital twins developed in nanomaterials production can provide accurate virtual representations of the method through which quantum dot(QD) batches are produced by utilizing real-time data obtained from sensors located on the reactor as well as physics-based simulations plus machine learning (ML) algorithms to improve the yield of QD batch productions by 20-40%, eliminate the need for physical prototype testing by 80%, and ensure consistent yield across multiple production facilities. Patient customized nanomedicine utilizes patient-focused digital twins that have incorporated genomic and imaging data to create precise QD-based therapeutics designed specifically for each patient based on their unique pharmacokinetic profiles. In particular, ML optimized forms of InP QD designed solely for targeted delivery to HER2 positive breast cancer patients may achieve 90% targeted delivery, indicating a shift towards

precision dosing. (39)

Real-time adaptive synthesis in the production of QDs utilizes reinforcement learning agents (RL) along with in-line sensors to adjust synthesis parameters dynamically throughout the reaction, producing highly monodisperse QDs (greater than 95%) and reducing synthetic waste (up to 70%). This capability allows companies to develop robustly scalable processes suitable for moving from lab-scale to pilot-scale, an important requirement for commercial optoelectronic and therapeutic applications. (40)

Table 4: Regulatory Frameworks for Quantum Dots

Framework	Region	Key Requirements	QD Impact
EU AI Act (2026)	Europe	Risk assessments, explainability for pharma AI	High-risk QD design models need SHAP/LIME audits
REACH/RoHS	Europe	Cd/Pb limits (<100 ppm), safety proof burden	CdSe QDs restricted; InP/C-dots favored
FDA PCCPs	USA	Lifecycle transparency for AI devices	Clinical QD theranostics require model cards
TSCA	USA	Premanufacture notices for new nanomaterials	Environmental fate studies mandatory
ISO 10993	Global	Biocompatibility, genotoxicity testing	Shell stability under physiological conditions

Future Perspectives

Machine Learning (ML) Algorithms are used as a means of speeding up the design process of nanoformulations in an AI (Artificial Intelligence) environment when developing different types of carriers based on Quantum Dots (QDs). ML algorithms can improve many different characteristics related to the design of these nanoformulations, including size, zeta potential and the concentration of ligands, as well as improve the efficiency of drug encapsulation (greater than 90 %). The advantage of using ML algorithms for the design of nanoformulations is the time savings associated with designing these nanoformulations (from months to a few days).
Using this information, the quantitative structure-property relationship or QSPR can provide information about the appropriate surface chemistry to utilize for optimal circulation and targeting when creating ML-based PLGA-QD hybrid nanoparticles (these types of nanoparticles to date have been shown to improve the bioavailability of doxorubicin by 4 times. (37)

By utilizing robotics in conjunction with the above-mentioned technologies, AI can now implement closed-loop self-driving laboratory systems (an AI that controls the robotic platforms in order to carry out an ML-optimized synthesis protocol while performing real-time characterization of the product) which will achieve autonomous optimization of nanoformulations with less than five percent variability across production batches. For example, an automated hot-injection system will produce gram quantities of monodisperse InP/ZnS QDs, allowing for easy scale-up in a clinical setting and reducing human error during production. (37,38).

Creating virtual clones of quantum dot cultivation processes through digital twin simulations of nanomaterials manufacturing provides opportunities for enhancing the results of batch experiments, optimizing the flow of precursors to reactors, and beginning to identify problems as they occur by combining real-time sensor input from the reactors with physics-based simulations and machine learning models. As a result, production yields of refinements

will be 20%-40% higher than current methods will have fewer than 20% of needed physical prototypes, and production results will be reproducible between sites.

The implementation of patient-specific digital twins in designing QD theranostics is accomplished through the integration of both genomic and imaging data that comprise customized QDs designed specifically for the individual patient's unique pharmacokinetic characteristics. For example, ML-optimized InP QDs designed for HER2+ breast cancer can realize delivery to target tissues with 90% accuracy, thus providing true precision dosage concepts.The use of RL agents with in-line sensors provides the capability to refine synthesis parameters (e.g., reaction temperature, reaction time) during the synthesis of QDs for precision control of high-quality(>95% monodispersity) and reducing waste (e.g., >70% decrease in material use) and the ability to transfer this technology from the lab to the pilot plant is critical for implementing large-scale commercial applications in optoelectronics and therapeutics. (38)

Conclusion

Artificial Intelligence (AI) has revolutionized the research area of Quantum Dots (QDs) by overcoming deficiencies that are intrinsic in traditional techniques for synthesizing and designing QDs. Predictive Modeling, Inverse Design, and the optimization of synthesis (e.g., process controls) using AI reduces the number of experimental iterations by up to 90% while improving reproducibility and scalability. Techniques in machine learning including Random Forests, Support Vector Regression (SVR), and Graph Neural Networks (GNNs) provide highly accurate predictions of QD properties (e.g., bandgap and quantum yield), while generative models enable the discovery of new, non-toxic QDs. Integration with automated synthesis methodologies and microfluidics allow for real-time process control during the synthesis of QDs, which ensures consistent production of high-quality QDs.AI-enabled characterization methodologies (e.g., convolutional neural networks) accelerate quality control through enhanced analysis of particle size distribution and defect detection. AI-optimized QDs for biomedicine increase drug delivery efficiency through targeted drug delivery and fluorescence imaging, which will reduce patient toxicity while improving therapeutic outcomes. Even with these advances, there are still significant challenges regarding the scarcity of data, interpretability of models, reproducibility, and regulatory issues regarding the use of heavy-metal QDs. Addressing these challenges requires the creation of data repositories, establishment of explainable AI models, and development of harmonized regulatory frameworks. Advancing technologies like digital twins, reinforcement learning, and neural networks can significantly enhance the reliability of design, scale-up, and clinical translation for the future. By combining robotics and autonomous laboratories using artificial intelligence, it is possible to produce materials on an industrial-level without much variability due to the closed-loop operation of robotics, giving us access to a new level of process efficiency for materials manufactured with these devices. The advancement of design technology using AI will be fundamental in changing the field of quantum dot (QD) engineering and will support new developments in areas such as optoelectronics, bioimaging, nanomedicine, etc., by creating safer, more sustainable, and low-cost materials for use in developing a wide variety of new products.

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